Introduction to Many-particle Physics

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Skulle nogen have spørgsmål til projektet kan Martin kontaktes på martinskogstad@gmail.com

En stor tak til professor emeritus Henrik Smith som også er forfatter til flere af bøgerne, og til lektor i fysik ved NBI Jens Paaske for samarbejde, opmuntring, valg af materiale og lån af fine eksemplarer af værkerne. This text is intended for use in a graduate-level one-semester course on many-particle physics. An effort has therefore been made to keep the number of pages below 150. There exist several comprehensive texts on many-body theory, starting with the classic treatise *Methods of Quantum Field Theory in Statistical Physics* by A. A. Abrikosov, L. P. Gorkov and I. E. Dzyaloshinski.

The challenge of teaching many-body theory is to avoid spending too much time on the formalism, but still provide a solid foundation which can be of later use. The general understanding of the structure of the theory must be combined with the insight obtained from calculating low-order diagrams. The present text attempts to meet these rather different goals by severely limiting the number of topics for which explicit calculations are carried out. Some of the topics left out of the main text are introduced in the homework problems, which are collected in the last chapter.

It is important that the student does not come away from an introductory course on many-body theory with the belief of being equipped to tackle any problem involving many particles. The Green function methods described in the present text complement a host of other important methods, including semiclassical transport theory, renormalization group analysis and bosonization techniques. The aim of the present course is to give the student sufficient understanding of the use of field-theoretical methods to be able to read the literature and to evaluate simple diagrams. It is important that the student learns to see the methods as alternatives to other methods. The derivation of the Drude-formula for the frequency-dependent electrical conductivity (Chapter 11) serves as an illustration. Here the use of elementary kinetic theory yields the answer in a few lines, as shown in Chapter 1. The advantage of the Green function method, on the other hand, is that it allows one to consider more general situations such as those involving weak localization.

The many-body course was given as a sequel to a course on semiclassical transport theory, based on *Transport Phenomena* by H. Smith and H. Højgaard Jensen. The first half of the problems in Chapter 12 of the present text (Problems 1-27) were used in the course on transport theory. In order to complement the lectures these homework problems deal exclusively with two-dimensional systems. The remaining homework problems (Problems 28-55) refer to the present text.

Ørsted Laboratory, May 2, 1994 Henrik Smith

List of corrections to Introduction to Many-particle Physics

- p. 13: fourth line from below should have "background".
- p. 17: left hand side of (2.49) should be $U(t, t_0)$.
- p. 36: line below (5.21) should have $u^2 v^2$
- p. 44: leave out the $\beta^{\dagger}\beta$ -term in (5.63).
- p. 45: line 2 from above: to be able.
- p. 45: replace H by K on left hand side of (5.69).
- p. 45: replace H by K on left hand side of (5.71).
- p. 45: in line below (5.69) remove "real" and add after Δ_k ", which we assume to be real,".
- p. 48: interchange e^{-iqa} and e^{iqa} in (5.90).
- p. 64: missing final] in (6.84).
- p. 76: multiply right hand side of (7.54) by \hbar .
- p. 80: multiply right hand side of (7.76) by \hbar .
- p. 81: multiply right hand side of (7.84) by -1.

p. 95: line 8 from above should have $1 - \lambda V(q) \Pi^{(0)} \simeq 1 + \lambda k_s^2/q^2$. In (8.63) $1 + k_s^2/q^2$ should be replaced by $1 + \lambda k_s^2/q^2$.

- p. 102: the minus-sign in front of the second fraction inside the parenthesis in (9.29) should be a plus-sign.
- p. 126: in third line below (11.13) change (8.49) to (8.50).
- p. 128: The second term inside the parenthesis on the right hand side of
- (11.21) should be $(\nabla \psi^{\dagger})\psi$ instead of $\bar{\psi}\nabla\psi^{\dagger}$.
- p. 128: Multiply the right hand side of (11.24) by $1/V^{1/2}$.
- p. 128: Multiply the right hand side of (11.25) by 1/V.
- p. 129: Multiply the integral in (11.32) by V/\hbar .
- p. 131: Multiply the right hand side of (11.47) by $1/\hbar$.
- p. 132: Multiply the right hand side of (11.49) by -1.
- p. 133: Multiply the right hand side of (11.57) by $1/V^2$.
- p. 133: Multiply the right hand side of (11.58) by $-1/\hbar\beta$.
- p. 135: Multiply the right hand side of (11.63) by $1/\omega$.
- p. 163 Problem 45: replace (A 89) by (12.90) in first line.
- p. 163 Problem 46: dispersion (in the long wavelength limit) of longitudinal plasma waves.
- p. 163 Problem 46: replace (8.37) by (8.38) and (8.33) by (8.34).
- p. 163 Problem 47: replace (8.37) by (8.38).
- p. 163 Problem 49: In first line add in the static limit after "determine".

HS April 16, 1997

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1 Introduction

A many-body problem, in the usual sense of the word, is a problem involving many particles. Not 3 or 11, but N, where $N \to \infty$, while the volume V of the system also tends to infinity in such a manner that the density N/V remains finite. This is the *thermodynamic limit*, in which statistical mechanics applies.

Even though the motion of, say, the conduction electrons in 1 cm³ of aluminum constitutes a many-body problem, it is possible for some purposes to treat it as an effective one-body problem. One of the first applications of quantum mechanics to metals was the free-electron model of Sommerfeld (1928). This model was remarkably successful in explaining the thermodynamic and transport properties of simple metals. The free-electron model reduced the many-body problem involving approximately 10^{23} electrons, which repel each other by Coulomb forces, to the motion of a single electron in a constant potential. A deeper understanding of the reasons for this success - as well as the limitations of the model - was obtained in the following decades by considering the effects of the periodic potential, the repulsion between the electrons and their interaction with the phonons.

In the following chapters we shall often use the electron gas to illustrate the use of the methods of many-body physics. This is not only due to the historical importance of the electron gas. It also reflects the fact that an understanding of its properties is the starting point for the understanding of the metals, semiconductors and superconductors that are being investigated in today's laboratories.

1.1 Specific heat and susceptibility

According to elementary statistical mechanics the heat capacity per unit volume (at constant volume) for a gas of non-interacting electrons is given at low temperatures by

$$C = \frac{\pi^2}{3} k^2 T g(\epsilon_{\rm F}), \qquad (1.1)$$

where k is the Boltzmann constant, and $g(\epsilon_{\rm F})$ is the density of states per unit volume at the Fermi energy. For a gas of free electrons the Fermi energy is $\epsilon_{\rm F} = \hbar^2 k_{\rm F}^2/2m$, where $k_{\rm F} = (3\pi^2 n)^{1/3}$, with n = N/V being the electron density and m the electron mass. The density of states at the Fermi energy is proportional to the electron mass, since

$$g(\epsilon)d\epsilon = \frac{1}{4\pi^3} 4\pi k^2 dk \tag{1.2}$$

together with $\epsilon = \hbar^2 k^2 / 2m$ implies that

$$g(\epsilon) = \frac{1}{\pi^2} \frac{m}{\hbar^3} \sqrt{2m\epsilon}, \qquad (1.3)$$

yielding

$$g(\epsilon_{\rm F}) = \frac{mk_{\rm F}}{\pi^2 \hbar^2}.$$
 (1.4)

Within the free-electron model, the electronic heat capacity (per unit volume) only depends on the number density n and the electron mass m apart from the temperature. This is no longer true, when the existence of a periodic potential and interaction effects are taken into account. For the purpose of comparing with the free-electron model it is often convenient to write the heat capacity in the form given by (1.1) and (1.4), but with m replaced by an effective mass m^* defined by

$$g(\epsilon_{\rm F}) = \frac{m^* k_{\rm F}}{\pi^2 \hbar^2}.$$
 (1.5)

When the periodic potential of the lattice as well as the effects of interactions are ignored, one thus has $m^* = m$.

The free-electron model may also be used to calculate the paramagnetic (spin) susceptibility χ of a degenerate electron gas. The result is

$$\chi = \beta^2 \mu_0 g(\epsilon_{\rm F}), \tag{1.6}$$

where $\beta = e\hbar/2m$ is the (spin) magnetic moment of the electron, while μ_0 is the permeability of empty space. Note that the susceptibility is an *intensive* quantity, proportional to the density of states per unit volume, $g(\epsilon_F)$.

In Section 1.3 below we shall compare the predictions of the free-electron model with experiment. The discrepancies will provide a motivation for the use of the methods of many-body physics. We stress, however, that the methods themselves are far more general. They may be applied to any interacting system of fermions and/or bosons, to spin systems, to a single magnetic impurity coupled to a non-interacting electron gas and to a host of other important problems. The experiments chosen are thus only meant to provide examples that illustrate the relation between quantities measured in the laboratory and results obtained by the methods of many-body theory.

1.2 Conduction of electricity and heat

In 1900 the German physicist Paul Drude introduced a statistical model describing the conduction of electricity and heat in a metal. He assumed that the electric current was carried by electrons in a steady state resulting from the balance of the acceleration due to the electric field and the deceleration due to collisions¹. Drude used a statistical description, by taking the average time

¹Drude imagined that these collisions were caused by the electrons bumping into the ions of the metal. Though the quantum theory of motion in a periodic potential showed this picture to be wrong, the Drude model has remained useful to this day, because the physical origin of the collisions played no explicit role in his theory.

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interval between two successive collisions to be a material-dependent constant τ , and assuming that the direction of the velocity of the electron immediately after a collison is random with respect to the electric field. During the time interval τ the electron therefore obtains an increase \mathbf{v}_d in velocity given by

$$\mathbf{v}_d = -\frac{e\mathbf{E}\tau}{m},\tag{1.7}$$

the charge of the electron being -e. Because of the assumption that the velocity of the electron is random immediately after a collision, the velocity increase \mathbf{v}_d may be identified with the drift velocity of the entire system of electrons. Now, since the current density \mathbf{j} is given by the conduction electron density n and the drift velocity \mathbf{v}_d according to

$$\mathbf{j} = -ne\mathbf{v}_d,\tag{1.8}$$

we obtain the desired relation between the electric field and the current density \mathbf{j} ,

$$\mathbf{j} = \boldsymbol{\sigma} \mathbf{E},\tag{1.9}$$

where the conductivity σ is given by

$$\sigma = \frac{ne^2\tau}{m}.\tag{1.10}$$

The resistivity $\rho = \sigma^{-1}$ is thus

$$\rho = \frac{m}{ne^2\tau}.\tag{1.11}$$

The Drude model would be of limited interest if it were only applied to the d. c. conductivity of a metal, since τ is an undetermined parameter. It is, however, straightforward to extend the model to the case of a time-varying electric field $\mathbf{E} = \mathbf{E}_0 \exp(-i\omega t)$. In this case the drift velocity is obtained from

$$\dot{\mathbf{v}}_d = -\frac{e}{m}\mathbf{E} - \frac{\mathbf{v}_d}{\tau},\tag{1.12}$$

resulting in $\mathbf{j} = \sigma(\omega) \mathbf{E}$, where

$$\sigma(\omega) = \frac{ne^2\tau}{m} \frac{1}{1 - i\omega\tau}.$$
(1.13)

The frequency dependence of the Drude conductivity (1.13) is compared with experiment in *Transport Phenomena*, Section 2.2.

As a final example of the use of the Drude model we quote the result for the thermal conductivity κ , which is defined as the coefficient relating the temperature gradient ∇T to the heat current density \mathbf{j}_{th} ,

$$\mathbf{j}_{\mathrm{th}} = -\kappa \nabla T. \tag{1.14}$$

According to the Drude model the thermal conductivity is

$$\kappa = \frac{1}{3}Cv^2\tau. \tag{1.15}$$

Here v is an average particle velocity (not the drift velocity), while C is the heat capacity per unit volume (at constant volume). In a classical gas, v is related to the thermal velocity $\sqrt{kT/m}$, but in a highly degenerate gas such as the conduction electrons in a metal the average velocity v should be identified with $v_{\rm F}$, since only states with energies close to the Fermi energy yield a significant contribution to the heat current.

1.2.1 Transport in a magnetic field

The classical Hall effect was first observed by E. H. Hall in 1880. When a current-carrying wire is placed in a magnetic field perpendicular to the direction of the current, one observes a potential difference across the wire, perpendicular to the direction of the current and to the magnetic field. This implies that the electric field and the current density in the wire are not parallel to each other. If the magnetic field is sufficiently strong, the electric field may be nearly perpendicular to the direction of the current.

The explanation for this effect is the following. When a current is passed through a wire in a magnetic field perpendicular to the direction of the current, the magnetic field acts to deflect the electrons in a direction perpendicular to itself and the velocity of the electrons. Since the drift velocity \mathbf{v}_d points along the direction of the wire, a component of the electric field must exist perpendicular to the current direction. The perpendicular field component has a magnitude which is just sufficient to ensure that the electrons move along the direction of the wire. The perpendicular field component is named the Hall field and denoted by $E_{\rm H}$. Its magnitude is determined by the requirement that the two forces perpendicular to the direction of the current, the Lorentz force due to the magnetic field and the force due to the perpendicular component of the electric field, cancel each other,

$$0 = -eE_{\rm H} + ev_d B. \tag{1.16}$$

The Hall field is thus proportional to both the drift velocity and the magnetic field. The current density \mathbf{j} and the drift velocity \mathbf{v}_d are connected by the relation $\mathbf{j} = -ne\mathbf{v}_d$, where *n* is the number density of the conduction electrons. This allows the Hall field to be written as

$$E_{\rm H} = R_{\rm H} j B, \tag{1.17}$$

where

$$R_{\rm H} = -\frac{1}{ne} \tag{1.18}$$

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is called the Hall constant. Within the simple treatment given here, the Hall constant is seen to depend solely on the charge of the electrons and their density.

If the magnetic field differs from zero, the conductivity thus becomes a tensor, since the application of an electric field in a direction perpendicular to the magnetic field gives rise to components of the current density both parallel and perpendicular to the electric field.

1.3 Three experiments

Let us now consider the results of three different types of experiment involving i) the specific heat, ii) the spin susceptibility and iii) the electrical resistivity of metals such as Al, Na and Cu. These results will be used in subsequent chapters for comparing theory with experiment.

1.3.1 Specific heat of aluminum

The low-temperature specific heat of metals is found experimentally to be linearly dependent on T, due to the contribution of the conduction electrons. In addition, the lattice vibrations at low temperatures contribute a term proportional to T^3 , and the measured specific heat of aluminum may therefore be fitted by an expression of the form

$$C = \gamma T + BT^3 \tag{1.19}$$

at sufficiently low temperatures². For aluminum one finds from such a fit that the molar specific heat C_{mol} is $\gamma_{mol}T$, where $\gamma_{mol} = 3.0 \cdot 10^{-4} \text{ cal/(mol K^2)}$.

Let us now compare this experimental observation with the results of the free-electron model. Since aluminum is trivalent, each atom in the metal contributes three electrons to the conduction electron gas. As the molar mass is $M_{\rm mol} = 26.982$ g/mol and the mass density is $\rho = 2.698$ g/cm³, the conduction electron density is $n = 3N_A\rho/M_{\rm mol} = 1.8 \cdot 10^{29}$ m⁻³, which allows us to determine $k_{\rm F}$ from $k_{\rm F} = (3\pi^2 n)^{1/3}$, resulting in

$$k_{\rm F} = 1.75 \cdot 10^8 {\rm cm}^{-1}. \tag{1.20}$$

Note that values of $k_{\rm F}$ for different metals are generally of this order of magnitude, roughly equal to the inverse of the distance between neighboring atoms in the metal. In the alkali metals $k_{\rm F}$ ranges from $1.12 \cdot 10^8 {\rm cm}^{-1}$ for Li to $0.65 \cdot 10^8 {\rm cm}^{-1}$ for Cs, reflecting the increase in ionic radius with increasing

² The temperature must be much less than the Debye temperature, which is a few hundred K for Al. Due to the existence of low-lying transverse phonon modes, the (frequency) density of phonon modes may deviate considerably from being proportional to ω^2 even at fairly low frequencies, thus further shrinking the temperature region in which a T^3 -term in the specific heat may be observed.

atomic number. Using $\gamma = \gamma_{mol} \rho / M_{mol}$ we may now express the experimentally measured value of γ in terms of an effective mass m^* according to

$$\gamma = \frac{\pi^2}{3} k^2 \frac{m^* k_{\rm F}}{\pi^2 \hbar^2}, \tag{1.21}$$

and determine m^* . By inserting in (1.21) the experimentally measured value of γ together with the fundamental constants and $k_{\rm F}$ from (1.20) one obtains that m^* is equal to 1.38 times the electron mass m.

The Sommerfeld theory explains why the heat capacity of the electrons is reduced drastically compared to its classical value, which would be temperature independent, equal to C = 3nk/2. The fact that the measured low-temperature specific heat is linear in T and that the calculated and observed values agree within 50 per cent constitutes a definite success of the free-electron model. From the point of view of many-body physics, the remaining discrepancy is however highly significant. One might think that the difference between theory and experiment is due to the fact that the electrons move in a periodic. rather than a constant potential. This effect turns out to be of negligible importance for aluminum though it plays a significant role in a number of other elements, notably the transition metals. As we shall see in Chapter 9, the interaction between the electrons and the phonons is responsible for the difference between the observed value of m^* and the free electron mass m. This is a real many-body effect. It implies that the electrons involved in a measurement of specific heat carry a 'cloud' of phonons with them in their motion, thereby obtaining a greater effective mass. Such a picture must, however, be used with great care. If we measure instead the spin susceptibility of the electrons, which in the free electron model is given by (1.6), we shall find that the electron-phonon interaction has no effect on the result. The density of states in (1.6) thus involves an effective mass which is different from the effective mass m^* appropriate to the specific heat. Likewise one may show that the Drude formula (1.10) is unaffected by the electron-phonon interaction, while the frequency-dependent generalization (1.13) is modified by it. These examples illustrate some of the subtleties involved in the description of many-body effects in metals. It is not in general possible to express many-body effects in terms of a single parameter m^*/m characterizing different physical quantities.

1.3.2 Spin susceptibility of sodium

As our second example of a physical quantity which may be measured experimentally, we shall now consider the electron spin susceptibility. Since the total magnetic moment of a metal in an external magnetic field contains both diamagnetic and paramagnetic contributions, it is not a simple matter to extract the paramagnetic part due to the spin of the conduction electrons. One method involves measuring a shift in the nuclear magnetic resonance (NMR) arising from the splitting of the nuclear energy levels in a magnetic

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field. Since the conduction electrons are coupled via their magnetic dipole moments to the nuclear magnetic moments, the nuclear magnetic resonance is shifted in frequency as the conduction electrons are polarized by the external field. This shift, known as the *Knight shift*, also depends on the value of the conduction-electron wave function at the site of the nucleus. Since the magnitude of the spin-polarization is proportional to the conduction-electron spin susceptibility, Knight shift measurements may therefore be used to deduce the conduction-electron spin susceptibility, provided something is known about the conduction-electron wave function at the site of the nucleus. A more direct method involves measurement of susceptibility by conduction-electron spin resonance. The method involves a measurement of the absolute intensity of the conduction-electron spin resonance signal by comparing it to the nuclear magnetic resonance signal in the same sample.

For sodium one finds experimentally that $\chi = 1.4 \cdot 10^{-5}$. In order to compare with the results of the free-electron model we evaluate (1.6) for the appropriate density of conduction electrons, $n = 2.65 \cdot 10^{28} \text{ m}^{-3}$, resulting in $k_{\rm F} = 0.92 \cdot 10^8 \text{ cm}^{-1}$, which yields $\chi = 0.83 \cdot 10^{-5}$. Thus $\chi_{\rm exp}/\chi_{\rm theory} = 1.7$. The origin of the discrepancy between the values is *not* the electron-phonon interaction, but rather the electron-electron interaction which we shall discuss in Section 4.3.2.

1.3.3 Electrical resistivity of copper

Our final example involves the measurement of the electrical resistivity of copper with a small amount of magnesium impurities. The temperature dependent resistivity of a normal metal usually³ decreases with decreasing temperature. Provided the metal does not become a superconductor below a certain critical temperature, the resistivity tends to a finite value, which depends on the number of impurities. This value is called the residual resistivity and denoted by ρ_0 . For Cu with 1 per cent of magnesium impurities one finds that $\rho_0 = 0.6 \cdot 10^{-6}$ Ω cm. For a sample of length L and cross-sectional area A the total resistance R is given by

$$R = \frac{\rho L}{A}.\tag{1.22}$$

We mention in passing that the generalization of (1.22) to two dimensions is

$$R = \frac{\rho_{2d}L_1}{L_2},$$
 (1.23)

for a rectangle with sidelengths L_1 and L_2 . The resistivity ρ_{2d} must therefore carry the same unit as that of R, namely ohm (in the SI-system). Note that the combination h/e^2 of the fundamental constants h and e has the same dimension as the two-dimensional resistivity.

³An exception to this rule is found in metals containing magnetic impurities.

Let us return to the three-dimensional case and again consider the value of the residual resistivity. It is convenient first to convert the resistivity into a characteristic rate $1/\tau$ by using the Drude-formula (1.10). Since $n = 8.47 \cdot 10^{28}$ m⁻³ for Cu, the rate obtained experimentally corresponding to the value $\rho_0 = 0.6 \cdot 10^{-6} \Omega$ cm is

$$\frac{1}{\tau} = \frac{ne^2}{m}\rho_0 = 1.4 \cdot 10^{13} \,\mathrm{s}^{-1}. \tag{1.24}$$

If this scattering rate is multiplied by the Planck constant we obtain the energy

$$\frac{\hbar}{\tau} = 0.9 \cdot 10^{-2} \,\mathrm{eV}.\tag{1.25}$$

Comparing this energy to the Fermi energy, which is 7 eV in Cu, we note that $\hbar/\tau \ll \epsilon_{\rm F}$. Since the mean free path is $l = v_{\rm F}\tau \simeq \hbar\tau/ma$ and $\epsilon_{\rm F} \simeq \hbar^2/ma^2$, with $a \simeq k_{\rm F}^{-1}$ being the distance between neighboring atoms, this inequality is equivalent to $l \gg a$ (or $k_{\rm F} l \gg 1$).

In Chapter 11 we shall use diagrammatic methods to calculate the resistivity of a simple metal in the limit $k_{\rm F} l \gg 1$. This will allow us to compare the calculated value of the residual resistivity for Cu with Mg impurities with that measured experimentally, as well as with that obtained by solving the Boltzmann equation.

2 Second quantization

In many-body physics it is very useful to express the Hamiltonian in terms of creation and annihilation operators for excitations, defined by some basis of one-electron states. Since the one-electron states satisfy the Schrödinger equation for the motion of a single particle, this procedure has traditionally been named 'second quantization'.

2.1 Creation and annihilation operators

For a single harmonic oscillator with force constant K and mass M it is wellknown from elementary quantum mechanics that the Hamiltonian may be written in the form

$$H = \hbar\omega(b^{\dagger}b + \frac{1}{2}), \quad \omega = \sqrt{K/M}, \quad (2.1)$$

where the operators b^{\dagger} and b create and annihilate, respectively, a quantum of energy $\hbar\omega$. For the case of lattice vibrations described in the harmonic approximation one may show, as demonstrated in Chapter 5, that the Hamiltonian can be written as a sum of independent harmonic oscillators according to

$$H = \sum_{\mathbf{q}\lambda} \hbar \omega_{\mathbf{q}\lambda} (b_{\mathbf{q}\lambda}^{\dagger} b_{\mathbf{q}\lambda} + \frac{1}{2}).$$
 (2.2)

Here $\omega_{q\lambda}$ is the frequency of the normal mode with wavevector \mathbf{q} and polarization index λ . If the Hamiltonian function for the lattice contains terms of higher order than two in the deviations of the atoms from their ideal lattice positions, the Hamiltonian contains additional terms involving three or more creation and annihilation operators.

Since we are mainly concerned with fermion operators in the following, we shall describe in detail how the Hamiltonian of interacting Fermi particles may be expressed in terms of creation and annihilation operators. As a basis for the description of a system of identical fermions we shall use Slater determinants, which are antisymmetrized products of single-particle states.

To gain familiarity with the field operators and their commutation properties we first consider the occupation of a single quantum state, in analogy with the single harmonic oscillator. While in the case of the harmonic oscillator the number of vibrational quanta could be anywhere in the range from zero to infinity, the antisymmetry requirement restricts the occupation of a given quantum state to be one or zero.

Let us denote by $|0\rangle$ the vacuum state in which no particle occupies the quantum state in question, and by $|1\rangle$ the occupied state. The fermion creation operator c^{\dagger} is then introduced by the definition

$$c^{\dagger}|0\rangle = |1\rangle; \quad c^{\dagger}|1\rangle = 0.$$
 (2.3)

Since c^{\dagger} is seen to be given by

$$c^{\dagger}:\left(\begin{array}{c}0&0\\1&0\end{array}\right) \tag{2.4}$$

in the basis $|0\rangle$, $|1\rangle$, we deduce that

$$c:\left(\begin{array}{cc} 0 & 1\\ 0 & 0 \end{array}\right) \tag{2.5}$$

and hence

$$c|0\rangle = 0; \quad c|1\rangle = |0\rangle. \tag{2.6}$$

By combining (2.3) and (2.6) we obtain the commutation rules

$$c^{\dagger}c^{\dagger} = cc = 0; \quad c^{\dagger}c + cc^{\dagger} = 1$$
 (2.7)

for the operators c^{\dagger} and c.

The next step is to examine how operators belonging to different singleparticle states commute. The simplest case is that of two particles. Consider a state obtained by adding particles in the two single-particle states and according to the rule of correspondence

$$c_i^{\dagger} c_k^{\dagger} |0\rangle \leftrightarrow \frac{1}{\sqrt{2}} (\phi_i(x_1) \phi_k(x_2) - \phi_k(x_1) \phi_i(x_2))$$

$$(2.8)$$

where $x_1(x_2)$ denote the coordinates of particle 1(2). When the single-particle states are filled in reverse order, corresponding to $c_k^{\dagger} c_i^{\dagger} |0\rangle$, we must obtain the same state. Since

$$c_k^{\dagger} c_i^{\dagger} | 0 \rangle \leftrightarrow \frac{1}{\sqrt{2}} (\phi_k(x_1) \phi_i(x_2) - \phi_i(x_1) \phi_k(x_2))$$
 (2.9)

the operators c_i^{\dagger} and c_k^{\dagger} must anticommute:

$$\{c_i^{\dagger}, c_k^{\dagger}\} = c_i^{\dagger} c_k^{\dagger} + c_k^{\dagger} c_i^{\dagger} = 0.$$
(2.10)

It is similarly seen that c_i and c_k satisfy the same relations as (2.10). The argument may readily be extended to an arbitrary number of particles. Together with (2.7) these relations lead to the Fermi commutation rules

$$\{c_i, c_k\} = \{c_i^{\dagger}, c_k^{\dagger}\} = 0; \quad \{c_i, c_k^{\dagger}\} = \delta_{ik}, \quad (2.11)$$

with i labelling a set of single-particle states.

Having introduced the creation and annihilation operators for fermions and noted the difference between their commutation rules (2.11) and those of boson

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operators, we next show how one- and two-body operators may be expressed in terms of c and c^{\dagger} operators.

Since a one-body operator is a sum of operators, each acting on functions of the coordinates of a single particle, it must have an expansion of the form

$$A = \sum_{ij} A(ij)c_i^{\dagger}c_j. \qquad (2.12)$$

Note that the validity of this equation does not depend on the state of the system being a Slater determinant. Since an arbitrary state may be expanded in terms of the complete set of Slater determinants, (2.12) holds generally, as an operator identity. The simplest way to determine the coefficients A(ij) of the expansion (2.12) is to form matrix elements of A between single-particle states $c_i^{\dagger}|0\rangle = \phi_i$ and $c_k^{\dagger}|0\rangle = \phi_k$. Then

$$A(ij) = \langle i|A|j \rangle = \int dx \phi_i^*(x) A \phi_j(x), \qquad (2.13)$$

where for simplicity we have suppressed the spin degrees of freedom. If spin is taken into account explicitly, the wave functions become spinors, and the integration over x should be supplemented by a summation over spin variables. The one-body operator A consequently has the form

$$A = \sum_{ij} \langle i|A|j \rangle c_i^{\dagger} c_j.$$
(2.14)

A two-body operator B may be treated in an analogous fashion. Since a two-body operator is a sum of operators, each acting on functions of the coordinates of two particles, it may be expanded according to

$$B = \sum_{ijkl(i>j,k>l)} B(ijkl)c_i^{\dagger}c_j^{\dagger}c_lc_k.$$
(2.15)

In writing (2.15) we have adopted a definite ordering of the single-particle states, written symbolically as i > j. The reason is that when we take matrix elements of (2.15) between states

$$|ij\rangle = c_i^{\dagger} c_j^{\dagger} |0\rangle \tag{2.16}$$

and

$$|kl\rangle = c_k^{\dagger} c_l^{\dagger} |0\rangle \tag{2.17}$$

we have adopted a definite order in which these states are filled, corresponding to i > j and k > l. We conclude that

$$B(ijkl) = \langle ij|B|kl\rangle, \qquad (2.18)$$

in analogy with (2.13). Note that the matrix (2.18) is antisymmetric with respect to interchange of i and j, as well as k and l. It is often convenient to abandon the restriction i > j, k > l and to introduce the non-symmetrized matrix elements $\langle ij|B|kl\rangle_{n.s.}$ given by

$$\langle ij|B|kl\rangle_{\rm n.s.} = \int \int dx_1 dx_2 \phi_i^*(x_1) \phi_j^*(x_2) B\phi_k(x_1) \phi_l(x_2)$$
 (2.19)

Thus we have

$$B = \frac{1}{4} \sum_{ijkl} \langle ij|B|kl \rangle c_i^{\dagger} c_j^{\dagger} c_l c_k = \frac{1}{2} \sum_{ijkl} \langle ij|B|kl \rangle_{\text{n.s.}} c_i^{\dagger} c_j^{\dagger} c_l c_k.$$
(2.20)

2.2 Hamiltonians

We now introduce the three Hamiltonians which we shall use in our effort to explain each of the three experiments discussed in Section 1.3 of the previous chapter. The three Hamiltonians involve electrons interacting with themselves (Section 2.2.1), electrons interacting with phonons (Section 2.2.2), and electrons interacting with impurities (Section 2.2.3).

2.2.1 Electron-electron interaction

The Hamiltonian of a homogeneous electron gas is

$$H = H_0 + H'$$
 (2.21)

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(2.22)

represents the kinetic energy, while the interaction between the electrons is described by

$$H' = \frac{1}{2V} \sum_{\mathbf{q}\neq 0,\mathbf{k},\mathbf{k}',\sigma,\sigma'} \frac{4\pi e_0^2}{q^2} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma}, \qquad (2.23)$$

since the matrix-element $\langle \mathbf{k} + \mathbf{q} \ \mathbf{k}' - \mathbf{q} | e_0^2 / r | \mathbf{k} \ \mathbf{k}' \rangle$ is equal to $4\pi e_0^2 / q^2 V$, as shown in App. A¹. The restriction on the **q** sum is due to the fact that the electrons are immersed in a positive background of charge due to the lattice

¹We use the form e_0^2/r with $e_0^2 = e^2/4\pi\epsilon_0$, appropriate to the SI system of units, for the Coulomb potential describing the interaction between two electrons separated by the distance r. The transition to the cgs system is then easily achieved by replacing everywhere e_0^2 by e^2 . Note that most of the literature on many-body physics still uses the cgs system of units.

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ions. This positive charge is assumed to be spread uniformly throughout the volume V under consideration. The $\mathbf{q} = 0$ term left out in (2.23) precisely cancels the contribution from the interaction between the ions of the positive background and the interaction between the electrons and the positive background. This may be seen by considering the $\mathbf{q} = \mathbf{0}$ term left out of (2.23), which is proportional to the operator \hat{O} given by

$$\hat{O} = \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} c^{\dagger}_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k}',\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma}.$$
(2.24)

By using the fermion commutation relations

$$\{c_{\mathbf{k},\sigma}, c^{\dagger}_{\mathbf{k}',\sigma'}\} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$$
(2.25)

 and

$$\{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}\} = 0, \qquad (2.26)$$

the operator \hat{O} is seen to be given by the operator \hat{N} for the total number of particles,

$$\hat{N} = \sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(2.27)

according to

$$\hat{O} = \hat{N}^2 - \hat{N}.$$
(2.28)

Since we are working with states corresponding to a definite number of particles, N, we may therefore replace \hat{N} and \hat{O} by their eigenvalues N and $N(N-1) \simeq N^2$, respectively. It follows that the $\mathbf{q} = 0$ term represents the energy $E_{\rm el-el}$ of a uniform charge distribution of density $n_0 = N/V$ due to the mutual repulsion of the negative charges, since $E_{\rm el-el}$ may be written as²

$$E_{\rm el-el} = \int d\mathbf{r} \int d\mathbf{r}' \frac{e_0^2}{2|\mathbf{r} - \mathbf{r}'|} n_0^2 \qquad (2.29)$$

which apart from the constant factor n_0^2 equals the $\mathbf{q} = 0$ Fourier-component of the electron-electron interaction. This electrostatic energy of the uniform electron charge distribution is, however, precisely cancelled by the sum of $E_{\rm el-ion}$, the energy due the interaction between the uniform electron charge density with the positive background, and $E_{\rm ion-ion}$, the energy due the interaction of the positive background with itself, as may be seen explicitly by writing out their contribution in the manner of (2.29). This results in $E_{\rm ion-ion} = E_{\rm el-el} = -E_{\rm el-ion}/2$, leading to $E_{\rm ion-ion} + E_{\rm el-el} + E_{\rm el-ion} = 0$.

²Stricly speaking the energy is infinite, corresponding to the divergence in $V(q) = 4\pi e_0^2/q^2 V$ as q tends to zero. The divergence may be handled by introducing a finite range of the Coulomb interaction by multiplying it by $\exp -|\mathbf{r} - \mathbf{r}'|/a$ and letting a go to infinity at the end. A detailed discussion of this procedure may be found in A. L. Fetter and J. D. Walecka 'Quantum Theory of Many-Particle Systems', McGrawHill 1971, p. 21.

2.2.2 Electron-phonon interaction

The Hamiltonian describing electrons interacting with phonons is

$$H_{\rm el-ph} = \sum_{\mathbf{k}\mathbf{k'q}\sigma\sigma'\alpha} g(\mathbf{k}, \mathbf{k'}, \mathbf{q}, \alpha) c^{\dagger}_{\mathbf{k'}, \sigma'} c_{\mathbf{k}, \sigma} (b_{\mathbf{q}\alpha} + b^{\dagger}_{-\mathbf{q}\alpha})$$
(2.30)

It will be derived in Chapter 9 with a simple model-form for the coupling function $g(\mathbf{k}, \mathbf{k}', \mathbf{q}, \alpha)$. In a real metal the coupling function g depends on the two separate wave vectors (Bloch vectors) \mathbf{k} and \mathbf{k}' . In Chapter 9 we shall discuss the simpler case of a gas of free electrons described by the Hamiltonian (2.22) coupled to the phonons via the interaction (2.30). In this case g only depends on the wave-vector difference $\mathbf{q} = \mathbf{k}' - \mathbf{k}$.

Note that the form of (2.30) is similar to that of a one-body operator, cf. (2.14), as far as the electrons are concerned, but unlike potential scattering associates the transition between two different electron states with the emission and absorption of a phonon. In a real metal the phonons interact not only with the electrons but also with themselves due to the presence of anharmonic terms (of the form $b^{\dagger}bb$ and $b^{\dagger}b^{\dagger}b$, etc.) in the lattice Hamiltonian. Also the phonons may interact with impurities and other defects. If these effects are important, one has to add such terms explicitly to the Hamiltonian.

2.2.3 Electron-impurity interaction

The Hamitonian for a single electron interacting with impurities which occupy fixed positions in a lattice is

$$H = \frac{\mathbf{p}^2}{2m} + \sum_i V(\mathbf{r} - \mathbf{R}_i).$$
(2.31)

Here the sum extends over the position vectors \mathbf{R}_i of the impurities.

The Hamiltonian for an electron gas which interacts with fixed impurities may be written in the second-quantized form

$$H = H_0 + H_1 \tag{2.32}$$

where H_0 is given by (2.22), while

$$H_1 = \sum_{\mathbf{q}} \rho_{\rm imp}(\mathbf{q}) V(-\mathbf{q}) \rho(\mathbf{q}).$$
(2.33)

Here $\rho(\mathbf{q})$ is the Fourier component of the density operator, given by

$$\rho(\mathbf{q}) = \sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} , \qquad (2.34)$$

while

$$\rho_{\rm imp}(\mathbf{q}) = \sum_{\mathbf{i}} e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{i}}},\tag{2.35}$$

and $V(\mathbf{q})$ is the Fourier-transform of $V(\mathbf{r})$ divided by the volume. When this Hamiltonian is used in Chapter 11 to evaluate the d. c. resistivity of a metal, we shall also need to average over the positions of the impurities. This allows us to relate the phenomenological Drude relaxation time τ introduced in Section 1.2 to the number density of impurities and the matrix-element $V(\mathbf{q})$ of the impurity potential, as well as the number density of the electrons and the electron mass. We shall evaluate the resistivity for a simple model-potential and compare the outcome with the value of τ obtained experimentally, cf. (1.24).

2.3 Pictures

Let us consider a general physical system described by the time-independent Hamiltonian H. The Schrödinger equation has the form

$$i\hbar\frac{\partial\Psi_S}{\partial t} = H\Psi_S,\tag{2.36}$$

where Ψ_S denotes the Schrödinger wave function. In the Schrödinger picture operators are independent of time, while the state vectors develop in time according to (2.36). It is sometimes convenient to work in an alternative picture, which is equivalent to the Schrödinger picture. In this Heisenberg picture the state vectors are independent of time, while the operators develop in time. It is also useful to employ an interaction picture, which in a certain sense is intermediate between the Heisenberg and Schrödinger pictures. Below we shall exhibit the unitary transformations that connect these different pictures and introduce the time-development operator in the interaction picture, U, which will be used extensively in the following.

2.3.1 The Heisenberg picture

The transition to the Heisenberg picture is accomplished by the unitary transformation

$$\Psi_H = e^{iHt/\hbar} \Psi_S \tag{2.37}$$

while the operator A_{S} in the Schrödinger picture becomes

$$A_H = e^{iHt/\hbar} A_S e^{-iHt/\hbar}.$$
(2.38)

This transformation of the operator ensures that any matrix element of an operator A_S in the Schrödinger picture equals the corresponding matrix element in the Heisenberg picture, since

$$\langle \Psi'_S, A_S \Psi_S \rangle = \langle \Psi'_H, e^{iHt/\hbar} A_S e^{-iHt/\hbar} \Psi_H \rangle.$$
(2.39)

Evidently A_H satisfies the equation of motion

$$i\hbar\frac{dA_H}{dt} = [A_H, H], \qquad (2.40)$$

provided A_s has no explicit dependence on time, as may be seen by differentiating A_H given by (2.38) with respect to time.

2.3.2 The interaction picture

One often deals with a time-independent Hamiltonian H, which may be separated in a part H_0 with known eigenvalues and eigenvectors, and a part H_1 (which does not commute with H_0) with unknown eigenvalues and eigenvectors. Typically, H_0 is the energy operator for independent particles, while H_1 describes the interaction. In the examples studied in the following, H_0 describes independent electrons, while H_1 may represent the mutual interaction between the electrons or the interaction between electrons and phonons. In order to do infinite-order perturbation theory it is convenient to introduce a 'mixed' picture, the interaction picture, in which state vectors develop according to

$$\Psi_I = e^{iH_0 t/\hbar} \Psi_S. \tag{2.41}$$

In the absence of any interaction, corresponding to $H_1 = 0$, the interaction picture becomes identical to the Heisenberg picture, implying that the states are time-independent. In the presence of the interaction, described by the Hamiltonian H_1 , the states develop in time in a manner determined by the interaction.

By taking the time derivative of the state Ψ_I and using the Schrödinger equation (2.36) one sees that

$$i\hbar\frac{\partial\Psi_I}{\partial t} = e^{iH_0t/\hbar}(-H_0 + H)e^{-iH_0t/\hbar}\Psi_I$$
(2.42)

or

$$i\hbar\frac{\partial\Psi_I}{\partial t} = H_1(t)\Psi_I, \qquad (2.43)$$

where

$$H_1(t) = e^{iH_0 t/\hbar} H_1 e^{-iH_0 t/\hbar}.$$
(2.44)

Since an arbitrary matrix element in the Schrödinger picture may be written as

$$\langle \Psi'_S, A_S \Psi_S \rangle = \langle \Psi'_I, e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar} \Psi_I \rangle, \qquad (2.45)$$

the operator A_I in the interaction picture is given by

~ ~

$$A_I = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar}.$$
 (2.46)

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The development in time of the state vectors in the interaction picture is described by the time-development operator $U(t, t_0)$, which is defined by

$$\Psi_I(t) = U(t, t_0) \Psi_I(t_0). \tag{2.47}$$

Clearly U satisfies the condition

$$U(t_0, t_0) = 1. (2.48)$$

By combining (2.37) and (2.41) one sees that

$$U(t) = e^{iH_0 t/\hbar} e^{-iHt/\hbar} e^{iHt_0/\hbar} e^{-iH_0 t_0/\hbar}.$$
(2.49)

It follows from (2.49) that U is unitary, $U^{\dagger}(t,t_0) = U^{-1}(t,t_0)$, and that $U(t_0,t) = U^{-1}(t,t_0) = U^{\dagger}(t,t_0)$. Furthermore, one sees from the combination of (2.43) with (2.47) that $U(t,t_0)$ satisfies the differential equation

$$i\hbar\frac{\partial U}{\partial t} = H_1(t)U. \tag{2.50}$$

For convenience we now set $t_0 = 0$. With the boundary condition U(0,0) = 1, the integrated form of the differential equation (2.50) becomes

$$U(t,0) = 1 + \frac{1}{i\hbar} \int_0^t dt' H_1(t') U(t',0)$$
(2.51)

The integral equation (2.51) may be iterated. Since $H_1(t')$ and $H_1(t'')$ do not necessarily commute when t' differs from t'' it is important to maintain the proper ordering of the operators,

$$U(t,0) = 1 + \frac{1}{i\hbar} \int_0^t dt' H_1(t') + \frac{1}{(i\hbar)^2} \int_0^t dt' H_1(t') \int_0^{t'} dt'' H_1(t'') + \cdots$$
(2.52)

This may be achieved by introducing the time-ordering operator T, which in the present context is defined by

$$T\{H_1(t')H_1(t'')H_1(t''')\cdots\} = C\{H_1(t')H_1(t'')H_1(t''')\cdots\},$$
(2.53)

where C is an operator which orders the operators $H_1(t')H_1(t'')H_1(t''')\cdots$ chronologically with earlier times to the right. As an example we have

$$T\{H_1(t')H_1(t'')\} = \Theta(t'-t'')H_1(t')H_1(t'') + \Theta(t''-t')H_1(t'')H_1(t'), \quad (2.54)$$

where $\Theta(x)$ is the Heaviside step-function, defined by

$$\Theta(x) = 1 \text{ for } x > 0, \ \Theta(x) = 0 \text{ for } x < 0, \ \Theta(x) = \frac{1}{2} \text{ for } x = 0.$$
 (2.55)

With the use of (2.54) we see that

$$\begin{split} \int_{0}^{t} dt' \int_{0}^{t'} dt'' H_{1}(t') H_{1}(t'') &= \frac{1}{2} \int_{0}^{t} dt' \int_{0}^{t''} dt'' H_{1}(t') H_{1}(t'') \\ &+ \frac{1}{2} \int_{0}^{t} dt'' \int_{0}^{t'''} dt' H_{1}(t'') H_{1}(t') \\ &= \frac{1}{2} \int_{0}^{t} dt' \int_{0}^{t} dt'' H_{1}(t') H_{1}(t'') \Theta(t' - t'') \\ &+ \frac{1}{2} \int_{0}^{t} dt' \int_{0}^{t} dt'' H_{1}(t'') H_{1}(t') \Theta(t'' - t') \\ &= \frac{1}{2} \int_{0}^{t} dt' \int_{0}^{t} dt'' T\{H_{1}(t')H_{1}(t'')\}, \quad (2.56) \end{split}$$

where the first equality is obtained by splitting the left hand side into two identical terms and interchanging the names of the integration variables in the second term.

By generalizing this procedure to all orders one finds the following expansion for U(t, 0)

$$U(t,0) = \sum_{n=0}^{\infty} \frac{1}{(i\hbar)^n} \frac{1}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n T\{H_1(t_1)H_1(t_2)\cdots H_1(t_n)\},$$
(2.57)

which may equivalently be written as

$$U(t,0) = T\{\exp[\frac{1}{i\hbar} \int_0^t dt' H_1(t')]\}.$$
(2.58)

The result (2.58) will be used in Chapter 6 for the purpose of expanding the time-ordered Green function in an infinite-order perturbation series. The individual terms in the series are associated with Feynman diagrams, which help visualizing the structure of the expansion and suggest how one may sum certain classes of diagrams (containing an infinite number of terms). The following chapters contain examples of the application of this technique and the specific evaluation of simple, but important diagrams.

3 Perturbation theory and the electron gas

The electron gas is a very important many-body system, which forms the starting point for the discussion of the properties of metals. The conduction electrons in a metal are immersed in the medium constituted by the positively charged ions. In this chapter we consider the *homogeneous* electron gas and treat the ions as a uniform, immobile background of positive charge, which compensates the total charge of the conduction electrons. Such a model is often referred to as *jellium*.

In the following we investigate the effect of treating the interaction between the electrons as a perturbation. As we shall see, the density of the electron gas must be *high* in order that the perturbative treatment of the interaction is valid. This may seem surprising at first sight. From classical gases we are used to think of ideal gases as being very dilute. The explanation of this paradox is the following: Although the contribution of the Coulomb repulsion to the energy of the electron gas increases for increasing density, the kinetic energy also increases, in fact more rapidly with the density. Measured relative to the kinetic energy the importance of the Coulomb repulsion therefore becomes less, when the density of the electron gas is increased.

While the first-order correction to the unperturbed ground-state energy is finite and small in the high-density limit, we shall discover an unpleasant surprise when going to second order: the second-order correction to the groundstate energy is infinite, thus signalling the break-down of ordinary perturbation theory. How this difficulty may be overcome is described in Chapters 6 and 8.

Before proceeding to do perturbation theory, we recall (Section 2.2.1) that the Hamiltonian of a homogeneous electron gas is

$$H = H_0 + H' \tag{3.1}$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(3.2)

represents the kinetic energy while

$$H' = \frac{1}{2V} \sum_{\mathbf{q}\neq 0,\mathbf{k},\mathbf{k}',\sigma,\sigma'} \frac{4\pi e_0^2}{q^2} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma}.$$
 (3.3)

is the interaction between the electrons.

3.1 First-order perturbation theory

Let us first determine the ground-state energy for the system of non-interacting electrons, described by the Hamiltonian H_0 . This may be found by calculating

the expectation value $E_0 = \langle H_0 \rangle$ in the ground state $|0\rangle$ of the unperturbed system. We have

$$E_0 = \langle 0|H_0|0\rangle = 2\sum_{\mathbf{k}} \epsilon_k \Theta(k_{\rm F} - k)$$
(3.4)

Since the total number of particles is

$$N = \langle 0 | \sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} | 0 \rangle = 2 \sum_{\mathbf{k}} \Theta(k_{\mathrm{F}} - k), \qquad (3.5)$$

the ground-state energy per particle, E_0/N , becomes

$$\frac{E_0}{N} = \frac{\hbar^2}{2m} \frac{\int_0^{k_{\rm F}} dk k^4}{\int_0^{k_{\rm F}} dk k^2} = \frac{3}{5} \frac{\hbar^2 k_{\rm F}^2}{2m}.$$
(3.6)

Next, we use first order perturbation theory to determine the change $E^{(1)}$ of the ground state energy due to H'. We exploit that $c_{\mathbf{k},\sigma}$ acting on the unperturbed ground state $|0\rangle$ yields zero, unless an electron occupies the single-particle state labelled by (\mathbf{k},σ) . Then $E^{(1)}$ may be written as

$$E^{(1)} = -\frac{1}{2V} \sum_{\mathbf{q}\neq 0, \mathbf{k}, \sigma} \frac{4\pi e_0^2}{q^2} \Theta(k_{\rm F} - |\mathbf{k} + \mathbf{q}|) \Theta(k_{\rm F} - k).$$
(3.7)

As usual, we convert the summations over the wave-vectors (\mathbf{k}, \mathbf{q}) to integrations. It is convenient to carry out the integral over q at the last stage. According to (3.7) we need to determine the volume of intersection in \mathbf{k} -space for two spheres with radius $k_{\rm F}$, their centers being separated by the distance q.

We shall express $(E_0 + E^{(1)})/N$ in terms of the dimensionless parameter r_s defined by

$$\frac{4\pi}{3}(r_s a_0)^3 = \frac{V}{N},\tag{3.8}$$

where a_0 is the Bohr radius, $a_0 = \hbar^2/me_0^2$. The parameter r_s is a convenient dimensionless measure of the density of the electron gas. Small values of r_s evidently imply high electron densities. The Fermi wave-vector $k_{\rm F}$ is inversely proportional to r_s . Using $k_{\rm F}^3 = 3\pi^2 N/V$ we obtain the relation

$$r_s = (9\pi/4)^{1/3} \frac{1}{k_{\rm F} a_0}.$$
 (3.9)

The values of r_s for the gas of conduction electrons in metals varies from about 2 to 6, with most metals having densities corresponding to r_s -values between 2 and 3.

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In order to determine the volume common to the two intersecting spheres and to complete the integration over q, we need to carry out the following two integrals $(x = q/k_{\rm F})$:

$$f(x) = \frac{1}{4\pi/3} 2\pi \int_{x/2}^{1} dy(1-y^2) = 1 - \frac{3}{4}x + \frac{1}{16}x^3$$
(3.10)

$$\int_{0}^{2} dx f(x) = \frac{3}{4} \tag{3.11}$$

Collecting these results we then get the final answer

$$\frac{E_0 + E^{(1)}}{N} = \frac{3}{5} \frac{\hbar^2 k_{\rm F}^2}{2m} - \frac{3}{4\pi} e_0^2 k_{\rm F}.$$
(3.12)

By introducing the parameter r_s defined in (3.8) and utilizing (3.9) we may write the result in the equivalent form

$$\frac{E_0 + E^{(1)}}{N} = \frac{e_0^2}{2a_0} \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right).$$
(3.13)

The result (3.13) shows that the kinetic energy per particle (proportional to r_s^{-2}) dominates the ground-state energy in the high-density limit $r_s \to 0$. The first-order contribution due to the Coulomb repulsion is proportional to r_s^{-1} . It is negative and may be thought of as an exchange effect, arising from the tendency of parallel-spin electrons to stay apart in accordance with the exclusion principle.

3.2 Second-order perturbation theory

According to the standard result of second-order perturbation theory the contribution $E^{(2)}$ to the energy of the ground state due to the perturbation H' is given by

$$E^{(2)} = \sum_{n \neq 0} \frac{\langle 0|H'|n\rangle\langle n|H'|0\rangle}{E_0 - E_n},$$
(3.14)

where n labels the eigenstates of the unperturbed Hamiltonian H_0 . To elucidate the structure of the problem involved in calculating the sum in (3.14) let us write H' in the symbolic form

$$H' = \sum_{1,2,3,4} U(1-4)c_1^{\dagger}c_2^{\dagger}c_3c_4$$
(3.15)

-(2)

with 1, 2, 3, 4 being short-hand notation for the momentum and spin variables in (3.3). By writing the interaction as a function of the variable 1-4 we indicate that it depends on the momentum transfer $\mathbf{q} = (\mathbf{k} + \mathbf{q}) - \mathbf{k}$ corresponding to 1-4. The conservation of momentum and spin implies with our symbolic notation that 1+2=3+4. We now have

$$\sum_{n \neq 0} \frac{\langle 0 | \sum_{1,2,3,4} U(1-4) c_1^{\dagger} c_2^{\dagger} c_3 c_4 | n \rangle \langle n | \sum_{1',2',3',4'} U(1'-4') c_1^{\dagger} c_2^{\dagger} c_{3'} c_{4'} | 0 \rangle}{E_0 - E_n} (3.16)$$

We must have either of the four possibilities

$$1' = 3, 2' = 4, 3' = 1, 4' = 2$$

$$1' = 4, 2' = 3, 3' = 2, 4' = 1$$

$$1' = 4, 2' = 3, 3' = 1, 4' = 2$$

$$1' = 3, 2' = 4, 3' = 2, 4' = 1$$
(3.17)

The first two involve $U(1-4)U(4-1) \propto 1/q^4$ while the last two involve $U(1-4)U(4-2) \propto 1/q^2 |\mathbf{k}' - \mathbf{k} - \mathbf{q}|^2$. For this reason, the contribution of the first two terms is called 'direct' while that of the last two is called 'exchange'.

Let us examine the contribution $E_{direct}^{(2)}$ due to the first two terms. In calculating $E_{direct}^{(2)}$ we shall postpone the integration over q to the last stage. If this integral is to be well-defined, the $1/q^4$ -singularity from the interaction matrix-elements must be compensated by the volume of the effective phase-space going to zero as q goes to zero at least as q^s with s greater than 1. If s were to be equal to 1, the integral would diverge logaritmically, since the volume element in q space is given by $4\pi q^2 dq$. In order to investigate this, we shall divide all wave-vector variables by $k_{\rm F}$. Then

$$E_{\rm direct}^{(2)} = -\frac{1}{\pi^4} V k_{\rm F}^3 \frac{m e_0^4}{\hbar^2} \int_0^\infty I(q) \frac{dq}{q^2}$$
(3.18)

where the weight-function I(q) is exhibited in the box below. Now, the energy denominator $E_0 - E_n$ is equal to $\epsilon_{k'} + \epsilon_k - \epsilon_{|\mathbf{k}+\mathbf{q}|} - \epsilon_{|\mathbf{k}'-\mathbf{q}|}$. We name the variable \mathbf{k}' by $-\mathbf{p}$ and obtain the more symmetric form for the energy denominator

$$E_0 - E_n = \epsilon_p + \epsilon_k - \epsilon_{|\mathbf{k}+\mathbf{q}|} - \epsilon_{|\mathbf{p}+\mathbf{q}|} = -\frac{\hbar^2 k_{\rm F}^2}{2m} (2q^2 + 2qkx + 2pqy), \quad (3.19)$$

where x equals cosine of the angle between \mathbf{k} and \mathbf{q} , while y equals cosine of the angle between \mathbf{p} and \mathbf{q} .

We are now ready to write down the four-dimensional integral determining the weight-function I(q) and evaluate it in the limit when $q \ll 1$, corresponding

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to q being much less than the Fermi wave vector $k_{\rm F}$:

$$I(q) = \int_{-1}^{1} dx \int_{-1}^{1} dy \int_{0}^{1} dk k^{2} \int_{0}^{1} dpp^{2}$$
$$\frac{\Theta(k^{2} + q^{2} + 2kqx - 1)\Theta(p^{2} + q^{2} + 2pqy - 1)}{q^{2} + qkx + qpy}.$$
(3.20)

The theta-functions arise from the requirement that the single-particle state with wave-vector $\mathbf{k} + \mathbf{q}$ is unoccupied, resulting in $|\mathbf{k} + \mathbf{q}| > k_{\rm F}$ or

$$k^2 + q^2 + 2kqx - 1 > 0 (3.21)$$

and similarly for the state with wave-vector $\mathbf{p} + \mathbf{q}$. Since x is less than or equal to 1, (3.21) implies that

$$1 - q < k < 1. \tag{3.22}$$

We assume in the following that

$$q \ll 1, \tag{3.23}$$

and introduce the new variable

$$\tilde{k} = \frac{1-k}{q}, \quad 0 < \tilde{k} < 1.$$
(3.24)

Since $q \ll 1$ the inequality (3.22) implies that $k^2 dk$ may be replaced by dk. Then

$$I(q) \simeq q \int_{\tilde{k}}^{1} dx \int_{\tilde{p}}^{1} dy \int_{0}^{1} d\tilde{k} \int_{0}^{1} d\tilde{p} \frac{1}{q+x+y}.$$
 (3.25)

Since we are interested in the small-q limit, we set q = 0 in the denominator. Then the integrals are all elementary. First we calculate

$$I_{1} = \int_{\tilde{k}}^{1} dx \int_{\tilde{p}}^{1} dy \frac{1}{x+y} = 2\ln 2 - (1+\tilde{k})\ln(1+\tilde{k}) - (1+\tilde{p})\ln(1+\tilde{p}) + (\tilde{p}+\tilde{k})\ln(\tilde{p}+\tilde{k})$$
(3.26)

and then carry out the two remaining integrations over \tilde{k} and \tilde{p} with the result

$$I(q) = \frac{2}{3}(1 - \ln 2)q.$$
 (3.27)

So we get a logarithmic divergence, when (3.27) is inserted into (3.18). Ordinary perturbation theory does not work, not even in principle. If the integration is cut off at $q = k_s$ we get a term proportional to $\ln k_s$. Later on (Chapter 8) we shall see that this is the result of the RPA-approximation with

$$k_s^2 = \frac{4k_{\rm F}}{\pi a_0}.$$
 (3.28)

Since $k_{\rm F} \propto r_s^{-1}$ we get $\ln(k_s/k_{\rm F}) = (1/2) \ln r_s + {\rm const.}$ and therefore

$$\frac{E^{(2)}}{N} = \frac{1}{\pi^2} (1 - \ln 2) \frac{me_0^4}{\hbar^2} \ln r_s.$$
(3.29)

We shall obtain this result in Chapter 8 by summing the most divergent terms in the perturbation series.

4 Hartree-Fock theory

In atomic physics the Hartree-Fock approximation is often used to describe in an approximate manner the influence of the electron-electron interaction on the energy levels of the atom. But the use of Hartree-Fock theory is by no means limited to atoms. In this chapter we shall first discuss the general features of the Hartree-Fock approximation. Subsequently we apply it to the homogeneous electron gas considered in the preceding chapter. It turns out that the Hartree-Fock approximation in this case gives the same result for the ground state energy as the use of first order perturbation theory. This is a special feature of the homogeneous electron gas and does not hold, for instance, for the electrons in an atom. As an example of the use of the Hartree-Fock approximation for a gas of interacting fermions we calculate the density of states at the Fermi surface and the (spin) susceptibility for a simple model interaction.

4.1 The Hartree-Fock approximation

In order to discuss the general nature of the Hartree-Fock approximation we consider a system of fermions interacting via two-body potentials, described by the Hamiltonian

$$H = H_0 + H', (4.1)$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(4.2)

represents the kinetic energy, while

$$H' = \frac{1}{2} \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}', \sigma, \sigma'} V_{\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q}, \sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}, \sigma'} c_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}$$
(4.3)

is the interaction.

Let us consider the Heisenberg equation of motion for the creation operator $c^{\dagger}_{\mathbf{k},\sigma}$,

$$i\hbar \dot{c}^{\dagger}_{\mathbf{k},\sigma} = [c^{\dagger}_{\mathbf{k},\sigma}, H],$$
(4.4)

where the dot denotes a derivative with respect to time. If we replace H by H_0 , thus neglecting the interaction entirely, we get the trivial result

$$[c_{\mathbf{k},\sigma}^{\dagger}, H_0] = -\epsilon_k c_{\mathbf{k},\sigma}^{\dagger}. \tag{4.5}$$

Let $|0\rangle$ denote the ground state for a non-interacting gas of fermions, with ground-state energy E_0 ($= 3\epsilon_F/5$ per particle). If we continue to neglect the interaction, the state

$$c_{\mathbf{k},\sigma}^{\dagger}|0\rangle \quad (k > k_{\mathrm{F}})$$
 (4.6)

is an eigenstate for a N + 1-particle system with energy $\epsilon_k = \hbar^2 k^2 / 2m$ relative to the ground-state energy of the N-particle system, since

$$H_0 c^{\dagger}_{\mathbf{k},\sigma} |0\rangle = (E_0 + \epsilon_k) c^{\dagger}_{\mathbf{k},\sigma} |0\rangle.$$
(4.7)

Next we shall include H' in the equation of motion for $c_{\mathbf{k},\sigma}^{\dagger}$. With use of the identities

$$[A, BC] = [A, B]C - B[C, A]$$
(4.8)

and

$$[A, BC] = \{A, B\}C - B\{C, A\},$$
(4.9)

we obtain

$$i\hbar \dot{c}^{\dagger}_{\mathbf{k},\sigma} = -\epsilon_{k}c^{\dagger}_{\mathbf{k},\sigma} - \sum_{\mathbf{q},\mathbf{k}',\sigma'} V_{\mathbf{q}}c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}c_{\mathbf{k}',\sigma'}.$$
(4.10)

This equation is exact but useless, as we must know the development in time of $c^{\dagger}c^{\dagger}c$ in order to solve it. The equation of motion for $c^{\dagger}c^{\dagger}c$ will introduce $c^{\dagger}c^{\dagger}cc^{\dagger}c$ and so on. In the Hartree-Fock approximation this infinite chain of equations is truncated by the approximation

$$c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}c_{\mathbf{k}',\sigma'} \simeq c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} < c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}c_{\mathbf{k}',\sigma'} > - < c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}c_{\mathbf{k}',\sigma'} > c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}$$
(4.11)

The minus sign in front of the second term is the result of interchanging the two creation operators. Now we identify the averages $\langle c_k^{\dagger} c_k \rangle$ with their value n_k in the non-interacting system, which is 0 if $k > k_{\rm F}$ and 1 if $k < k_{\rm F}$. This results in

$$c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}c_{\mathbf{k}',\sigma'} \simeq c^{\dagger}_{\mathbf{k},\sigma}n_{\mathbf{k}'}\delta_{\mathbf{q},0} - n_{\mathbf{k}+\mathbf{q},\sigma}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta_{\sigma,\sigma'}c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}.$$
(4.12)

With this approximation the equation of motion becomes

$$i\hbar \dot{c}^{\dagger}_{\mathbf{k},\sigma} = -(\epsilon_k + V_{\mathrm{HF}}(k))c^{\dagger}_{\mathbf{k},\sigma}, \qquad (4.13)$$

where $V_{\rm HF}(k)$ is

$$V_{\rm HF}(k) = \sum_{k',\sigma'} V_0 n_{k'} - \sum_{k'} V_{k-k'} n_{k'}.$$
 (4.14)

In the first term we may carry out the \mathbf{k}' -sum immediately, since the V_0 is a constant, independent of \mathbf{k}' . This introduces the number N of the electrons and the Hartree-Fock approximation thus results in

$$V_{\rm HF}(k) = V_0 N - \sum_{k'} V_{k-k'} n_{k'}.$$
 (4.15)

Note that the Hartree-Fock term for symmetry reasons can be a function only of k, the magnitude of the wave vector, but not of its direction.

The new energy spectrum is consequently given by

$$E_{k} = \epsilon_{k} + V_{\rm HF}(k). \tag{4.16}$$

The first of the terms in $V_{\rm HF}(k)$, the so-called Hartree term, is absent in the homogeneous electron gas due to the restriction $q \neq 0$. Physically, the reason for the cancellation is that the Hartree term describes the effect of the mean electrostatic field associated with the homogeneous charge distribution of the electrons, which is precisely cancelled by the uniform positive background due to the ions.

4.1.1 The variational method

The Hartree-Fock approximation may be carried out directly from the Schrödinger equation, without the use of second quantization, for a many-body system consisting of N electrons with spin σ with Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i,j=1}^{N} V(|\mathbf{r}_i - \mathbf{r}_j|).$$
(4.17)

For an electron gas the interaction is described by the potential $V(|\mathbf{r}|) = e_0^2/|\mathbf{r}|$.

The Hartree-Fock method is based on the use of a variational trial function $\psi_{\rm HF}$, which is an antisymmetrized product of single-particle wave functions (a Slater determinant), and the minimization of the total energy $E = \langle \psi_{\rm HF} | H | \psi_{\rm HF} \rangle$. For a homogeneous electron gas the single-particle wave functions $\psi(\mathbf{r})$ may be labelled with the quantum numbers \mathbf{k}, σ , where \mathbf{k} is a wave vector. As a result of the variational procedure one finds that each of the wave functions $\psi_{\mathbf{k},\sigma}$ should satisfy the equations

$$H_{\rm eff}\psi_{\mathbf{k},\sigma} = \epsilon_{\mathbf{k},\sigma}\psi_{\mathbf{k},\sigma},\tag{4.18}$$

where

$$H_{\text{eff}}\psi_{\mathbf{k},\sigma}(\mathbf{r}) = -(\hbar^2/2m)\nabla^2\psi_{\mathbf{k},\sigma}(\mathbf{r}) + \int d\mathbf{r}' \sum_{\mathbf{k}'(\mathbf{k}' < \mathbf{k}_{\text{F}}),\sigma'} |\psi_{\mathbf{k}',\sigma'}(\mathbf{r}')|^2 V(|\mathbf{r} - \mathbf{r}'|)\psi_{\mathbf{k},\sigma}(\mathbf{r}) - \int d\mathbf{r}' \sum_{\mathbf{k}'(\mathbf{k}' < \mathbf{k}_{\text{F}})}\psi_{\mathbf{k}',\sigma}^*(\mathbf{r}')\psi_{\mathbf{k}',\sigma}(\mathbf{r})V(|\mathbf{r} - \mathbf{r}'|)\psi_{\mathbf{k},\sigma}(\mathbf{r}').$$
(4.19)

Here $k_{\rm F} = (3\pi^2 N/V)^{1/3}$ is the length of the Fermi wave vector for N non-interacting electrons in the volume V.

The first term on the right hand side of (4.19) represents the kinetic energy of a single electron, while the second one, the Hartree term, may be interpreted as the mean electrostatic potential due to all other electrons. The third term may be written symbolically as

$$V_{\mathbf{F}}\psi_{\mathbf{k},\sigma}(\mathbf{r}),\tag{4.20}$$

but it should be noted that $V_{\rm F}$ is a non-local integral operator, cf. (4.19). Note that the summation in (4.19) only involves the occupied states and that the summation in the third term (the Fock term) is limited to states which have the same spin σ as the one under consideration.

4.2 The electron gas

For the homogeneous electron gas it is possible to determine an exact solution to the Hartree-Fock equations, which must normally be solved with the help of numerical methods. We shall show that (4.18) is satisfied by plane waves,

$$\psi_{\mathbf{k}} = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}}.$$
(4.21)

Since we assume that the electrons move in a uniform positive charge distribution due to the positive ions, the Hartree term is cancelled by the positive background. The third term in (4.19) becomes

$$-e_0^2 \frac{1}{V^{3/2}} \int d\mathbf{r}' \sum_{\mathbf{k}'(\mathbf{k}' < \mathbf{k}_{\mathrm{F}})} e^{-i\mathbf{k}' \cdot \mathbf{r}'} e^{i\mathbf{k}' \cdot \mathbf{r}} |\mathbf{r} - \mathbf{r}'|^{-1} e^{i\mathbf{k} \cdot \mathbf{r}'}$$
(4.22)

upon insertion of (4.21) and $V(r) = e_0^2/r$. By multiplying this expression by

$$1 = e^{-i\mathbf{k}\cdot\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{r}} \tag{4.23}$$

we observe that it assumes the form

$$V_{\rm F}(k) \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{4.24}$$

with

$$V_{\rm F}(k) = -\sum_{\mathbf{k}'(k' < k_{\rm F})} \tilde{V}(\mathbf{k}' - \mathbf{k})$$
(4.25)

where

$$\tilde{V}(\mathbf{q}) = \frac{1}{V} \int d\mathbf{r} V(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}$$
(4.26)

is the Fourier-transform of the interaction¹. In the case of the Coulomb interaction we have

$$\tilde{V}(\mathbf{q}) = \frac{4\pi e_0^2}{q^2 V}$$
(4.27)

as shown in Appendix A.

The eigenvalues $\epsilon_{\mathbf{k},\sigma}$ are then seen to be

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} + V_{\rm F}(k). \tag{4.28}$$

We shall first determine the energy eigenvalues (4.28) in a few limiting cases and then proceed to evaluate them for general k.

Let us consider the case when $k \gg k_F$. Then we may approximate $\tilde{V}(\mathbf{k}' - \mathbf{k})$ by $\tilde{V}(\mathbf{k})$ and carry out the sum over \mathbf{k}' , resulting in

$$V_{\rm F}(k) \simeq -\frac{1}{(2\pi)^3} \frac{4\pi}{3} k_{\rm F}^3 \frac{4\pi e_0^2}{k^2} = -\frac{2}{3\pi} e_0^2 k_{\rm F} \frac{k_{\rm F}^2}{k^2}$$
(4.29)

For large k, the interaction effects become small. Note that the kinetic energy rises as k^2 .

Next we consider the limit k = 0. In this case we get from (4.25)

$$V_{\rm F}(0) = -\frac{1}{(2\pi)^3} \int_0^{k_{\rm F}} dk' 4\pi k'^2 \frac{4\pi e_0^2}{k'^2} = -\frac{2}{\pi} e_0^2 k_{\rm F}.$$
 (4.30)

Note that the energy is decreased by an amount given by $e_0^2 k_{\rm F}$ except for a numerical constant.

Finally, we explore what happens at $k = k_F$. By changing the integration variable to $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ we may write $V_F(k)$ as

$$V_{\rm F}(k) = -\sum_{\mathbf{q}(|\mathbf{k}+\mathbf{q}| < k_{\rm F})} \frac{4\pi e_0^2}{q^2 V}.$$
(4.31)

¹It is common in the literature to distinguish a function and its Fourier-transform by their arguments only, hence leaving out the tilde.

When $k = k_F$, the constraint on $|\mathbf{k} + \mathbf{q}|$ that it should be less than the Fermi wave-vector becomes

$$k_{\rm F}^2 + 2k_{\rm F}q\cos\theta + q^2 < k_{\rm F}^2. \tag{4.32}$$

or

$$\cos\theta < -\frac{q}{2k_{\rm F}},\tag{4.33}$$

which puts the upper limit $2k_{\rm F}$ on the integration over q, since $\cos\theta$ cannot be less than -1. As the integrand does not depend on θ the integration over $\cos\theta$ simply introduces the additional factor $(1 - q/2k_{\rm F})$ in the integral over q, because of the constraint (4.33). We thus get

$$V_{\rm F}(k_{\rm F}) = -\frac{1}{(2\pi)^3} \int_0^{2k_{\rm F}} dq 2\pi q^2 (1 - \frac{q}{2k_{\rm F}}) \frac{4\pi e_0^2}{q^2} = -\frac{1}{\pi} e_0^2 k_{\rm F}.$$
 (4.34)

By comparing (4.30) and (4.34) we note that the energy separation between the highest and the lowest occupied state (the 'bandwidth') in the Hartree-Fock approximation is changed by $e_0^2 k_{\rm F}/\pi$ (in practice a few eV) compared to the free-electron value. This is in strong disagreement with what is known experimentally about the bandwidth in metals. Another unphysical feature of the Hartree-Fock approximation has to do with the form of the density of states near the Fermi surface. This may be seen by carrying out the integration in general, for arbitrary values of $k/k_{\rm F}$, starting from (4.25). By first integrating over the angle between \mathbf{k}' and \mathbf{k} and subsequently carrying out the integration over k' one gets

$$V_{\rm F}(k) = -\frac{e_0^2 k_{\rm F}}{\pi} \left[1 + \frac{k_{\rm F}^2 - k^2}{2kk_{\rm F}} \ln \frac{|k + k_{\rm F}|}{|k - k_{\rm F}|}\right]. \tag{4.35}$$

From this general expression the previous special cases may easily be recovered. Thus (4.30) and (4.29) are obtained by expanding the logarithm for small and large k, respectively, while (4.34) may be read off from (4.35) directly. Since the derivative of (4.35) with respect to k diverges as $-\ln |(k - k_{\rm F})/k_{\rm F}|$ for $k \to k_{\rm F}$, the density of states vanishes in this limit, yielding a specific heat which is proportional to $T/\ln T$, in disagreement with experiment.

We emphasize that the ground-state energy of the electron gas may not be obtained simply by summing the single-particle energies in (4.28) over the occupied states. To illustrate this point, let us sum $V_{\rm F}(k)$ over the occupied states, thereby obtaining

$$-\sum_{\mathbf{k},\sigma,\mathbf{k}'(\mathbf{k},\mathbf{k}'<\mathbf{k}_{\mathrm{F}})}\tilde{V}(\mathbf{k}'-\mathbf{k}).$$
(4.36)

By comparison with (3.7) we see that (4.36) is exactly twice the former, which is the contribution (to first order) to the total energy from the interaction. In general there is no simple connection between the single-particle energies in an interacting many-body system and its ground state energy.
4.3 Effective mass and spin susceptibility

In this concluding section we illustrate the use of the Hartree-Fock approximation for an interacting system of fermions, with a general interaction potential given by the Fourier-transform $V_{\mathbf{q}}$. The Hartree-Fock energy spectrum is according to (4.15-4.16)

$$E_k = \epsilon_k + V_0 N - \sum_{\mathbf{q}} V_{\mathbf{q}} n_{\mathbf{k}+\mathbf{q}}.$$
(4.37)

We shall calculate the effective mass, which determines the density of states at the Fermi surface, and the spin susceptibility on the basis of (4.37) and a specific choice of $V_{\mathbf{q}}$, corresponding to a screened Coulomb interaction.² For convenience, we consider in the following a unit volume and thus set V equal to unity.

4.3.1 The effective mass

The effective mass enters, when the integration over \mathbf{k} is transformed into an integration over the energy E_k . Let us therefore define the effective mass m^* by

$$\frac{m}{m^*} = \frac{m}{\hbar^2 k_{\rm F}^2} \mathbf{k} \cdot \frac{\partial E_k}{\partial \mathbf{k}} |_{k=k_{\rm F}}.$$
(4.38)

When interactions are neglected, the effective mass is seen to be equal to the bare mass m. Since the Hartree-term is independent of k, only the Fock-term contributes to the effective mass. Since $n_{\mathbf{k+q}} = \Theta(k_{\mathrm{F}} - |\mathbf{k+q}|)$, we get

$$\frac{\partial n_{\mathbf{k}+\mathbf{q}}}{\partial \mathbf{k}} = -\delta(k'-k_{\mathrm{F}})\hat{\mathbf{k}}', \qquad (4.39)$$

where $\mathbf{\hat{k}}' = \mathbf{k}'/k'$ and $\mathbf{k}' = \mathbf{k} + \mathbf{q}$. Then

$$\frac{m}{m^*} = 1 + \frac{m}{\hbar^2 k_{\rm F}} \int \frac{d\mathbf{k}'}{(2\pi)^3} \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}' \delta(k' - k_{\rm F}) V_{\mathbf{k}' - \mathbf{k}}.$$
(4.40)

Since the effective mass is defined at $k = k_{\rm F}$, the expression (4.40) may be written as an average involving the angle θ between **k** and **k'**

$$\frac{m}{m^*} = 1 + \frac{mk_{\rm F}}{2\pi^2\hbar^2} \int_{-1}^1 \frac{d(\cos\theta)}{2} \cos\theta V(\theta) \tag{4.41}$$

² It should be noted that we have already gone beyond Hartree-Fock theory as applied to the interacting electron gas by using a screened instead of a bare interaction. As we shall see later on, the screening enters when we do the so-called random-phase approximation. The expression (4.37) for the single-particle energies is the result of doing Hartree-Fock theory starting from a screened as opposed to a bare interaction.

where $V(\theta) = V_q$ with $q = 2k_F \sin \theta/2$ being the length of $\mathbf{q} = \mathbf{k}' - \mathbf{k}$. To evaluate m/m^* we need to specify V_q . If we take V_q to have the form of a screened Coulomb interaction,

$$V_q = \frac{4\pi e_0^2}{q^2 + k_s^2},\tag{4.42}$$

then the integration over θ (or q) may be carried out analytically with the result

$$\frac{m}{m^*} = 1 + \alpha (\frac{1}{2} + \alpha) \ln \frac{\alpha + 1}{\alpha} - \alpha \tag{4.43}$$

where $\alpha = (k_s/2k_F)^2 \simeq 0.166r_s$, when $k_s^2 = 4k_F/\pi a_0$, cf. (3.28). For $\alpha = 1/2$ we obtain from (4.43) the value $m/m^* = 1.05$. When r_s varies from 2 to 5, m/m^* varies between 1.05 and 1.04. In all cases we obtain a very small decrease of the effective mass relative to the free electron value.

4.3.2 The spin susceptibility

We may use the Hartree-Fock expression for the energy to determine the spin susceptibility of a degenerate Fermi gas. The presence of an external magnetic field B, which we take to be in the z-direction, changes the relative number of spin-up and spin-down particles. Since the exchange contribution to the Hartree-Fock energy only involves particles with the same spin as the state under consideration, one therefore expects the exchange term to influence the susceptibility, which is defined as $M = \chi B/\mu_0$, where M is the magnitude of the resulting magnetization. For electrons with gyromagnetic ratio g = 2 the magnetization is $M = g\mu_B\delta N = 2\mu_B\delta N$, with δN being the change per unit volume in the number of down-spin electrons (which equals minus the change per unit volume in the number of up-spin electrons) while $\mu_B = e\hbar/2m$ is the Bohr magneton. It is convenient to express the result in terms of the density of states for the non-interacting system, N(0), per spin at the Fermi energy, which is given by $N(0) = mk_{\rm F}/2\pi^2\hbar^2$.

The presence of the magnetic field causes the Fermi wavevector of the spinup electrons to differ in magnitude from the Fermi wavevector of the spin-down electrons. The associated energy change of a spin-up electron at the Fermi surface is

$$\delta E_{k_{\rm F}-\delta k_{\rm F},\uparrow} = g\mu_B \frac{1}{2}B - \frac{\partial E}{\partial k} \delta k_{\rm F} + \delta N < V > . \tag{4.44}$$

Here the terms on the right hand side have the following origin: The first one is the energy change due to the interaction between the magnetic moment of the electron and the external field, while the second is due to the explicit wavevector dependence of E_k . Finally $\langle V \rangle$ is the average of the potential $V(\theta)$ over angle,

$$\langle V \rangle = \frac{1}{2} \int_{-1}^{1} d(\cos \theta) V(\theta),$$
 (4.45)

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which is the change in energy originating from the exchange term. The average involves the undistorted Fermi surface, since we are only considering small changes $\delta k_{\rm F}$.

For spin-down electrons we get correspondingly

$$\delta E_{k_{\rm F}+\delta k_{\rm F},\downarrow} = -g\mu_B \frac{1}{2}B + \frac{\partial E}{\partial k} \delta k_{\rm F} - \delta N < V > . \tag{4.46}$$

In equilibrium these two changes in energy must be equal to each other, since the chemical potential for each of the two spin species must be the same. Since

$$\frac{\partial E}{\partial k} \delta k_{\rm F} = \frac{\partial E}{\partial k} \frac{\delta k_{\rm F}}{\delta N} \delta N = \frac{m}{m^* N(0)} \delta N \tag{4.47}$$

we get

$$2\delta N = \frac{g\mu_B B}{m/m^* N(0) - \langle V \rangle}$$
(4.48)

and

$$\chi = \frac{M}{B/\mu_0} = \chi_0 \frac{m^*/m}{1 - N(0) < V > m^*/m},$$
(4.49)

where $\chi_0 = \mu_0 (g\mu_B)^2 N(0)/2$ is the Pauli susceptibility.

Let us use the screened Coulumb potential (4.42) to calculate the angular average $\langle V \rangle$ according to

$$\langle V \rangle = \int_{-1}^{1} \frac{d(\cos\theta)}{2} V(\theta) = \int_{0}^{1} d(q/2k_{\rm F})(q/k_{\rm F})V_q.$$
 (4.50)

The result is seen to be

$$N(0) < V >= \frac{\alpha}{2} \ln \frac{\alpha + 1}{\alpha}.$$
(4.51)

For large α the dimensionless quantity N(0) < V > approaches 1/2. For $\alpha = 1/2$ we obtain N(0) < V >= 0.275. Thus we find considerable enhancement of the susceptibility. The ratio χ/χ_0 is 1.22, 1.28 and 1.34 for r_s equal to 2, 3 and 4, respectively, while experimentally (cf. Section 1.3.2) the enhancement factor for Na ($r_s = 4$) is found to be 1.7.

5 Canonical transformations

It is sometimes fruitful to simplify a many-particle Hamiltonian to a degree that its eigenvalues may be obtained by doing a canonical transformation of the operators in the simplified Hamiltonian. In this case one no longer has a true many-body problem, since the Hamiltonian is reduced to a form that describes non-interacting *elementary excitations.*¹

In this chapter we first illustrate the use of a particular canonical transformation, the *Bogoliubov transformation*, by considering a Hamiltonian of a simple, bilinear form. Subsequently we discuss some examples of the use of canonical transformations involving phonons in crystal lattices and in superfluid helium, quasiparticles in superconductors and spin waves in magnets.

5.1 The Bogoliubov transformation

We consider a bilinear Hamiltonian of the general form

$$H = E_0(a^{\dagger}a + b^{\dagger}b) + E_1(a^{\dagger}b^{\dagger} + ba)$$

$$(5.1)$$

where $a, b (a^{\dagger}, b^{\dagger})$ denote annihilation (creation) operators, while E_0 and E_1 are constants. By a suitable canonical transformation to a new set of operators α and β it is possible to determine the eigenvalues of the Hamiltonian by expressing it in a form involving only $\alpha^{\dagger}\alpha$ and $\beta^{\dagger}\beta$. In the following we shall treat the boson and the fermion case separately.

5.1.1 Bosons

In the boson case the operators obey the commutation rules

$$[a, a^{\dagger}] = [b, b^{\dagger}] = 1, \ [a, b^{\dagger}] = [b, a^{\dagger}] = 0.$$
 (5.2)

We introduce new operators α and β by the transformation

$$a = u\alpha - v\beta^{\dagger}, \quad b = u\beta - v\alpha^{\dagger}, \tag{5.3}$$

and require that they satisfy the same boson commutation rules,

$$[\alpha, \alpha^{\dagger}] = [\beta, \beta^{\dagger}] = 1, \ [\alpha, \beta^{\dagger}] = [\beta, \alpha^{\dagger}] = 0.$$
(5.4)

By inserting (5.3) into (5.2) and using (5.4) one sees that u and v must satisfy the condition

$$u^2 - v^2 = 1. \tag{5.5}$$

¹ In real systems, the terms left out of the original Hamiltonian will modify the energy of these elementary excitations and cause them to have a finite lifetime.

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We now insert (5.3) into (5.1) and obtain the result

$$H = 2v^{2}E_{0} - 2uvE_{1} + (E_{0}(u^{2} + v^{2}) - 2uvE_{1})(\alpha^{\dagger}\alpha + \beta^{\dagger}\beta) + (E_{1}(u^{2} + v^{2}) - 2uvE_{0})(\alpha\beta + \beta^{\dagger}\alpha^{\dagger}).$$
(5.6)

It is evidently possible to choose u and v in such a manner that the term proportional to $(\alpha\beta + \beta^{\dagger}\alpha^{\dagger})$ vanishes, by setting the coefficient in front equal to zero,

$$E_1(u^2 + v^2) - 2uvE_0 = 0. (5.7)$$

The condition (5.5) is satisfied by adopting the following parametrization of u and v,

$$u = \cosh t, \quad v = \sinh t, \tag{5.8}$$

which in turn implies that the condition (5.7) may be written as

$$E_1(\cosh^2 t + \sinh^2 t) - 2E_0 \sinh t \cosh t = 0$$
(5.9)

or

$$\tanh 2t = \frac{E_1}{E_0}.$$
 (5.10)

It is now a simple matter to express $u^2 + v^2$ and 2uv in terms of the ratio E_1/E_0 and insert these expressions into (5.6). The result is

$$H = \lambda(\alpha^{\dagger}\alpha + \beta^{\dagger}\beta) + \text{const.}, \qquad (5.11)$$

where λ is given in terms of E_0 and E_1 as

$$\lambda = \sqrt{E_0^2 - E_1^2}.$$
 (5.12)

We have chosen the positive sign, since we define λ as the energy needed to create an elementary excitation. Note that the magnitude of E_0 must exceed that of $|E_1|$ in order for this result to make sense.

5.1.2 Fermions

The fermion case is very similar to the boson case treated above. The operators now obey the fermion commutation rules

$$\{a, a^{\dagger}\} = \{b, b^{\dagger}\} = 1, \ \{a, b^{\dagger}\} = \{b, a^{\dagger}\} = 0.$$
 (5.13)

As before we introduce new operators α and β by the transformation

$$a = u\alpha + v\beta^{\dagger}, \quad b = u\beta - v\alpha^{\dagger},$$
 (5.14)

and demand that they satisfy fermion commutation rules,

$$\{\alpha, \alpha^{\dagger}\} = \{\beta, \beta^{\dagger}\} = 1, \ \{\alpha, \beta^{\dagger}\} = \{\beta, \alpha^{\dagger}\} = 0.$$
 (5.15)

When (5.14) is inserted into (5.13) one obtains the condition

$$u^2 + v^2 = 1 \tag{5.16}$$

corresponding to (5.5). As in the boson case we proceed by inserting (5.14) into (5.1). The result is

$$H = 2v^{2}E_{0} + 2uvE_{1} + (E_{0}(u^{2} - v^{2}) - 2uvE_{1})(\alpha^{\dagger}\alpha + \beta^{\dagger}\beta) - (E_{1}(u^{2} - v^{2}) + 2uvE_{0})(\alpha\beta + \beta^{\dagger}\alpha^{\dagger}).$$
(5.17)

Again, it is possible to choose u and v in such a manner that the term proportional to $(\alpha\beta + \beta^{\dagger}\alpha^{\dagger})$ vanishes by requiring

$$E_1(u^2 - v^2) + 2uvE_0 = 0. (5.18)$$

The condition (5.16) is satisfied by parametrizing u and v according to

$$u = \cos t, \quad v = \sin t, \tag{5.19}$$

which implies that (5.18) becomes

$$E_1(\cos^2 t - \sin^2 t) + 2E_0 \sin t \cos t = 0 \tag{5.20}$$

or

$$\tan 2t = -\frac{E_1}{E_0}.$$
 (5.21)

When the resulting expressions for $u^2 + v^2$ and 2uv are inserted into (5.17) we obtain

$$H = \lambda(\alpha^{\dagger}\alpha + \beta^{\dagger}\beta) + \text{const.}, \qquad (5.22)$$

where λ is given by E_0 and E_1 as

$$\lambda = \sqrt{E_0^2 + E_1^2}.$$
 (5.23)

In the case of superconductivity (which is treated in Section 5.4 below) it is sometimes convenient to choose λ to have the same sign as E_0 (which is negative for states below the Fermi surface), thereby facilitating the comparison to the normally conducting state.

5.2 Phonons in a crystal lattice

Each of the atoms in a crystalline solid carries out vibrations around its equilibrium position, but these vibrations are not independent, since the vibrations of a given atom will influence those of its neighbors. A crystalline solid is therefore a large system of coupled oscillators, in fact as many as the number of atoms times three.

Our discussion of lattice vibrations proceeds in two steps, the first one involving only classical mechanics and the second quantum mechanics. First, we seek to turn the problem of coupled oscillators into a simpler one, for which the oscillations are independent of each other. Such a transformation is achieved by a transition to normal coordinates, and the resulting oscillations are called normal modes. As a simple example we shall see how the normal modes are determined for the simplest possible 'crystal' consisting of a linear chain of atoms.

5.2.1 Normal modes

In this subsection we treat the classical equations of motion for a linear chain of identical atoms which are connected by springs with the same force constant K. The mass of an atom is called M. By u_n we denote the deviation of the n'th atom from its equilibrium position. The atoms are only allowed to move along the direction of the chain. Later on we shall see how the model is generalized to the case when the atoms occupy positions in a three-dimensional lattice and are allowed to move in different directions.

According to Newton's second law the acceleration \ddot{u}_n of the *n*'th atom is given by

$$M\ddot{u}_n = -K(u_n - u_{n-1}) - K(u_n - u_{n+1}).$$
(5.24)

For a chain of N atoms we shall use the periodic boundary conditions

$$u_N = u_0; \quad u_{N+1} = u_1 \tag{5.25}$$

on the solutions to (5.24). The distance between two neighboring atoms in equilibrium is a, which means that the total length L of the chain is L = Na. The boundary conditions (5.25) evidently correspond to joining together the two ends of the linear chain.

In solving the equations of motion it is convenient to regard u_n as the real part of a complex quantity. We note that (5.24) is satisfied by

$$u_n = u_0 e^{iqna - i\omega t} \tag{5.26}$$

provided ω and q are related by the condition

$$M\omega^2 = 4K\sin^2\frac{qa}{2}.$$
(5.27)

The solution (5.26) has the form of a plane wave

$$e^{iqx-i\omega t},\tag{5.28}$$

where the position coordinate x assumes the discrete values x = na with $n = 1, \dots, N$. The wave number is evidently $q/2\pi$, while the angular frequency is ω . The actual deviation u_n is of course real, and (5.26) should strictly speaking be written as

$$u_n = \operatorname{Re} u_0 e^{iqna - i\omega t} = u_0 \cos(qna - \omega t), \qquad (5.29)$$

where u_0 is chosen to be real. The symbol Re denotes that the real part is taken, but it is usually suppressed with the understanding that the real part is taken at the end. By inserting (5.29) in (5.24) we obtain again the condition (5.27), which may be written as

$$\omega = 2\sqrt{\frac{K}{M}} |\sin\frac{qa}{2}|, \qquad (5.30)$$

the sign of ω being chosen to be positive. An equation such as (5.30), which connects the wave vector with the frequency, is called a dispersion relation. The particular pattern of oscillations u_n associated with a definite value of q(and hence ω), is called a normal mode. Note that the connection between ω and q is linear for small values of q. In this limit the mode corresponds to a sound wave, with dispersion relation

$$\omega = sq, \tag{5.31}$$

where the sound velocity s is given by

$$s = a\sqrt{\frac{K}{M}}.$$
(5.32)

The reason why the frequency ω becomes small for small values of q is that neighboring atoms oscillate very nearly in phase and therefore only move slightly with respect to each other. However, if q assumes the value π/a , neighboring atoms oscillate in opposite phase $(u_n = -u_{n-1})$, giving rise to the maximum frequency equal to $2\sqrt{K/M}$.

The boundary conditions (5.25) determine the allowed values of q. This is of course a purely classical consideration. The condition (5.25) requires that

$$e^{iqNa} = 1, \tag{5.33}$$

which implies that q may assume the values

$$q = \frac{m}{N} \frac{2\pi}{a},\tag{5.34}$$

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where m is an integer (positive, negative or zero).

Besides (5.34) the allowed wave vectors must satisfy another condition, which is a consequence of the fact that the only physically significant values of the plane wave (5.26) are those associated with the lattice points x = na. If we replace in (5.26) the wave vector q by $q + 2\pi/a$, the mode u_n remains the same. The two different values of q thus correspond to exactly the same mode pattern. We therefore limit q to the interval

$$-\frac{\pi}{a} < q \le \frac{\pi}{a},\tag{5.35}$$

which is also known as the first Brillouin zone. Note that q may then assume precisely N different values.

In summary, we have shown that the oscillations of the atoms in the crystal may be described in terms of normal modes such as (5.26), provided ω and q are related by the dispersion relation (5.30). There exist N different modes, namely as many as the allowed values of q in the interval $-\pi/a < q \leq \pi/a$.

5.2.2 Quantization

Having solved the classical linear-chain problem of the motion of N atoms, each with mass M, interacting via harmonic forces, we shall now prove that the Hamiltonian \hat{H} for the linear chain is a sum over q of terms having the same form as for a single oscillator,

$$\hat{H} = \sum_{q} \hbar \omega_q (\hat{b}_q^{\dagger} \hat{b}_q + \frac{1}{2}).$$
(5.36)

In the following we prove (5.36) starting from the Hamiltonian

$$H = \sum_{n=1}^{N} \left(\frac{p_n^2}{2M} + \frac{K}{2}(u_n - u_{n-1})^2\right), \tag{5.37}$$

where

$$[\hat{u}_m, \hat{p}_n] = i\hbar\delta_{mn}. \tag{5.38}$$

The operators \hat{u}_n og \hat{p}_n are expressed in terms of \hat{Q}_q and \hat{P}_q through

$$\hat{u}_n = \frac{1}{\sqrt{N}} \sum_q \hat{Q}_q e^{iqna} \tag{5.39}$$

and

$$\hat{p}_n = \frac{1}{\sqrt{N}} \sum_q \hat{P}_q e^{-iqna}.$$
(5.40)

The periodic boundary conditions are satisfied provided that q satisfies the condition $e^{iqNa} = 1$. The allowed values of q are thus

$$q = \left(-\frac{N}{2} + 1, \cdots, \frac{N}{2} - 1, \frac{N}{2}\right)\frac{2\pi}{Na},\tag{5.41}$$

where we have assumed for definiteness that N is even.

After inserting (5.39) and (5.40) in the Hamiltonian we carry out the summation over n, using

$$\sum_{n=1}^{N} e^{i(q-q')na} = N\delta_{qq'}.$$
(5.42)

The inverse relation

$$\sum_{q} e^{i(n-n')qa} = N\delta_{nn'},\tag{5.43}$$

is also valid, since q according to (5.41) assumes N different values.

As a result the Hamiltonian (5.37) becomes

$$\hat{H} = \sum_{q} \left(\frac{1}{2M} \hat{P}_{q} \hat{P}_{-q} + K(1 - \cos qa) \hat{Q}_{q} \hat{Q}_{-q} \right).$$
(5.44)

From the inverse relations of (5.39) and (5.40)

$$\hat{Q}_{q} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \hat{u}_{n} e^{-iqna}$$
(5.45)

and

$$\hat{P}_{q} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \hat{p}_{n} e^{iqna}, \qquad (5.46)$$

which follow from (5.39) and (5.40) together with (5.43), we find the following commutation relations satisfied by \hat{Q} and \hat{P} ,

$$[\hat{Q}_{q},\hat{P}_{q'}] = \frac{1}{N} \sum_{n,n'=1}^{N} (\hat{u}_{n}\hat{p}_{n'} - \hat{p}_{n'}\hat{u}_{n})e^{i(q'n'-qn)a} = i\hbar\delta_{qq'}.$$
 (5.47)

We introduce creation and annihilation operators by the definition

$$\hat{b}_{q}^{\dagger} = -i\frac{1}{\sqrt{2M\hbar\omega_{q}}}(\hat{P}_{q} + iM\omega_{q}\hat{Q}_{-q})$$
(5.48)

and

$$\hat{b}_q = i \frac{1}{\sqrt{2M\hbar\omega_q}} (\hat{P}_{-q} - iM\omega_q \hat{Q}_q).$$
(5.49)

This turns \hat{H} into the form (5.36), with ω_q being the classical oscillation frequency given by (5.30). Note that the creation and annihilation operators satisfy the commutation relations

$$[\hat{b}_q, \hat{b}_{q'}^{\dagger}] = \delta_{qq'} \tag{5.50}$$

as a consequence of (5.47).

We have thus shown that the Hamiltonian H for the linear chain is

$$\hat{H} = \sum_{q} \hbar \omega_q (\hat{b}_q^{\dagger} \hat{b}_q + \frac{1}{2}).$$
(5.51)

The Hamiltonian for a linear chain has thus a very simple form, since it is a sum of operators associated with each independent harmonic oscillator that belongs to one of the N possible values of q. The different possible energy eigenvalues are obtained in a way analogous to the single harmonic oscillator by specifying the number of quanta n_q associated with each normal mode. The resulting contribution to the energy is thus $\hbar \omega_q (n_q + 1/2)$, and the total energy in the state under consideration is therefore the sum over q of all these energies. The state is labelled by the values of the quantum numbers n_{q_i} , where the index *i* runs through N different values 1 to N,

$$|n_{q_1}, n_{q_2}, \cdots, n_{q_N}\rangle. \tag{5.52}$$

The energy quanta in a normal mode are called phonons. In the long wavelength limit $(qa \ll 1)$ the normal modes have linear dispersion just like sound, cf. (5.30). Instead of considering the different energy eigenvalues of the total energy as a sum of energies associated with each normal mode specified by the quantum numbers n_q , one may just as well denote the eigenstate by giving the number of phonons, n_q , associated with each normal mode. The lattice has thus been transformed from a system of N atoms that are mutually interacting to a non-interacting gas of phonons. The phonon gas is non-interacting, because the Hamiltonian only contains terms that are quadratic in the deviations u_n of the atoms from their equilibrium position. If higher-order terms are retained in the Hamiltonian, it is possible to describe these to a first approximation as perturbations. This gives the phonons a finite lifetime. A given phonon may for instance decay into two other phonons. Such processes play an important role in the thermal conduction in insulators. In the absence of interaction between the phonons and neglecting any effects of boundaries such an insulator would have infinite thermal conductivity.

The number of phonons is not a conserved quantity, unlike the number of molecules in ordinary gases such as air in a closed container. The number of phonons depends on the temperature. In the ground state of the lattice the number of phonons is zero, since $n_{q_i} = 0$ for all *i*.

A linear chain of atoms is not a satisfactory model for a solid. In a real three-dimensional crystal each atom has typically six, eight or twelve nearest neighbors, depending on the crystal structure. The determination of the classical lattice vibrations must take the crystal structure into account and consider the coupling between an atom and its nearest neighbors - and possibly its more distant neighbors as well. This complicates the calculation of the frequencies of the normal modes, but involves no conceptual changes. In the three-dimensional case a normal mode is characterized by a wave vector **q** with an associated angular frequency $\omega_{\mathbf{q}}$, corresponding to the replacement of (5.26) by

$$\mathbf{u} = \mathbf{u}_0 \exp(i\mathbf{q} \cdot \mathbf{R} - i\omega t), \tag{5.53}$$

where **R** is a lattice vector. Since the atoms may vibrate in three directions, there are three normal modes associated with each value of **q**. The lattice vibrations are therefore characterized not only by the wave vector **q**, but also by polarization vectors, which may be chosen to be orthogonal to each other. If the direction of **q** is along a symmetry axis in the crystal, it becomes possible to choose the polarization vectors to be parallel with or perpendicular to **q**, and the phonons are called longitudinal and transverse, respectively. Many crystals have a unit cell containing more than one atom. In this case one has not only branches that are acoustic as in the one-dimensional case (meaning that the frequency goes to zero when q goes to zero), but there are also optical branches, in which the frequency tends towards a non-zero value as q goes to zero.

The quantization of the lattice vibrations proceeds as in the one-dimensional case. The Hamiltonian is given by (5.51), provided q is interpreted as (\mathbf{q}, α) , where α is a polarization index. According to the discussion given above α may assume three different values ($\alpha = 1, 2, 3$), which label the three unit vectors \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 giving the polarization directions for the normal modes associated with a given \mathbf{q} . This enables us to write down the different possible energy eigenvalues E_i for the crystal as a whole,

$$E_{i} = \sum_{\mathbf{q},\alpha} \hbar \omega_{\mathbf{q}\alpha} (n_{\mathbf{q}\alpha} + \frac{1}{2}), \qquad (5.54)$$

where i is an index labelling the set of quantum numbers $n_{q\alpha}$.

5.3 Phonons in a Bose gas

From elementary statistical mechanics it is known that the non-interacting Bose gas undergoes a phase transition in three dimensions at a temperature equal to $\hbar^2 (N/V)^{2/3}/mk$, except for a numerical constant. Here N is the total number of bosons, V is the volume, m the mass of a boson and k the Boltzmann constant. At T = 0 K the lowest single-particle quantum state is macroscopically occupied, the occupation number N_0 being equal to N. In general one uses the term macroscopic occupation when the occupation number N_0 divided by N has a limiting value differing from zero, when N tends towards infinity.

In this section we shall treat the interaction between the bosons as a perturbation. We assume that in the interacting system the lowest-lying singleparticle state is macroscopically occupied, ensuring that N_0/N tends towards a finite value when N goes to infinity, and approximate the corresponding operators a_0 and a_0^{\dagger} by c-numbers. In the unperturbed system we have $a_0^{\dagger}|N_0\rangle = \sqrt{N_0 + 1}|N_0 + 1\rangle$ and $a_0|N_0\rangle = \sqrt{N_0}|N_0 - 1\rangle$. We shall therefore approximate both operators by $\sqrt{N_0}$.

The Hamiltonian of a system of interacting bosons is

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{q} a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}'-\mathbf{q}}^{\dagger} a_{\mathbf{k}'} a_{\mathbf{k}} \quad , \tag{5.55}$$

where $\epsilon_k = \hbar^2 k^2/2m$. The operators satisfy Bose commutation relations

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}, \mathbf{k}'}, \quad [a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0, \quad [a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}'}^{\dagger}] = 0.$$
(5.56)

We have furthermore assumed that the interaction potential $V(\mathbf{r}, \mathbf{r}')$ only depends on the length $|\mathbf{r} - \mathbf{r}'|$, implying that the matrix element - its Fourier transform $V_{\mathbf{q}}$ - only depends on the length q of the vector \mathbf{q} .

The simplest possible model for the interaction is the delta function potential

$$V(\mathbf{r}, \mathbf{r}') = U\delta(\mathbf{r} - \mathbf{r}'), \qquad (5.57)$$

where U(>0) is a constant. The associated matrix element is given by the Fourier transform of the delta function,

$$V_q = \frac{U}{V} \tag{5.58}$$

and is therefore independent of q. We now replace a_0 and a_0^{\dagger} by $\sqrt{N_0}$ in accordance with the assumption that the lowest quantum state is macroscopically occupied and discard in the interaction all terms which are not (at least) proportional to N_0 . This results in the Hamiltonian

$$H \simeq \frac{UN_0^2}{2V} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{UN_0}{V} \sum_{\mathbf{k}(\mathbf{k}\neq0)} (a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger} a_{-\mathbf{k}} + \frac{1}{2} a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} + \frac{1}{2} a_{\mathbf{k}} a_{-\mathbf{k}}).$$

$$(5.59)$$

Next we introduce the total particle number

$$N = N_0 + \frac{1}{2} \sum_{\mathbf{k}(\mathbf{k}\neq 0)} (a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger} a_{-\mathbf{k}})$$
(5.60)

in the Hamiltonian, which becomes

$$H \simeq \frac{UN^2}{2V} + \frac{1}{2} \sum_{\mathbf{k}(\mathbf{k}\neq\mathbf{0})} [(\epsilon_{\mathbf{k}} + \frac{NU}{V})(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger}a_{-\mathbf{k}}) + \frac{NU}{V}(a_{\mathbf{k}}^{\dagger}a_{-\mathbf{k}}^{\dagger} + a_{\mathbf{k}}a_{-\mathbf{k}})],$$
(5.61)

when we neglect terms in the potential energy, which are not (at least) proportional to N.

The structure of the Hamiltonian is now very simple, since each of the terms in the k-sum has the form

$$E_0(a^{\dagger}a + b^{\dagger}b) + E_1(a^{\dagger}b^{\dagger} + ba), \qquad (5.62)$$

where $[a, a^{\dagger}] = [b, b^{\dagger}] = 1$, while a and a^{\dagger} commute with b^{\dagger} as well as b.

We may now use the result (5.12) to bring the Hamiltonian (5.61) into diagonal form,

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} (\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}}) + \text{const.}$$
(5.63)

with

$$E_{k} = \sqrt{(\epsilon_{k} + NU/V)^{2} - (NU/V)^{2}}$$
(5.64)

Note that E_k for small k is a linear function of k, $E_k \simeq s\hbar k$. The velocity s is seen to be

$$s = \sqrt{UN/Vm}.$$
 (5.65)

The repulsive interaction has thus turned the energy spectrum, which is quadratic in the non-interacting case, into a linear one, in agreement with what is observed experimentally in liquid ⁴He. The measured slope of the dispersion curve at q = 0 corresponds to a velocity s which is 240 m/s at a temperature of 1 K.

5.4 Quasiparticles in a superconductor

The BCS-theory of superconductivity will be discussed in a later chapter. Here we shall demonstrate how the method of canonical transformations allows one to derive the energy spectrum of a superconductor starting from a simplified Hamiltonian of the form (5.1). The starting point is an effective electronelectron interaction, which keeps only part of the complete Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{2V} \sum_{\mathbf{q}\neq 0,\mathbf{k},\mathbf{k}',\sigma,\sigma'} V(\mathbf{k},\mathbf{k}',\mathbf{q}) c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} ,$$
(5.66)

namely the part that connects pairs with total momentum equal to zero. An important feature of the BCS-Hamiltonian is that the term $\mu \hat{N}$, where \hat{N} is the

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particle number operator, is subtracted from the original Hamiltonian in order to able to describe a state of broken (gauge) symmetry. The procedure is analogous to the transition to a grand canonical ensemble in statistical mechanics and allows one to consider anomalous averages of the form $\langle c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow} \rangle$.

The simplified BCS-Hamiltonian $K = H - \mu \hat{N}$ is thus given by

$$K = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) (c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} + c^{\dagger}_{-\mathbf{k},\downarrow} c_{-\mathbf{k},\downarrow}) - \sum_{\mathbf{k},\mathbf{k}'} V(\mathbf{k},\mathbf{k}') c^{\dagger}_{\mathbf{k}',\uparrow} c^{\dagger}_{-\mathbf{k}',\downarrow} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow},$$
(5.67)

where the interaction matrix elements $V(\mathbf{k}, \mathbf{k}')$ are taken to be constant within a shell of thickness $2\hbar\omega_{\rm D}$ around the Fermi surface, $\omega_{\rm D}$ being the Debye frequency (which is roughly equal to the maximum phonon frequency),

$$V(\mathbf{k}, \mathbf{k}') = V \text{ for } |\epsilon_{\mathbf{k}} - \mu|, |\epsilon_{\mathbf{k}'} - \mu| \le \hbar \omega_{\mathrm{D}}$$

= 0 otherwise. (5.68)

The constant V is positive, corresponding to an attractive interaction in the BCS-Hamiltonian (5.67). In order to obtain the energy spectrum one makes a Hartree-like approximation to the BCS-Hamiltonian with the result

$$H = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) (c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} + c^{\dagger}_{-\mathbf{k},\downarrow} c_{-\mathbf{k},\downarrow}) - \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow} + \Delta_{\mathbf{k}} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow}),$$
(5.69)

where the real quantity Δ_k is

$$\Delta_{k} = \sum_{\mathbf{k}'} V(\mathbf{k}, \mathbf{k}') < c^{\dagger}_{\mathbf{k}',\uparrow} c^{\dagger}_{-\mathbf{k}',\downarrow} > .$$
(5.70)

We can now use the result of (5.23) and write down the diagonalized Hamiltonian in the form

$$H = \text{const.} + \sum_{\mathbf{k}} E_{k} (\alpha_{\mathbf{k},\uparrow}^{\dagger} \alpha_{\mathbf{k},\uparrow} + \alpha_{-\mathbf{k},\downarrow}^{\dagger} \alpha_{-\mathbf{k},\downarrow})$$
(5.71)

where

$$E_k^2 = \Delta_k^2 + \xi_k^2 \tag{5.72}$$

with the definition

$$\xi_k = \epsilon_k - \mu. \tag{5.73}$$

The gap parameter Δ_k , which in the present model is independent of k, is obtained by solving the selfconsistency equation (5.70), as we shall see in a later chapter. It turns out to be a non-analytic function of the strength V of the attractive interaction, indicating that the superconducting ground state cannot be obtained by simple perturbation theory starting from the normal state.

5.5 Spin waves in a magnet

In Section 5.2 above we have characterized the possible states of a crystalline lattice by the number of phonons associated with each normal mode. We shall now see how ferromagnets at low temperatures may be described in terms of spin waves, the so-called magnons. Like phonons the magnons represent excited states of the system, i. e. states with higher energy than the ground state.

5.5.1 Ferromagnet

A simple model of a ferromagnet is a linear chain of atoms interacting with their nearest neighbors.² The Hamiltonian of the magnetic chain is

$$\hat{H} = -J \sum_{n} \hat{\mathbf{S}}_{n} \cdot \hat{\mathbf{S}}_{n+1} = -J \sum_{n} (\hat{S}_{n,z} \hat{S}_{n+1,z} + \frac{1}{2} (\hat{S}_{n}^{+} \hat{S}_{n+1}^{-} + \hat{S}_{n}^{-} \hat{S}_{n+1}^{+})), \quad (5.74)$$

where J is a positive constant. The Hamiltonian is thus a sum of terms which describe the exchange interaction between neighboring atoms. As usual $\hat{S}^+ = \hat{S}_x + i\hat{S}_y$ and $\hat{S}^- = \hat{S}_x - i\hat{S}_y$. For convenience we have made the eigenvalues of the spin operators dimensionless by dividing them by \hbar . This gives J the dimension of energy. The positions of the atoms in the chain have been numbered by $n = 1, 2, 3, \dots, N$, where N is the number of atoms. As in the phonon case we use periodic boundary conditions. By using the properties of the operators of angular momentum one finds that the state $|0\rangle$ given by

$$|0\rangle = |s_1, s_2, \cdots s_N\rangle \tag{5.75}$$

is an eigenstate of \hat{H} ,

$$\hat{H}|0\rangle = -JNs^2|0\rangle, \tag{5.76}$$

with $s_i = s$ denoting the maximum value of the z-component of the spin of the *i*'th atom (s = 1/2 for a single electron, but in general s may be larger than this value, since the atomic spin is the result of the addition of the angular momenta of the atomic electrons). The state $|0\rangle$ is thus characterized by the eigenvalue of each $\hat{S}_{n,z}$ being s. It is not difficult to show that the eigenvalue in (5.76) is the lowest one possible, corresponding to the ground state, but we leave out the proof. From a classical point of view it is plausible that the lowest energy is obtained when the spins all line up in the same direction, since J is taken to be positive.

²We discuss the one-dimensional case because of its transparency, but it should be remembered that one-dimensional systems with finite-range interactions do not order at any finite temperature. The methods described in the following are however easily generalized to the three-dimensional case, in which the magnetic order occurs at a temperature roughly equal to the exchange constant J divided by k.

Canonical transformations

Let us now try to find excited states of the system, i. e. eigenstates of the Hamiltonian with energies larger than the ground-state energy $-JNs^2$. We consider a (normalized) state $|n\rangle$ given by

$$|n\rangle = \frac{1}{\sqrt{2s}}\hat{S}_n^-|0\rangle. \tag{5.77}$$

It is readily seen that the state is not an eigenstate for \hat{H} , since one obtains

$$\hat{H}|n\rangle = -Js(|n+1\rangle + |n-1\rangle) - J(N-2)s^{2}|n\rangle - s(s-1)2J|n\rangle$$
 (5.78)

by using the properties of the angular momentum operators. Let us, however, attempt to build an eigenstate by forming the linear combination

$$|q\rangle = \frac{1}{\sqrt{N}} \sum_{n} e^{iqna} |n\rangle, \qquad (5.79)$$

where a is the distance between neighboring atoms. We find that (5.79) is indeed an eigenstate, since

$$\hat{H}|q\rangle = (-JNs^2 + 2Js(1 - \cos qa))|q\rangle.$$
 (5.80)

Evidently $|q\rangle$ is an energy eigenstate with energy

$$\hbar\omega_q = 2Js(1 - \cos qa) = 4Js\sin^2 qa/2$$
 (5.81)

relative to the ground state. Note that this state is also an eigenstate of the z-component of the total spin with eigenvalue Ns - 1 (in units of \hbar), since it is a superposition of states such as (5.77) which are eigenstates of the z-component of the total spin with eigenvalue Ns - 1, the operator \hat{S}_n^- reducing the eigenvalue by 1 relative to the ground state.

The determination of the magnon energies in the three-dimensional case proceeds just as for one dimension. For simplicity we assume that the magnetic material is ordered in a simple cubic lattice. In three dimensions the magnon energy thus becomes

$$\hbar\omega_{\mathbf{q}} = 4Js(\sin^2(q_x a/2) + \sin^2(q_y a/2) + \sin^2(q_z a/2)), \tag{5.82}$$

since the magnon state is characterized by a three-dimensional wave vector \mathbf{q} as in the case of phonons. The dispersion relation (5.82) has cubic symmetry, since the magnon energy does not change by interchange of the axes in \mathbf{q} -space. It is anisotropic in the sense that the energy depends not only on the length of \mathbf{q} , but also on its direction.

5.5.2 The Holstein-Primakoff transformation

There exists a transformation, known as the Holstein-Primakoff transformation, which allows one to write a spin-Hamiltonian like (5.74) in terms of boson creation and annihilation operators. It is

$$S^{+} = (2s)^{1/2} (1 - a^{\dagger} a/2s)^{1/2} a; \quad S^{-} = (2s)^{1/2} a^{\dagger} (1 - a^{\dagger} a/2s)^{1/2}, \tag{5.83}$$

which implies that

$$S_z^2 = s(s+1) - \frac{1}{2}(S^+S^- + S^-S^+) = (s - a^{\dagger}a)^2.$$
 (5.84)

The operators a and a^{\dagger} satisfy the commutation rule

$$[a_m, a_n^{\dagger}] = \delta_{mn}, \qquad (5.85)$$

where we have restored the site index. The boson commutation rules ensure that the spin operators given by these expressions satisfy the usual angularmomentum commutation relations.

The transition to collective coordinates proceeds in analogy with (5.39),

$$a_n = \frac{1}{\sqrt{N}} \sum_q b_q e^{iqna}.$$
(5.86)

At low temperatures the number of spin waves (which depends on temperature) is small. It is therefore possible to neglect the interaction between the spin waves and approximate S^+ and S^- by

$$S^+ \simeq (2s)^{1/2} a; \quad S^- \simeq (2s)^{1/2} a^{\dagger},$$
 (5.87)

while S_z is given by the positive root of (5.84),

$$S_z = s - a^{\dagger}a. \tag{5.88}$$

The Hamiltonian (5.74) is then approximated to be bilinear in a, a^{\dagger} , with quartic terms being neglected, and is thus readily solvable. To obtain the energy spectrum one must carry out sums of the type

$$\sum_{n} a_{n}^{\dagger} a_{n} = \sum_{n} a_{n+1}^{\dagger} a_{n+1} = \frac{1}{N} \sum_{n,q,q'} b_{q}^{\dagger} b_{q'} e^{i(q-q')na} = \sum_{q} b_{q}^{\dagger} b_{q}$$
(5.89)

and

$$\sum_{n} a_{n}^{\dagger} a_{n+1} = \sum_{q} e^{-iqa} b_{q}^{\dagger} b_{q}; \quad \sum_{n} a_{n} a_{n+1}^{\dagger} = \sum_{q} e^{iqa} b_{q}^{\dagger} b_{q}, \quad (5.90)$$

which is seen to result in the energy dispersion relation (5.81).

In the antiferromagnetic case, J is negative. If one assumes that the ground state is one in which the spins are aligned in opposite directions on each of the two sublattices (corresponding to $S_{n,z} = s, S_{n+1,z} = -s$), then we must treat each sublattice separately by making the transformations

$$S_{n,z} = s - a^{\dagger}a, \quad S_n^- = (2s)^{1/2}a^{\dagger}, \quad S_n^+ = (2s)^{1/2}a, \quad (5.91)$$

and

$$S_{n+1,z} = -s + c^{\dagger}c, \quad S_{n+1}^{-} = (2s)^{1/2}c, \quad S_{n+1}^{+} = (2s)^{1/2}c^{\dagger}.$$
 (5.92)

Here we have introduced boson operators c and c^{\dagger} associated with those sites, in which the z-component of the spin has the value -s in the ground state. As shown in Problem 33, one then obtains a Hamiltonian of the form (5.1), which may readily be diagonalized, resulting in spin waves with a *linear* dispersion. It should be noted that our initial assumption about the nature of the ground state is actually incorrect in the antiferromagnetic case, cf. Problem 34.

6 Green functions at zero temperature

Green functions in many-particle physics come in many different forms, depending on the particular problem that is being considered. In this chapter we shall introduce *time-ordered*, *single-particle* Green functions at zero temperature, and discuss the properties of *free-particle* Green functions which form the basic building blocks needed for carrying out perturbation theory to infinite order.

Not all Green functions are time-ordered. One frequently needs to consider *retarded* or *advanced* functions as well. The use of time-ordered Green functions allows a perturbation series to be written in a convenient form. Retarded and advanced functions arise naturally when one considers the linear response of a system to an external disturbance. While a physical quantity like the ground-state energy of an interacting many-body system may be obtained from the time-ordered, single-particle Green function, other physical quantities, such as the electrical or thermal conductivity, requires the knowledge of two-particle Green functions are determined by infinite-order perturbation series in which one-particle Green functions form the building blocks. Many-body theory therefore starts with the study of the Green function, or *propagator*, for noninteracting particles.

For a general interacting system the single-particle Green function G is defined by

$$G_{\sigma\sigma'}(\mathbf{x},t;\mathbf{x}',t') = -i < T\{\psi_{\sigma}(\mathbf{x},t)\psi_{\sigma'}^{\dagger}(\mathbf{x}',t')\} > .$$
(6.1)

Here $\psi_{\sigma}^{\dagger}(\mathbf{x}, t)$ and $\psi_{\sigma}(\mathbf{x}, t)$ are operators in the Heisenberg picture, which add and remove, respectively, a particle in a spin-state σ (= ±1) to the interacting system at the space-time point (\mathbf{x}, t). We shall here treat the case when the particles are fermions. The time-ordering operator T is in the fermion case defined by

$$T\{A(t_1)B(t_2)C(t_3)\cdots\} = (-1)^p C\{A(t_1)B(t_2)C(t_3)\cdots\},$$
(6.2)

where C is an operator which orders the fermion operators $A(t_1)B(t_2)C(t_3)\cdots$ chronologically with earlier times to the right, while p is the number of interchanges needed to achieve this chronological ordering. Thus

$$T\{\psi(t_1)\psi^{\dagger}(t_2)\} = \psi(t_1)\psi^{\dagger}(t_2) \text{ if } t_1 > t_2, \qquad (6.3)$$

while

$$T\{\psi(t_1)\psi^{\dagger}(t_2)\} = -\psi^{\dagger}(t_2)\psi(t_1) \text{ if } t_1 < t_2.$$
(6.4)

¹The definition of an N-particle Green function involves N creation and N annihilation operators.

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The average $\langle \cdots \rangle$ in (6.1) is the quantum-mechanical expectation value involving the exact Heisenberg ground state of the interacting system. Naturally, this state is not known for a general many-body system, and (6.1) is therefore not a practical starting point for the calculation of G. If the Green function G is known, one may obtain from (6.1) physical quantities such as the particle density or the total energy of the system, as we shall see in Section 6.2 below.

6.1 Translational invariance

As we shall be dealing with systems that are translationally invariant (in both space and time) it is convenient to introduce operators $c_{\mathbf{k},\sigma}$ and $c_{\mathbf{k},\sigma}^{\dagger}$ that remove and add, respectively, a particle in a definite momentum and spin state \mathbf{k}, σ . This is accomplished by the transformation

$$\psi_{\sigma}(\mathbf{x},t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k},\sigma}(t)$$
(6.5)

and the corresponding expression for the Hermitian conjugate

$$\psi_{\sigma}^{\dagger}(\mathbf{x},t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k},\sigma}^{\dagger}(t).$$
(6.6)

Then

$$G_{\sigma\sigma'}(\mathbf{x}, t; \mathbf{x}', t') = -\frac{i}{V} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} e^{-i\mathbf{k}' \cdot \mathbf{x}'} e^{i\mathbf{k} \cdot \mathbf{x}} < T\{c_{\mathbf{k},\sigma}(t)c_{\mathbf{k}',\sigma'}^{\dagger}(t')\} > .$$
(6.7)

Since the system is translationally invariant, $G_{\sigma\sigma'}(\mathbf{x}, t; \mathbf{x}', t')$ is a function of only the relative coordinate $\mathbf{x} - \mathbf{x}'$, implying that the terms in the sum with $\mathbf{k}' \neq \mathbf{k}$ are zero. Similarly, if the Hamiltonian is time-independent, the invariance with respect to displacement in time implies that $G_{\sigma\sigma'}(\mathbf{x}, t; \mathbf{x}', t')$ only depends on the difference t - t' of the time-arguments. We thus obtain

$$G_{\sigma\sigma'}(\mathbf{x}, t; \mathbf{x}', t') = \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} G_{\sigma\sigma'}(\mathbf{k}, t-t')$$
(6.8)

where

$$G_{\sigma\sigma'}(\mathbf{k},t) = -i < T\{c_{\mathbf{k},\sigma}(t)c_{\mathbf{k},\sigma'}^{\dagger}(0)\} > .$$
(6.9)

In the problems we shall consider, the Green function is proportional to the unit matrix in spin-space²

$$G_{\sigma\sigma'}(\mathbf{k},t) = \delta_{\sigma\sigma'}G(\mathbf{k},t). \tag{6.10}$$

²Whenever the Hamiltonian and its ground state is invariant under spatial rotation and reflection, the Green function is proportional to the unit matrix $I = \delta_{\sigma\sigma'}$ in spin space.

We shall frequently need to work with the Fourier-transform of G with respect to time. This is given by

$$G(\mathbf{k},\omega) = \int dt e^{i\omega t} G(\mathbf{k},t), \qquad (6.11)$$

together with the inverse

$$G(\mathbf{k},t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} G(\mathbf{k},\omega).$$
(6.12)

We shall generally follow the commonly used convention of distinguishing between a function and its Fourier-transform by their explicit argument only, except in special cases such as the example treated in Section 6.5.1 below, where an additional 'tilde' is introduced to prevent misunderstanding. The integrations always extend from minus infinity to plus infinity unless the limits are explicitly indicated.

6.2 Physical observables

We shall now show how the Green function in a translationally invariant system yields information on the occupation of the single-particle states \mathbf{k} . The occupation number $n_{\mathbf{k}}$ of the state \mathbf{k} is seen to be given by

$$n_{\mathbf{k}} = \langle c_{\mathbf{k},\sigma}^{\dagger}(0)c_{\mathbf{k},\sigma}(0) \rangle = -i \lim_{t \to 0^{-}} G(\mathbf{k},t) = -i \int \frac{d\omega}{2\pi} e^{i\omega\eta} G(\mathbf{k},\omega). \quad (6.13)$$

Here η denotes a positive infinitesimal, $\eta = 0^+$.

The total number of particles N therefore equals

$$N = 2\sum_{\mathbf{k}} n_{\mathbf{k}} = -2i\sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} e^{i\omega\eta} G(\mathbf{k},\omega).$$
(6.14)

In general, an arbitrary single-particle operator (such as the spin density or the current density) may be related to the single-particle Green function, because the latter involves one creation and one annihilation operator.

It is also possible to express the total energy in terms of the single-particle Green function. One might expect that this would require knowledge of a two-particle Green function, but since the field operators ψ satisfy the Heisenberg equation of motion involving the Hamiltonian of the system, one may relate

The proof of that is obtained by expanding G in terms of the unit matrix and the three Pauli matrices, which together form a complete basis in spin space. Since G by assumption is a scalar under spatial rotation, G must be a linear combination of I and $\tau \cdot \mathbf{k}$, with τ denoting the three Pauli-matrices. The invariance under reflection implies, however, that the coefficient of the term involving $\tau \cdot \mathbf{k}$ is zero.

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the expectation value of the total energy to the single-particle Green function. This is shown as follows:

For definiteness we shall assume a Hamiltonian of the form

$$H = H_0 + H' (6.15)$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(6.16)

represents the kinetic energy, while

$$H' = \frac{1}{2V} \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}', \sigma, \sigma'} V_{\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q}, \sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}, \sigma'} c_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}$$
(6.17)

is the interaction energy. The Fourier-transform of the (spin-independent) interaction potential is denoted by $V_{\mathbf{q}}$.

The Heisenberg equation of motion is

$$i\hbar\frac{\partial}{\partial t}c_{\mathbf{k}}(t) = e^{iHt/\hbar}[c_{\mathbf{k}}, H]e^{-iHt/\hbar}, \qquad (6.18)$$

where H is the Hamiltonian given in (6.15).

In calculating the time derivative of an annihilation operator c_1 in the Heisenberg-picture we encounter a commutator of the form

$$[c_1, c_2^{\dagger} c_3^{\dagger} c_4 c_5]. \tag{6.19}$$

When working out such expressions it is convenient to exploit the identities (4.8) and (4.9). Using (4.8) we get

$$[c_1, c_2^{\dagger} c_3^{\dagger} c_4 c_5] = [c_1, c_2^{\dagger} c_3^{\dagger}] c_4 c_5 - c_2^{\dagger} c_3^{\dagger} [c_4 c_5, c_1] = [c_1, c_2^{\dagger} c_3^{\dagger}] c_4 c_5,$$
(6.20)

while the use of (4.9) yields

$$[c_1, c_2^{\dagger} c_3^{\dagger} c_4 c_5] = \delta_{1,2} c_3^{\dagger} c_4 c_5 - \delta_{1,3} c_2^{\dagger} c_4 c_5.$$
(6.21)

Note that (6.21) implies that

$$\sum_{12345} c_1^{\dagger}[c_1, c_2^{\dagger}c_3^{\dagger}c_4c_5] = 2 \sum_{2345} c_2^{\dagger}c_3^{\dagger}c_4c_5.$$
(6.22)

The time derivative of $\langle c_{\mathbf{k}\sigma}^{\dagger}(0)c_{\mathbf{k}\sigma}(t) \rangle$ is determined by working out the commutators with the help of (6.21),

$$i\hbar\frac{\partial}{\partial t}\sum_{\mathbf{k}\sigma} \langle c^{\dagger}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle = \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}} \langle c^{\dagger}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle$$

$$+\frac{1}{2V}\sum_{\mathbf{k}\sigma\mathbf{p}\sigma'\mathbf{p}'\sigma''\mathbf{q}}V_{\mathbf{q}}(\delta_{\mathbf{p+q,k}}\delta_{\sigma\sigma'} < c^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{\mathbf{p}'-\mathbf{q}\sigma''}(t)c_{\mathbf{p}'\sigma''}(t)c_{\mathbf{p}\sigma}(t) > -\delta_{\mathbf{p}'-\mathbf{q,k}}\delta_{\sigma\sigma''} < c^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{\mathbf{p+q}\sigma'}(t)c_{\mathbf{p}'\sigma''}(t)c_{\mathbf{p}\sigma'}(t) >), \quad (6.23)$$

which implies that

$$-i \lim_{t \to 0^{-}} \sum_{\mathbf{k}\sigma} i\hbar \frac{\partial}{\partial t} G(\mathbf{k}, t) = -i \lim_{t \to 0^{-}} \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} G(\mathbf{k}, t) + 2 < H' > \quad (6.24)$$

on using (6.22). By means of (6.12) we then obtain from (6.24)

$$\langle H' \rangle = -\frac{iV}{(2\pi)^4} \int d\mathbf{k} \int d\omega e^{i\omega\eta} (-\epsilon_k + \hbar\omega) G(\mathbf{k},\omega),$$
 (6.25)

which yields the final result for the ground-state energy

$$E = \langle H \rangle = \langle H_0 + H' \rangle = -\frac{iV}{(2\pi)^4} \int d\mathbf{k} \int d\omega e^{i\omega\eta} (\epsilon_k + \hbar\omega) G(\mathbf{k}, \omega).$$
(6.26)

Knowledge of the single-particle Green-function $G(\mathbf{k}, \omega)$ thus allows one to determine the ground-state energy E, by carrying out the integrations in (6.26) over \mathbf{k} and ω .

It is sometimes convenient to separate the ground-state energy in two terms, $E = E_0 + E_1$, where E_0 is the ground-state energy of the noninteracting system, while E_1 is that due to the interaction. This is achieved by introducing a variable coupling constant λ defined as follows: Let $H = H_0 + H'$ be the Hamiltonian of the system, with H' being the interaction. The operator $H(\lambda)$ defined by

$$H(\lambda) = H_0 + \lambda H' \tag{6.27}$$

then has the properties that $H(0) = H_0$, while H(1) = H. We let λ vary between 0 and 1, and imagine that we have calculated the total energy $E(\lambda)$ associated with the Hamiltonian $H(\lambda)$. Denoting the ground-state wavefunction by $\Psi(\lambda)$ we thus have

$$E(\lambda) = \langle \Psi(\lambda) | H(\lambda) | \Psi(\lambda) \rangle.$$
(6.28)

By differentiating with respect to λ we obtain

$$\frac{dE(\lambda)}{d\lambda} = E(\lambda)\frac{d}{d\lambda}\langle\Psi(\lambda)|\Psi(\lambda)\rangle + \langle\Psi(\lambda)|H'|\Psi(\lambda)\rangle.$$
(6.29)

Since $\langle \Psi(\lambda)|\Psi(\lambda)\rangle = 1$, the first term on the right-hand side of (6.29) equals zero. By integrating with respect to λ we finally obtain the identity

$$E - E_0 = \int_0^1 \frac{d\lambda}{\lambda} \langle \Psi(\lambda) | \lambda H' | \Psi(\lambda) \rangle.$$
 (6.30)

In order to evaluate (6.30) we must calculate $\langle \Psi(\lambda) | \lambda H' | \Psi(\lambda) \rangle$ for each λ . This is accomplished with the help of (6.25), resulting in

$$E - E_0 = -i\frac{V}{(2\pi)^4} \int_0^1 \frac{d\lambda}{\lambda} \int d\mathbf{k} \int d\omega e^{i\omega\eta} (-\epsilon_k + \hbar\omega) G^\lambda(\mathbf{k},\omega), \qquad (6.31)$$

where the superscript λ indicates that the Green function belongs to the Hamiltonian $H(\lambda) = H_0 + \lambda H'$.

6.3 Green functions for free fermions

The Green function $G(\mathbf{k}, t)$ for free fermions is

$$G_{\sigma\sigma'}(\mathbf{k},t) = -i < T\{c_{\mathbf{k}\sigma}(t)c_{\mathbf{k}\sigma'}^{\dagger}(0)\} >_0, \qquad (6.32)$$

where the expectation value involves the ground state of the free-particle Hamiltonian H_0 given by

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (6.33)$$

where $\epsilon_k = \hbar^2 k^2 / 2m$.

The use of the Heisenberg equations of motion and the Hamiltonian (6.33) results in the equation of motion

$$i\hbar\frac{\partial}{\partial t}c_{\mathbf{k}} = \epsilon_k c_{\mathbf{k}}(t) \tag{6.34}$$

with the solution

$$c_{\mathbf{k}}(t) = e^{-i\epsilon_{\mathbf{k}}t/\hbar}c_{\mathbf{k}}(0).$$
(6.35)

This allows us to determine the free-particle Green function $G(\mathbf{k}, t)$. By considering first t > 0 and subsequently t < 0, we obtain the result

$$G(\mathbf{k},t) = -i[(1-n_{\mathbf{k}})\Theta(t) - n_{\mathbf{k}}\Theta(-t)]e^{-i\epsilon_{\mathbf{k}}t/\hbar},$$
(6.36)

where $\Theta(t) = 1$ if t > 0 and $\Theta(t) = 0$ if t < 0. Here $n_{\mathbf{k}} = 1$ if $k < k_{\mathbf{F}}$, while $n_{\mathbf{k}} = 0$ if $k > k_{\mathbf{F}}$. Thus $n_{\mathbf{k}}$ are the occupation numbers in the ground state of the non-interacting system.

In later applications of many-body theory we shall find that the poles of the single particle Green function $G(\mathbf{k}, \omega)$ in the complex ω -plane yields information about the energy and lifetime of the *quasiparticles*, which is the commonly used name for the elementary excitations of the system. In order to see how this works for free fermions we use the identity

$$\Theta(\pm t) = \mp \int \frac{d\omega}{2\pi i} \frac{e^{-i\omega t}}{\omega \pm i\eta},$$
(6.37)

where η as usual is a positive infinitesimal, to prove that

$$G^{(0)}(\mathbf{k},\omega) = \frac{1-n_{\mathbf{k}}}{\omega - (\epsilon_{\mathbf{k}}/\hbar) + i\eta} + \frac{n_{\mathbf{k}}}{\omega - (\epsilon_{\mathbf{k}}/\hbar) - i\eta},$$
(6.38)

where the superscript on G indicates that it is the Green function for noninteracting particles. Note the different location of the pole in the complex ω -plane for $k < k_{\rm F}$ and for $k > k_{\rm F}$.

The Green functions for free electrons do not by themselves contain any information which may not be obtained by using elementary quantum mechanics. By doing infinite-order perturbation theory in the presence of interactions we shall find that the poles of the Green functions are shifted in the complex frequency plane. Provided the poles remain sufficiently close to the real axis, their real and imaginary parts represent, respectively, the energy and (\hbar times) the inverse lifetime of the elementary excitations.

6.4 Infinite-order perturbation theory

In using perturbation theory to evaluate the Green function we shall employ the method of *adiabatic* turning-on of the interaction: we imagine that at some time in the distant past the interaction between the particles is absent, while for increasing times it is gradually being turned on in such a way that it assumes its full value at a definite instant of time t = 0. This could be described by the Hamiltonian

$$H = H_0 + e^{-\epsilon |t|} H'$$
 (6.39)

where ϵ is an infinitesimal positive quantity. According to (6.39) the interaction vanishes for $t \to \pm \infty$, while the Hamiltonian equals its full value $H = H_0 + H'$ at t = 0. The limit $\epsilon \to 0$ corresponds to turning on the interaction adiabatically, i. e. infinitely slowly.

In the interaction picture the wave function $\Psi_I(t)$ develops in time according to

$$\Psi_I(t) = U_\epsilon(t, t_0) \Psi_I(t_0), \qquad (6.40)$$

where we have indicated by the subscript ϵ that the time-development operator depends on this parameter. It is given by expression (2.57) or (2.58), with $H_1(t') = e^{-\epsilon|t'|}H'(t')$. If the time t_0 approaches $-\infty$, then the Schrödinger wave function $\Psi_S(t_0)$ must be given by

$$\Psi_S(t_0) = e^{-iH_0 t_0/\hbar} \Phi_0 \tag{6.41}$$

where Φ_0 is a stationary eigenstate for H_0 ,

$$H_0 \Phi_0 = E_0 \Phi_0. \tag{6.42}$$

The wave function in the interaction picture at time $t = t_0 = -\infty$ is therefore

$$\Psi_I(t_0) = e^{iH_0 t_0/\hbar} \Psi_S(t_0) = \Phi_0.$$
(6.43)

At time t = 0 all three pictures coincide as before. We thus have

$$\Psi_S(0) = \Psi_H(0) = \Psi_I(0) = U_{\epsilon}(0, -\infty)\Phi_0.$$
(6.44)

Strictly speaking $\Psi_0 = U_{\epsilon}(0, -\infty)\Phi_0$ does not exist in the limit $\epsilon \to 0$, since it acquires a phase which increases in proportion to $1/\epsilon$. In stating the *Gell-Mann* Low theorem it is therefore necessary to consider instead the quantity

$$\lim_{\epsilon \to 0} \frac{|U_{\epsilon}(0, -\infty)\Phi_{0}\rangle}{\langle \Phi_{0}|U_{\epsilon}(0, -\infty)\Phi_{0}\rangle} = \frac{|\Psi_{0}\rangle}{\langle \Phi_{0}|\Psi_{0}\rangle}.$$
(6.45)

The theorem due to Gell-Mann and Low³ says the following: If (6.45) exists to all orders in perturbation theory, then it is an eigenstate of H,

$$H\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = E\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle}.$$
(6.46)

We shall not give the proof of the theorem here.⁴ It should be noted that the state which develops adiabatically from the ground-state of the non-interacting system is ordinarily, but not necessarily, the ground-state of the interacting system. If - as in a superconductor - the ground-state energy does not possess a perturbation series in the coupling constant, then the eigenvalue E is not the ground-state energy.

The theorem of Gell-Mann and Low shows how an eigenstate (usually the ground state) of the Hamiltonian H is generated by adiabatically turning on the interaction. We shall make use of the theorem in evaluating the single-particle Green function, which involves a time-ordered expectation value of two Heisenberg operators in the ground state of the interacting system. As we shall see below, this expectation value may in turn be expressed in terms of expectation values of operators given in the interaction picture, evaluated in the ground-state Φ_0 of the non-interacting system.

First we calculate the norm of the state vector entering the eigenvalue equation (6.46). We observe that the state given by (6.45) may equally well be obtained by letting the system develop backwards in time from $t = +\infty$ to zero. Thus we have

$$\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = \lim_{\epsilon \to 0} \frac{|U_{\epsilon}(0,\infty)\Phi_0\rangle}{\langle\Phi_0|U_{\epsilon}(0,\infty)\Phi_0\rangle}.$$
(6.47)

³M. Gell-Mann and F. Low, Phys. Rev. 84, 350, 1951

⁴A detailed discussion may be found in A. L. Fetter and J. D. Walecka, *Quantum Theory* of Many-particle Systems, McGraw-Hill 1971.

By using $U(0,\infty)^{\dagger} = U^{-1}(0,\infty) = U(\infty,0)$ we obtain

$$\frac{\langle \Psi_0 | \Psi_0 \rangle}{\langle \Psi_0 | \Phi_0 \rangle \langle \Phi_0 | \Psi_0 \rangle} = \frac{\langle \Phi_0 | U(\infty, 0) U(0, -\infty) | \Phi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2} = \frac{\langle \Phi_0 | U(\infty, -\infty) | \Phi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2}.$$
(6.48)

Let us consider the quantity I(t,t') defined by in terms of the operators A_H and B_H

$$I(t,t') = \frac{\langle \Psi_0 | T\{A_H(t)B_H(t')\} | \Psi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2}.$$
 (6.49)

First we treat the case t > t' and obtain

$$I(t,t')|\langle \Phi_0|\Psi_0\rangle|^2 = \langle \Psi_0|U_{\epsilon}(0,t)A_I(t)U_{\epsilon}(t,0)U_{\epsilon}(0,t')B_I(t')U_{\epsilon}(t',0)|\Psi_0\rangle.$$
(6.50)

Using the property $U(t,0) = U(0,t)^{-1}$ of the time-development operator, we get

$$I(t,t')|\langle \Phi_0|\Psi_0\rangle|^2 = \langle \Psi_0|U_{\epsilon}(0,t)A_I(t)U_{\epsilon}(t,0)U_{\epsilon}(0,t')B_I(t')U_{\epsilon}(t',0)|\Psi_0\rangle$$

= $\langle \Phi_0|T\{U_{\epsilon}(\infty,-\infty)A_I(t)B_I(t')\}|\Phi_0\rangle.$ (6.51)

The opposite case t < t' may be treated in a similar fashion.

In the following 1 stands for $(\mathbf{x}_1, t_1, \sigma_1)$ and $\int d1 \cdots$ for $\sum_{\sigma_1} \int d\mathbf{x}_1 \int dt_1 \cdots$. The Green function G(1, 2) may therefore with the help of (2.58) be expressed as

$$iG(1,2) = \sum_{n=0}^{\infty} (-\frac{i}{\hbar})^n \frac{1}{n!} \int_{-\infty}^{\infty} dt'_1 \cdots \int_{-\infty}^{\infty} dt'_n \\ \frac{\langle T\{H'(t'_1) \cdots H'(t'_n)\psi(1)\psi^{\dagger}(2)\} >_0}{\langle S \rangle_0}.$$
(6.52)

Here the operators are written in the interaction picture. The average $< ... >_0$ involves the ground state of the non-interacting system. The denominator $< S >_0$ is given by the expression

$$\langle S \rangle_{0} = \sum_{n=0}^{\infty} (-\frac{i}{\hbar})^{n} \frac{1}{n!}$$
$$\int_{-\infty}^{\infty} dt_{1}^{'} \cdots \int_{-\infty}^{\infty} dt_{n}^{'} \langle T\{H'(t_{1}^{'}) \cdots H'(t_{n}^{'})\} \rangle_{0} .$$
(6.53)

The result (6.52) forms the starting point for the diagrammatic perturbation theory described in the following subsection.

6.5 Diagrams

In general, the Green function cannot be determined exactly. Instead, one does perturbation theory and sums selected terms to infinite order by expanding the numerator and denominator of (6.52) in powers of H'. This procedure generates time-ordered products of strings of field-operators, corresponding to *n*-particle Green functions for the non-interacting system. We shall therefore need to consider many-particle Green functions $G_n^{(0)}$ for the non-interacting system,

$$G_n^{(0)}(1\cdots n; n'\cdots 1') = (-i)^n \langle \Phi_0 | T\{\psi(1)\cdots\psi(n)\psi^{\dagger}(n')\cdots\psi^{\dagger}(1')\} | \Phi_0 \rangle.$$
(6.54)

For short we have written n for the argument $(\mathbf{x}_n, t_n, \sigma_n)$.

First we derive a differential equation for $G_1^{(0)}$, the one-particle Green function for the *non-interacting* system with Hamiltonian H given by

$$H = \sum_{\sigma_1} \int d\mathbf{x}_1 \psi^{\dagger}_{\sigma_1}(\mathbf{x}_1) H_0(\mathbf{x}_1) \psi_{\sigma_1}(\mathbf{x}_1).$$
(6.55)

We have

$$G_{1}^{(0)}(1,1') = -i\langle \Phi_{0}|T\{\psi(1)\psi^{\dagger}(1')\}|\Phi_{0}\rangle$$

= $-i\langle \Phi_{0}|\psi(1)\psi^{\dagger}(1')|\Phi_{0}\rangle\Theta(t_{1}-t_{1'})$
+ $i\langle \Phi_{0}|\psi^{\dagger}(1')\psi(1)|\Phi_{0}\rangle\Theta(t_{1'}-t_{1}).$ (6.56)

Since

$$i\hbar \frac{\partial \psi(1)}{\partial t_1} = [\psi(1), H] \\ = [\psi(1), \sum_{\sigma_2} \int d\mathbf{x}_2 \psi^{\dagger}(2) H_0(2) \psi(2)] \\ = H_0(1) \psi(1), \qquad (6.57)$$

we get

$$i\hbar \frac{\partial}{\partial t_1} G_1^{(0)}(1,1') = H_0(1) G_1^{(0)}(1,1') + \hbar \delta(t_1 - t_1') \langle \Phi_0 | \psi(1) \psi^{\dagger}(1') + \psi^{\dagger}(1') \psi(1) | \Phi_0 \rangle = H_0(1) G_1^{(0)}(1,1') + \hbar \delta(t_1 - t_1') \delta(\mathbf{x}_1 - \mathbf{x}_{1'}). \quad (6.58)$$

In operator form we thus have

$$G_1^{(0)}(1,1') = (i\hbar\frac{\partial}{\partial t_1} - H_0(1))^{-1}\hbar\delta(1-1').$$
(6.59)

We now proceed to consider the equation of motion satisfied by the twoparticle Green function $G_2^{(0)}(1,2;2',1')$. In this case we must consider separately⁵ the intervals $t_1 < t'_1$ and $t_1 > t'_1$ together with $t_1 < t'_2$ and $t_1 > t'_2$. We therefore get

$$(i\hbar\frac{\partial}{\partial t_{1}} - H_{0}(1))G_{2}^{(0)}(1,2;2',1')$$

$$= -i\hbar\delta(t_{1} - t_{1}')\langle\Phi_{0}|\{\psi(1),\psi^{\dagger}(1')\}T\{\psi(2)\psi^{\dagger}(2')\}|\Phi_{0}\rangle$$

$$+i\hbar\delta(t_{1} - t_{2}')\langle\Phi_{0}|\{\psi(1),\psi^{\dagger}(2')\}T\{\psi(2)\psi^{\dagger}(1')\}|\Phi_{0}\rangle$$

$$= \hbar\delta(1 - 1')G_{1}^{(0)}(2,2') - \hbar\delta(1 - 2')G_{1}^{(0)}(2,1'). \quad (6.60)$$

On using (6.59) we see that

$$G_2^{(0)}(1,2;2',1') = G_1^{(0)}(1,1')G_1^{(0)}(2,2') - G_1^{(0)}(1,2')G_1^{(0)}(2,1'),$$
(6.61)

which may be written as a determinant

$$G_2^{(0)}(1,2;2',1') = \begin{vmatrix} G_1^{(0)}(1,1') & G_1^{(0)}(1,2') \\ G_1^{(0)}(2,1') & G_1^{(0)}(2,2'). \end{vmatrix}$$
(6.62)

It is left as an exercise for the reader to show that the corresponding result for a three-particle Green function may be written as

$$G_{3}^{(0)}(1,2,3;3',2',1') = \begin{vmatrix} G_{1}^{(0)}(1,1') & G_{1}^{(0)}(1,2') & G_{1}^{(0)}(1,3') \\ G_{1}^{(0)}(2,1') & G_{1}^{(0)}(2,2') & G_{1}^{(0)}(2,3') \\ G_{1}^{(0)}(3,1') & G_{1}^{(0)}(3,2') & G_{1}^{(0)}(3,3') \end{vmatrix}$$
(6.63)

These results are readily generalized to a n-particle Green function, which is given by

$$G_{n}^{(0)}(1,\cdots n;n'\cdots 1') = \begin{vmatrix} G_{1}^{(0)}(1,1') & G_{1}^{(0)}(1,2') & \cdots & G_{1}^{(0)}(1,n') \\ G_{1}^{(0)}(2,1') & G_{1}^{(0)}(2,2') & \cdots & G_{1}^{(0)}(2,n') \\ \cdots & \cdots & \cdots & \cdots \\ G_{1}^{(0)}(n,1') & G_{1}^{(0)}(n,2') & \cdots & G_{1}^{(0)}(n,n') \end{vmatrix}$$
(6.64)

The result (6.64) is *Wick's theorem*. It forms the basis for the diagrammatic expansion of the Green function given by (6.52).

As an example of the use of diagrams we derive in the following subsection the results of Hartree-Fock theory discussed in Chapter 4.

⁵Note that we do not have to consider the intervals $t_1 < t_2$ and $t_1 > t_2$ separately, since the anticommutator $\{\psi(1), \psi(2)\}$ is zero and therefore gives a vanishing contribution to $\delta(t_1 - t_2)$.



Figure 6.1: Contributions to $\langle S \rangle_0$ to first order in V.

6.5.1 Hartree-Fock theory with diagrams

Let us consider a system of identical spin-1/2 fermions with Hamiltonian $H = H_0 + V$, where the interaction V is given in the Schrödinger picture by

$$V = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d\mathbf{x}_1 \int d\mathbf{x}_2 \psi^{\dagger}_{\sigma_1}(\mathbf{x}_1) \psi^{\dagger}_{\sigma_2}(\mathbf{x}_2) V(\mathbf{x}_1 - \mathbf{x}_2) \psi_{\sigma_2}(\mathbf{x}_2) \psi_{\sigma_1}(\mathbf{x}_1). \quad (6.65)$$

For simplicity we have assumed that the potential $V(\mathbf{x}_1 - \mathbf{x}_2)$ is spinindependent and only depends on the relative coordinates $\mathbf{x}_1 - \mathbf{x}_2$. It is convenient to introduce time explicitly by the definition

$$U(1,2) = V(\mathbf{x}_1 - \mathbf{x}_2)\delta(t_1 - t_2).$$
(6.66)

When we expand the Green function, we must remember to take into account that the creation operators appear before the annihilation operators in the interaction (6.65). It is therefore convenient to shift the time argument in the creation operators appearing in V(t) by a positive infinitesimal 0⁺. When we subsequently use Wick's theorem on (6.53), we shall encounter Green functions of the type $G^{(0)}(1', 1')$, where the two time arguments are $t_{1'}$ and $t_{1'}+0^+$, while the spatial arguments are $\mathbf{x}_{1'}$ and $\mathbf{x}_{1'}$,

$$G^{(0)}(1',1') = G^{(0)}_{\sigma_{1'}\sigma_{1'}}(\mathbf{x}_{1'},t_{1'};\mathbf{x}_{1'},t_{1'}+0^+).$$
(6.67)

Correspondingly there appear Green functions of the type $G^{(0)}(1', 2')$, where the two time arguments are $t_{1'}$ and $t_{1'} + 0^+$, respectively, while the spatial arguments are $\mathbf{x}_{1'}$ and $\mathbf{x}_{2'}$. In this case we have

$$G^{(0)}(1',2') = G^{(0)}_{\sigma_{1'}\sigma_{2'}}(\mathbf{x}_{1'},t_{1'};\mathbf{x}_{2'},t_{1'}+0^+).$$
(6.68)

To first order in the interaction $\langle S \rangle_0$ becomes

$$\langle S \rangle_{0} \simeq 1 - \frac{i}{\hbar} \int dt'_{1} \langle T\{V(t'_{1})\} \rangle_{0}$$

$$= 1 - \frac{i}{2\hbar} \int d1' \int d2' U(1', 2')$$

$$\langle T\{\psi^{\dagger}(1')\psi^{\dagger}(2')\psi(2')\psi(1')\} \rangle_{0},$$
(6.69)



Figure 6.2: Unlinked diagrams to first order in V.

where $\int d1 \cdots$ stands for $\sum_{\sigma_1} \int d\mathbf{x}_1 \int dt_1 \cdots$. We now use

$$< T\{\psi^{\dagger}(1')\psi^{\dagger}(2')\psi(1')\} >_{0} =$$

$$< T\{\psi(1')\psi^{\dagger}(1')\} >_{0} < T\{\psi(2')\psi^{\dagger}(2')\} >_{0} -$$

$$< T\{\psi(1')\psi^{\dagger}(2')\} >_{0} < T\{\psi(2')\psi^{\dagger}(1')\} >_{0},$$
 (6.70)

cf. (6.62). Diagrammatically, (6.69) and (6.70) may be illustrated as in Fig. 6.1.

By expanding in similar fashion the numerator in (6.52) to first order it is seen to contain terms in which the space-time point 1 is connected directly to 2, while 1' and 2' are connected as in the denominator (6.69). Symbolically we may combine these terms as shown in Fig. 6.2, and we observe that their contribution to first order is cancelled by those of the denominator. A similar cancellation appears in all higher orders, and we therefore only need to to consider the linked diagrams in the numerator, provided we replace the denominator $\langle S \rangle_0$ by 1.

The first-order contribution $iG^{(1)}(1,2)$ to the Green function is thus seen to be

$$iG^{(1)}(1,2) = -\frac{i}{\hbar} \frac{1}{2} \int d1' \int d2' U(1',2') < T\{\psi^{\dagger}(1')\psi^{\dagger}(2')\psi(2')\psi(1')\psi(1)\psi^{\dagger}(2)\} >_{0}, \quad (6.71)$$

where it is understood that only the linked diagrams are included. The corresponding diagrams are illustrated in Fig. 6.3 (a) and (b). Note that these diagrams have the same topological structure. They only differ by having the names of the internal variables interchanged, and they give therefore exactly the same contribution to $G^{(1)}$. The diagrams (c) and (d) likewise yield the same contribution, which means that the expression for $G^{(1)}(1,2)$ becomes

$$G^{(1)}(1,2) = \frac{i}{\hbar} \int d1' \int d2' [-G^{(0)}(1,2')U(1',2')G^{(0)}(1',1')G^{(0)}(2',2) + G^{(0)}(1,1')U(1',2')G^{(0)}(1',2')G^{(0)}(2',2)].$$
(6.72)

Green functions at zero temperature



Figure 6.3: Contributions to $G^{(1)}$.

Note that the factor 1/2 appearing in the original interaction (6.65) is cancelled in the expression (6.72), since the diagrams (a) and (b) (as well as (c) and (d)) yield precisely the same contribution.

For a system which is translationally invariant in space and time it is convenient to Fourier-transform from the (\mathbf{x}, t) -variables to (\mathbf{k}, ω) -variables,

$$G(1,2) = \frac{1}{(2\pi)^4} \int d\mathbf{k} \int d\omega e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-i\omega(t_1-t_2)} \tilde{G}(\mathbf{k},\omega) \delta_{\sigma_1\sigma_2}.$$
 (6.73)

The Fourier-transformation yields

$$\tilde{G}^{(1)}(\mathbf{k},\omega) = \frac{i}{\hbar} (\tilde{G}^{(0)}(\mathbf{k},\omega))^2 \frac{1}{(2\pi)^4} \int d\mathbf{k}' \int d\omega' \\ [-2\tilde{U}(0)\tilde{G}^{(0)}(\mathbf{k}',\omega')e^{i\omega'0^+} \\ + \tilde{U}(\mathbf{k}-\mathbf{k}',\omega-\omega')\tilde{G}^{(0)}(\mathbf{k}',\omega')e^{i\omega'0^+}], \qquad (6.74)$$

which may be shown as follows: In order to Fourier-transform an expression of the form

$$F(x_1, x_2) = \int dx_3 \int dx_4 A(x_1 - x_3) B(x_3 - x_4) C(x_3 - x_4) D(x_4 - x_2) \quad (6.75)$$

we insert

$$A(x) = \frac{1}{2\pi} \int dk e^{ikx} \tilde{A}(k) \tag{6.76}$$

etc. This results in

$$F(x_1, x_2) = (2\pi)^{-4} \int dx_3 \int dx_4 \int dk_1 \int dk_2 \int dk_3 \int dk_4$$

$$\tilde{A}(k_1)\tilde{B}(k_2)\tilde{C}(k_3)\tilde{D}(k_4)$$

$$\exp i[(x_1 - x_3)k_1 + (x_3 - x_4)k_2 + (x_3 - x_4)k_3 + (x_4 - x_2)k_4]$$

$$= (2\pi)^{-2} \int dk_1 \int dk_2 \int dk_3 \int dk_4 \exp i(x_1k_1 - x_2k_4)$$

$$\delta(k_1 - k_2 - k_3)\delta(k_2 + k_3 - k_4)\tilde{A}(k_1)\tilde{B}(k_2)\tilde{C}(k_3)\tilde{D}(k_4)$$

= $(2\pi)^{-2}\int dk_1 \int dk_2 e^{i(x_1 - x_2)k_1}\tilde{A}(k_1)\tilde{B}(k_2)\tilde{C}(k_1 - k_2)\tilde{D}(k_1),$ (6.77)

which shows that the Fourier-transform of F is

$$\tilde{F}(k) = \frac{1}{2\pi} \int dk' \tilde{A}(k) \tilde{B}(k') \tilde{C}(k-k') \tilde{D}(k).$$
(6.78)

In a similar fashion we obtain from an expression of the form

$$G(x_1, x_2) = \int dx_3 \int dx_4 A(x_1 - x_4) B(x_3 - x_4) C(x_3 - x_3) D(x_4 - x_2) \quad (6.79)$$

that

$$\tilde{G}(k) = \frac{1}{2\pi} \int dk' \tilde{A}(k) \tilde{B}(0) \tilde{C}(k') \tilde{D}(k), \qquad (6.80)$$

since the integration over x_3 and x_4 introduces $\delta(k_2)$ and $\delta(k_1 + k_2 - k_4)$, respectively. Note that it is necessary to take into account the infinitesimal difference 0⁺ between the time arguments of the Green function, resulting in the multiplication of the function corresponding to \tilde{C} in the two expressions above by $\exp(i\omega'0^+)$. This guarantees the convergence of the subsequent contour integration in the ω' -plane.

We have thus verified (6.74), which yields the first-order correction to the Green function in terms of a product of two zero-order Green functions. In order to obtain the Hartree-Fock approximation treated in Chapter 4 we need to *shift* the poles of the Green function, and it is therefore necessary to sum an infinity of diagrams. Symbolically, we may write (6.74) as

$$\tilde{G}^{(1)} = \tilde{G}^{(0)} \Sigma \tilde{G}^{(0)}, \tag{6.81}$$

where Σ is a function of **k** and ω . If we now include terms like $\tilde{G}^{(0)}\Sigma\tilde{G}^{(0)}\Sigma\tilde{G}^{(0)}$ etc. we get a geometric series for \tilde{G} ,

$$\tilde{G} = \tilde{G}^{(0)} + \tilde{G}^{(0)} \Sigma \tilde{G}^{(0)} + \tilde{G}^{(0)} \Sigma \tilde{G}^{(0)} \Sigma \tilde{G}^{(0)} + \cdots, \qquad (6.82)$$

which may easily be summed. It is convenient to write the result in terms of the inverse of \tilde{G} :

$$(\tilde{G})^{-1} = (\tilde{G}^{(0)})^{-1} - \Sigma.$$
 (6.83)

The expression for Σ is according to (6.74) given by

$$\Sigma(\mathbf{k},\omega) = -\frac{i}{\hbar} \frac{1}{(2\pi)^4} \int d\mathbf{k}' \int d\omega' [2\tilde{U}(0)\tilde{G}^{(0)}(\mathbf{k}',\omega')e^{i\omega'0^+} - \tilde{U}(\mathbf{k}-\mathbf{k}',\omega-\omega')\tilde{G}^{(0)}(\mathbf{k}',\omega')e^{i\omega'0^+}.$$
 (6.84)

By carrying out the integration over ω' and using (6.13) we obtain

$$\hbar\Sigma(\mathbf{k}) = V_0 \frac{2}{(2\pi)^3} \int d\mathbf{k}' n_{\mathbf{k}'} - \frac{1}{(2\pi)^3} \int d\mathbf{k}' n_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'}.$$
 (6.85)

Since Σ is a real quantity and a function of k) only, it shifts the pole of the Green function along the real axis from ϵ_k to $E_k = \epsilon_k + \hbar \Sigma(k)$. The shifted energies are seen to be identical to the result (4.15), thus demonstrating the equivalence of the summation of selected diagrams with the Hartree-Fock approximation in a translationally invariant system.⁶

6.6 Feynman rules

We shall now discuss the Feynman rules for the contribution to the Green function to a given order in the interaction. Note that the content of the Feynman rules in general depends on the particular physical problem being considered. In a later chapter we discuss the Feynman rules that apply to the electron-phonon problem. In the present section we deal with a Fermi system of interacting particles. A particular example is an electron gas, in which the interaction between the particles is given by the Coulomb law, but the rules apply equally well to other types of interaction.

In performing the expansion of (6.52) and (6.53) we must remember that the operators appearing in these expressions are understood to be given in the interaction picture. It is convenient to write the interaction in the form

$$V(t_{1}) = \frac{1}{2} \sum_{\sigma_{1}\sigma_{2}} \int d\mathbf{x}_{1} \int d\mathbf{x}_{2} \int dt_{2} \psi^{\dagger}_{\sigma_{1}}(\mathbf{x}_{1}, t_{1}) \psi^{\dagger}_{\sigma_{2}}(\mathbf{x}_{2}, t_{2})$$
$$V(\mathbf{x}_{1}, \mathbf{x}_{2}) \delta(t_{1} - t_{2}) \psi_{\sigma_{2}}(\mathbf{x}_{2}, t_{2}) \psi_{\sigma_{1}}(\mathbf{x}_{1}, t_{1})$$
(6.86)

by introducing a delta-function in time. This allows us to write the subsequent expansion in a form where space and time variables occur in a symmetric fashion. For brevity we introduce $\int d1 \cdots = \sum_{\sigma_1} \int d\mathbf{x}_1 dt_1 \cdots$ and thus have

$$\int dt_1 V(t_1) = \frac{1}{2} \int d1 \int d2\psi^{\dagger}(1)\psi^{\dagger}(2)V(1,2)\psi(2)\psi(1).$$
(6.87)

Here V(1,2) denotes $V(\mathbf{x}_1, \mathbf{x}_2)\delta(t_1 - t_2)$, and we have suppressed the spin-dependence⁷ of the interaction.

$$V_{\sigma_{1'},\sigma_{2'},\sigma_{2},\sigma_{1}} = V_{0}\delta_{\sigma_{1'},\sigma_{1}}\delta_{\sigma_{2'},\sigma_{2}} + V_{1}\tau_{\sigma_{1'},\sigma_{1}}\cdot\tau_{\sigma_{2'},\sigma_{2}}$$
(6.88)

where τ denotes the three Pauli-matrices, while V_0 and V_1 are scalars in spin-space.

 $^{^{6}}$ This simple equivalence only holds for translationally invariant systems. For atoms, the diagrams yielding the Hartree-Fock approximation must be calculated selfconsistently, leading to equations of the form (4.18-19).

⁷The most general form of the interaction involves an interaction matrix-element $V_{\sigma_1',\sigma_2',\sigma_2,\sigma_1}$ depending on four spin-variables. In the absence of external fields the Hamiltonian must be invariant under rotations in spin space, implying that the interaction has the form

$$1' 2' + (1) + (1) + (2) + (2)$$

Figure 6.4: Closed fermion loop.

Now we start the expansion through second order in the interaction. First we work out $\langle S \rangle_0$:

$$< S>_{0} = 1 + \frac{1}{i\hbar} \frac{1}{2} \int d1' \int d2' V(1', 2') < T\{\psi^{\dagger}(1')\psi^{\dagger}(2')\psi(2')\psi(1')\}>_{0} \\ + \frac{1}{(i\hbar)^{2}} \frac{1}{2^{2}} \frac{1}{2!} \int d1' \int d2' \int d3' \int d4' V(1', 2')V(3', 4') \\ < T\{\psi^{\dagger}(1')\psi^{\dagger}(2')\psi(2')\psi(1')\psi^{\dagger}(3')\psi^{\dagger}(4')\psi(4')\psi(3')\}>_{0} (6.89)$$

A similar expansion of the numerator may be carried out to second order in the interaction. In Problem 42 we examine the terms generated in the process. We have already mentioned the cancellation of the terms in the denominator against the unlinked diagrams in the numerator. This persists in all orders of perturbation theory, thereby allowing a considerable simplification in collecting the *n*-th order terms. Furthermore, the factor $1/2^n$ arising from the interaction raised to the *n*-th power disappears, since each interaction line may be 'flipped'. The flipping simply corresponds to interchanging the names of two integration variables. The factor of 1/n! also disappears, since the interaction lines may be ordered in n! different ways, giving rise to diagrams that yield the same contribution, since their only difference comes from the names of the internal variables.

In a translationally invariant system it is advantageous to Fourier-transform the Green function according to

$$G(1,2) = G(1-2) = \int \frac{d\mathbf{k}d\omega}{(2\pi)^4} G(\mathbf{k},\omega) e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-i\omega(t_1-t_2)}.$$
 (6.90)

This implies that we must conserve four-momentum at each vertex, the reason being that the integration over internal variables yields

$$\int d\mathbf{x}_1 \int dt_1 e^{i(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3) \cdot \mathbf{x}_1} e^{-i(\omega_1 - \omega_2 + \omega_3)t_1} = (2\pi)^4 \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3) \delta(\omega_1 - \omega_2 + \omega_3).$$
(6.91)

Finally, the sign of the contribution must be discussed: Each power of the interaction yields $(1/i\hbar)$, corresponding to the factor $(1/i\hbar)^n$. When the
Green functions at zero temperature

Feynman rules are formulated in terms of non-interacting Green functions G_0 , of which there are 2n + 1 in a *n*-th order diagram, one obtains from each a factor of *i* or altogether i^{2n+1} . The *n*-th order contribution to the Green function therefore has the factor

$$-i\frac{1}{(i\hbar)^n}i^{2n+1} = \frac{i^n}{\hbar^n}.$$
 (6.92)

In addition it is necessary to consider separately those diagrams that contain a closed fermion line. Since such a diagram arises from the pairing illustrated on Fig. 6.4, it gives rise to an odd number of interchanges of the fermion operators. A given contribution to the *n*-th order diagram must therefore be multiplied by $(-1)^F$ where F is the number of closed fermion loops.

We are now in a position to formulate the Feynman rules in momentumfrequency space for the n-th order contribution to the Green function G:

- Draw all topologically different diagrams with n interaction lines and 2n + 1 oriented fermion lines, i. e. free-particle Green functions $G^{(0)}$.
- Associate an oriented four-momentum with each interaction line and fermion line and conserve four-momentum at each vertex.
- Associate with each fermion line the factor

$$G^{(0)}(\mathbf{k},\omega) = \frac{1}{\omega - \omega_k + i\eta \operatorname{sgn}(k - k_{\mathrm{F}})} \delta_{\sigma\sigma'}, \qquad (6.93)$$

where $\hbar\omega_k = \hbar^2 k^2/2m$ is the free-particle (kinetic) energy.

- Associate $V(\mathbf{q})$ with each interaction line.
- Sum over the internal spin variables and integrate over the internal momentum and frequency variables.
- Multiply by

$$\frac{i^n}{\hbar^n}(-1)^F \frac{1}{(2\pi)^{4n}}.$$
(6.94)

• Interpret

as $e^{i\omega\eta}G^{(0)}(\mathbf{k},\omega)$.

$$\sim$$
 \vec{k}, ω \vec{k}, ω



Figure 6.5: Second order contributions to the reducible self-energy.

6.7 Dyson equations

It is evident from the previous discussion that the Green function may be written in the form

$$G(\mathbf{k},\omega) = G^{(0)}(\mathbf{k},\omega) + G^{(0)}(\mathbf{k},\omega)\Sigma^{\text{red}}(\mathbf{k},\omega)G^{(0)}(\mathbf{k},\omega).$$
(6.95)

The quantity $\Sigma^{\text{red}}(\mathbf{k}, \omega)$ is called the reducible self-energy. Its diagrammatic expansion is identical with that of G, except for the absence of the zero'th order term $G^{(0)}$ and the removal of the two external lines on the remaining diagrams.

In Fig. 6.5 we illustrate two second order contributions to $\Sigma^{red}(\mathbf{k},\omega)$. They are characterized by an important difference. The diagram (a) may be cut into two pieces by the cutting of a single fermion line. Such a diagram is called reducible. The diagram (b) does not, however, fall into two separate pieces by the cutting of a single fermion line. This property is named *irreducibility*. We shall define the *irreducible* self-energy $\Sigma(\mathbf{k},\omega)$ as the sum of all those contributions to $\Sigma^{red}(\mathbf{k},\omega)$, which cannot be cut into two pieces by the cutting of a single line. One therefore has

$$G(\mathbf{k},\omega) = G^{(0)}(\mathbf{k},\omega) + G^{(0)}(\mathbf{k},\omega)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega), \qquad (6.96)$$

as may be verified by iteration. The equation (6.96) is called the Dyson equation. By determining $\Sigma(\mathbf{k},\omega)$ in some approximation one therefore sums up infinitely many diagrams in the expansion of $G(\mathbf{k},\omega)$. It is evidently necessary to consider $\Sigma(\mathbf{k},\omega)$ rather than $\Sigma^{\text{red}}(\mathbf{k},\omega)$ in order to obtain a shift in the position of the poles of the Green function. This may be seen by writing (6.96) in the form

$$(G(\mathbf{k},\omega))^{-1} = (G^{(0)}(\mathbf{k},\omega))^{-1} - \Sigma(\mathbf{k},\omega).$$
(6.97)

In Section 6.5.1 we demonstrated this explicitly in carrying out the Hartree-Fock approximation.

7 Green functions at finite temperature

The operator $\exp(-iHt/\hbar)$ that describes the development in time of the Schrödinger states clearly resembles the operator $\exp(-H/kT)$, which enters the statistical average of a physical quantity belonging to a many-particle system at temperature T. This simple observation forms the basis for the introduction of temperature Green functions. Since temperature corresponds to imaginary time, one is led to define creation and annihilation operators that depend on the variable τ according to

$$\psi_{\sigma}(\mathbf{x},\tau) = e^{K\tau/\hbar} \psi_{\sigma}(\mathbf{x}) e^{-K\tau/\hbar}$$
(7.1)

and

$$\psi_{\sigma}^{\dagger}(\mathbf{x},\tau) = e^{K\tau/\hbar} \psi_{\sigma}^{\dagger}(\mathbf{x}) e^{-K\tau/\hbar}.$$
(7.2)

Here K equals the Hamiltonian H minus the chemical potential μ times the number operator N,

$$K = H - \mu N, \tag{7.3}$$

since we shall perform the statistical averaging in the grand canonical ensemble in which the particle number is varying. The variable τ has thus dimension of time. It should be noted that $\psi^{\dagger}_{\sigma}(\mathbf{x},\tau)$ is *not* the Hermitian conjugate of $\psi_{\sigma}(\mathbf{x},\tau)$, because τ is taken to be a real variable. For a general interacting system, the single-particle temperature Green function G is defined by

$$G_{\sigma\sigma'}(\mathbf{x},\tau;\mathbf{x}',\tau') = - \langle T_{\tau}\{\psi_{\sigma}(\mathbf{x},\tau)\psi_{\sigma'}^{\dagger}(\mathbf{x}',\tau')\}\rangle \rangle.$$
(7.4)

Here $< \cdots >$ denotes a statistical average over the grand-canonical ensemble,

$$\langle A \rangle = \frac{\operatorname{Tr}(e^{-\beta K}A)}{\operatorname{Tr}e^{-\beta K}} = e^{\beta \Omega} \operatorname{Tr}(e^{-\beta K}A),$$
 (7.5)

with Ω being the grand thermodynamic potential defined by

$$e^{-\beta\Omega} = \mathrm{Tr}e^{-\beta K}.$$
 (7.6)

We shall only treat the case when the particles are fermions. The tau-ordering operator T_{τ} is in the fermion case defined by

$$T_{\tau}\{A(\tau_1)B(\tau_2)C(\tau_3)\cdots\} = (-1)^p C\{A(\tau_1)B(\tau_2)C(\tau_3)\cdots\},$$
 (7.7)

where C is an operator which orders the fermion operators $A(\tau_1)B(\tau_2)C(\tau_3)\cdots$ chronologically with earlier 'times' to the right, while p is the number of interchanges needed to achieve this chronological ordering. In the boson case, the tau-ordering operator is given by the same expression as (7.7) except the factor of $(-1)^p$.

7.1 Translational invariance

Since we shall be dealing with systems that are translationally invariant in both space and time, it is convenient to introduce operators $c_{\mathbf{k},\sigma}$ and $c_{\mathbf{k},\sigma}^{\dagger}$ that remove and add, respectively, a particle in a definite momentum and spin state \mathbf{k}, σ . This is accomplished by the transformation

$$\psi_{\sigma}(\mathbf{x},\tau) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k},\sigma}(\tau).$$
(7.8)

Then

$$G_{\sigma\sigma'}(\mathbf{x},\tau;\mathbf{x}',\tau') = -\frac{1}{V} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} e^{-i\mathbf{k}'\cdot\mathbf{x}'} e^{i\mathbf{k}\cdot\mathbf{x}} < T_{\tau} \{ c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k}',\sigma'}^{\dagger}(\tau') \} > .$$
(7.9)

Since the system is translationally invariant in space and time, $G_{\sigma\sigma'}(\mathbf{x}, \tau; \mathbf{x}', \tau')$ is a function of only the relative coordinate $\mathbf{x} - \mathbf{x}'$, and of $\tau - \tau'$, implying that the terms in the sum with $\mathbf{k}' \neq \mathbf{k}$ are zero. We thus obtain

$$G_{\sigma\sigma'}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} G_{\sigma\sigma'}(\mathbf{k},\tau-\tau')$$
(7.10)

where

$$G_{\sigma\sigma'}(\mathbf{k},\tau) = - \langle T_{\tau} \{ c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma'}^{\dagger}(0) \} \rangle .$$
(7.11)

In the absence of spin-dependent forces G is proportional to the unit-matrix in spin-space,

$$G_{\sigma\sigma'}(\mathbf{k},\tau) = \delta_{\sigma\sigma'}G(\mathbf{k},\tau). \tag{7.12}$$

Each τ -variable ranges from 0 to $\hbar\beta$, and since the Green function G only depends on the difference between its two τ -variables, it is sufficient to consider the Green function in the interval

$$-\hbar\beta \le \tau < \hbar\beta$$
 or $-\frac{\hbar}{kT} \le \tau < \frac{\hbar}{kT}$. (7.13)

The Green function may therefore be expanded in a Fourier-series with Fouriercoefficients given by

$$G(\mathbf{k},\omega_n) = \frac{1}{2} \int_{-\hbar\beta}^{\hbar\beta} d\tau e^{i\omega_n \tau} G(\mathbf{k},\tau).$$
(7.14)

In the fermion case the Green function has an important symmetry property with respect to finite translations in τ -space,

$$G(\mathbf{k}, \tau + \hbar\beta) = -G(\mathbf{k}, \tau). \tag{7.15}$$

Green functions at finite temperature

In order to prove (7.15) we shall assume for definiteness that $0 > \tau > -\hbar\beta$. Then

$$\exp(-\beta\Omega)G(\mathbf{k},\tau) = \operatorname{Tr}(c_{\mathbf{k}}^{\dagger}(0)e^{K\tau/\hbar}c_{\mathbf{k}}(0)e^{-K\tau/\hbar}e^{-\beta K}).$$
(7.16)

Likewise we have

$$-\exp(-\beta\Omega)G(\mathbf{k},\tau+\hbar\beta) = \operatorname{Tr}(e^{-\beta K}e^{K(\tau+\hbar\beta)/\hbar}c_{\mathbf{k}}(0)e^{-K(\tau+\hbar\beta)/\hbar}c_{\mathbf{k}}^{\dagger}(0)).$$
(7.17)

Using the cyclic invariance of the trace, the right hand side of (7.16) is seen to be equal to the right hand side of (7.17), resulting in (7.15).

For bosons the minus-sign in (7.15) is replaced by a plus sign. In both cases we therefore have

$$G(\mathbf{k},\tau-\hbar\beta) = G(\mathbf{k},\tau+\hbar\beta). \tag{7.18}$$

The Fourier-expansion in the fermion case is thus

$$G(\mathbf{k},\tau) = \frac{1}{\beta\hbar} \sum_{n} e^{-i\omega_{n}\tau} G(\mathbf{k},\omega_{n}), \qquad (7.19)$$

where the Matsubara frequencies ω_n are given by

$$\omega_n = (2n+1)\frac{\pi}{\beta\hbar}, \quad n = 0, \pm 1, \pm 2, \pm 3 \cdots.$$
(7.20)

The symmetry property (7.15) together with the relation $\exp(-i\omega_n \hbar\beta) = -1$ allows one to write the Fourier-coefficients $G(\mathbf{k}, \omega_n)$ as

$$G(\mathbf{k},\omega_n) = \int_0^{\hbar\beta} d\tau e^{i\omega_n\tau} G(\mathbf{k},\tau).$$
(7.21)

The corresponding expansion in the case of bosons is identical to (7.14) and (7.19), while (7.20) is replaced by the even-numbered frequencies

$$\omega_n = 2n \frac{\pi}{\beta \hbar}, \quad n = 0, \pm 1, \pm 2, \pm 3 \cdots$$
 (7.22)

7.2 Physical observables

In close analogy with the zero-temperature case discussed in Chapter 6, we may verify that the Green function in a translationally invariant system yields information on the mean (thermal) occupation of the single-particle states \mathbf{k} . The mean occupation number $n_{\mathbf{k}}$ of the state \mathbf{k} is given by

$$n_{\mathbf{k}} = \langle c_{\mathbf{k},\sigma}^{\dagger}(0)c_{\mathbf{k},\sigma}(0) \rangle = G(\mathbf{k},\tau \to 0^{-}) = \frac{1}{\beta\hbar} \sum_{n} e^{i\omega_{n}\eta} G(\mathbf{k},\omega_{n}).$$
(7.23)

Here η denotes a positive infinitesimal, $\eta = 0^+$.

The total number of particles N is therefore

$$N = 2\sum_{\mathbf{k}} n_{\mathbf{k}} = \frac{2V}{(2\pi)^3 \beta \hbar} \int d\mathbf{k} \sum_{n} e^{i\omega_n \eta} G(\mathbf{k}, \omega_n).$$
(7.24)

In general, the thermal average of an arbitrary single-particle quantity (such as the spin density or the current density) may be related to the single-particle temperature Green function, because the latter involves one creation and one annihilation operator.

In analogy with the zero-temperature case it is also possible to express the internal energy in terms of the single-particle temperature Green function, as we shall now demonstrate. For definiteness we assume that the Hamiltonian has the form

$$H = H_0 + H'$$
(7.25)

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(7.26)

represents the kinetic energy, while

$$H' = \frac{1}{2V} \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}', \sigma, \sigma'} V_{\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q}, \sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}, \sigma'} c_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}$$
(7.27)

is the interaction energy. The Fourier-transform of the (spin-independent) interaction potential is denoted by $V_{\mathbf{q}}$.

By working out the τ -derivative of the operator $c_{\mathbf{k}}(\tau)$ given by

$$c_{\mathbf{k}}(\tau) = e^{K\tau/\hbar} c_{\mathbf{k}}(0) e^{-K\tau/\hbar}$$
(7.28)

we obtain its equation of motion

$$-\hbar \frac{\partial}{\partial \tau} c_{\mathbf{k}}(\tau) = [c_{\mathbf{k}}(\tau), K] = e^{K\tau/\hbar} [c_{\mathbf{k}}(0), K] e^{-K\tau/\hbar}.$$
 (7.29)

In working out the equation of motion we may thus first determine the commutator $[c_k, K]$, where the operators are both Schrödinger operators.

The internal energy U, which is the thermal average of the Hamiltonian, is obtained from

$$U = \langle H \rangle = \langle K \rangle + \mu \langle N \rangle.$$
 (7.30)

Here we may use the equation of motion for the field operators to determine $\langle K \rangle$, in precisely the same manner as we obtained $\langle H \rangle$ at zero temperature,

with ϵ_k being replaced by $\epsilon_k - \mu$, while ω is replaced by $i\omega_n$. The result is seen to be

$$U = \frac{V}{(2\pi)^3 \beta \hbar} \int d\mathbf{k} \sum_{n} e^{i\omega_n \eta} (\mu + \epsilon_k + i\hbar\omega_n) G(\mathbf{k}, \omega_n).$$
(7.31)

The knowledge of the single-particle Green-function $G(\mathbf{k}, \omega_n)$ thus allows one to determine the internal energy U, by carrying out the integrations over wave vector and the sum over Matsubara frequencies in (7.31).

7.3 Green functions for free fermions

The Green function $G(\mathbf{k}, \tau)$ for free fermions is

$$G_{\sigma\sigma'}(\mathbf{k},\tau) = - \langle T_{\tau} \{ c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}\sigma'}^{\dagger}(0) \} \rangle_{0}, \qquad (7.32)$$

where the thermal average $\langle \cdots \rangle_0$ involves the free-particle Hamiltonian H_0 given by

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (7.33)$$

where $\epsilon_k = \hbar^2 k^2 / 2m$. The operator $K = K_0$ is thus

$$K_0 = \sum_{\mathbf{k},\sigma} (\epsilon_k - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (7.34)$$

The use of the equation of motion (7.29) with (7.34) results in

$$-\hbar \frac{\partial}{\partial \tau} c_{\mathbf{k}} = (\epsilon_k - \mu) c_{\mathbf{k}}(\tau)$$
(7.35)

with the solution

$$c_{\mathbf{k}}(\tau) = e^{-(\epsilon_{\mathbf{k}} - \mu)\tau/\hbar} c_{\mathbf{k}}(0).$$
(7.36)

This allows us to determine the free-particle Green function $G(\mathbf{k}, \tau)$. By considering first $\tau > 0$ and subsequently $\tau < 0$, we obtain the result

$$G(\mathbf{k},\tau) = -[(1-n_{\mathbf{k}})\Theta(\tau) - n_{\mathbf{k}}\Theta(-\tau)]e^{-(\epsilon_{\mathbf{k}}-\mu)\tau/\hbar}, \qquad (7.37)$$

where $\Theta(\tau) = 1$ if $\tau > 0$ and $\Theta(\tau) = 0$ if $\tau < 0$. Here $n_{\mathbf{k}}$ are mean occupation numbers for the non-interacting system, given by the well-known expression from equilibrium statistical mechanics

$$n_{\mathbf{k}} = \langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \rangle_{0} = \frac{1}{e^{(\epsilon_{\mathbf{k}} - \mu)\beta} + 1}.$$
 (7.38)

The Fourier-coefficients are found by inserting (7.37) into (7.21) and integrating over τ ,

$$G(\mathbf{k},\omega_n) = -\int_0^{\beta\hbar} d\tau (1-n_{\mathbf{k}}) e^{-(\epsilon_k-\mu)\tau/\hbar} e^{i\omega_n\tau}.$$
 (7.39)

The Fourier-transform $G(\mathbf{k}, \omega_n)$ thus becomes

$$G(\mathbf{k},\omega_n) = \frac{1}{i\omega_n - (\epsilon_k - \mu)/\hbar}.$$
(7.40)

In the following 1 stands for $(\mathbf{x}_1, \tau_1, \sigma_1)$ and $\int d1 \cdots$ for $\sum_{\sigma_1} \int d\mathbf{x}_1 \int d\tau_1 \cdots$. We shall introduce an interaction picture in which operators develop according to

$$A_I(\tau) = e^{K_0 \tau/\hbar} A_S e^{-K_0 \tau/\hbar}.$$
(7.41)

The Heisenberg operator $A_H(\tau)$ is then related to the operator in the interaction picture by

$$A_H(\tau) = e^{K\tau/\hbar} e^{-K_0\tau/\hbar} A_I(\tau) e^{K_0\tau/\hbar} e^{-K\tau/\hbar}.$$
(7.42)

By introducing the operator $U(\tau_1, \tau_2)$ by the definition

$$U(\tau_1, \tau_2) = e^{K_0 \tau_1/\hbar} e^{-K \tau_1/\hbar} e^{K \tau_2/\hbar} e^{-K_0 \tau_2/\hbar}$$
(7.43)

we may write (7.42) in the form

$$A_H(\tau) = U(0,\tau)A_I(\tau)U(\tau,0).$$
 (7.44)

The operator U satisfies the condition

$$U(0,0) = 1. \tag{7.45}$$

and we have

$$U(\tau) \equiv U(\tau, 0) = e^{K_0 \tau/\hbar} e^{-K\tau/\hbar}.$$
(7.46)

It follows from (7.43) and (7.46) that $U(0, \tau) = U^{-1}(\tau, 0)$. By differentiating (7.46) one finds that $U(\tau)$ satisfies the differential equation

$$-\hbar \frac{\partial U}{\partial \tau} = K_1(\tau) U(\tau), \qquad (7.47)$$

where

$$K_1(\tau) = e^{K_0 \tau / \hbar} K_1 e^{-K_0 \tau / \hbar}, \qquad (7.48)$$

with $K_1 = K - K_0$ being the interaction part of the Hamiltonian. This corresponds to (2.50) in the zero-temperature case. With the boundary condition U(0) = 1, the integrated form of the differential equation (7.47) becomes

$$U(\tau) = 1 - \frac{1}{\hbar} \int_0^{\tau} d\tau' K_1(\tau') U(\tau')$$
(7.49)

The integral equation (7.49) may be iterated, just as in the zero temperature case, and the subsequent development closely parallels that of chapter 6. Note that the statistical operator $\exp(-\beta K)$ is given by

$$e^{-\beta K} = e^{-\beta K_0} U(\hbar\beta, 0). \tag{7.50}$$

We may therefore take over the final result, which is an expression for the Green function as an infinite series in the interaction part of the Hamiltonian, provided we integrate over τ from 0 to $\hbar\beta$. The Green function G(1,2) thus becomes

$$G(1,2) = -\sum_{n=0}^{\infty} (-\frac{1}{\hbar})^n \frac{1}{n!} \int_0^{\beta\hbar} d\tau_1' \cdots \int_0^{\beta\hbar} d\tau_n' \frac{\langle T_\tau \{K_1(\tau_1') \cdots K_1(\tau_n')\psi(1)\psi^{\dagger}(2)\} \rangle_0}{\langle S \rangle_0}.$$
(7.51)

The operators are written in the interaction picture, and $\langle \cdots \rangle_0$ is the usual thermal average for the non-interacting system. The operator S is $S = U(\hbar\beta, 0)$, and the denominator $\langle S \rangle_0$ is given by the expansion

$$< S >_{0} = \sum_{n=0}^{\infty} (-\frac{1}{\hbar})^{n} \frac{1}{n!} \int_{0}^{\beta\hbar} d\tau_{1}^{'} \cdots \int_{0}^{\beta\hbar} d\tau_{n}^{'} < T_{\tau} \{K_{1}(\tau_{1}^{'}) \cdots K_{1}(\tau_{n}^{'})\} >_{0} .$$
(7.52)

The result (7.51) forms the starting point for the diagrammatic perturbation theory.

7.4 Diagrams

In general, the Green function cannot be determined exactly. Instead, one does perturbation theory and sums selected terms to infinite order by expanding the numerator and denominator of (7.51) in powers of K_1 . This procedure generates time-ordered products of strings of field-operators, corresponding to *n*-particle Green functions for the non-interacting system. In analogy with the zero-temperature case we shall therefore need to consider many-particle Green functions $G_n^{(0)}$ for the non-interacting system,

$$G_n^{(0)}(1\cdots n; n'\cdots 1') = (-1)^n < T_\tau\{\psi(1)\cdots\psi(n)\psi^{\dagger}(n')\cdots\psi^{\dagger}(1')\} >_0.$$
(7.53)

For short we have written n for the argument (\mathbf{x}_n, τ_n) .

First we may derive a differential equation for $G_1^{(0)}$, the one-particle Green function for the non-interacting system. In analogy with the zero-temperature case we obtain

$$G_1^{(0)}(1,1') = (-\hbar \frac{\partial}{\partial \tau_1} - K_0(1))^{-1} \delta(1-1').$$
(7.54)

The equation of motion for the two-particle Green function $G_2^{(0)}(1,2;2',1')$ leads to

$$G_2^{(0)}(1,2;2',1') = \begin{vmatrix} G_1^{(0)}(1,1') & G_1^{(0)}(1,2') \\ G_1^{(0)}(2,1') & G_1^{(0)}(2,2'), \end{vmatrix}$$
(7.55)

just as in chapter 6.

These results are readily generalized to a n-particle Green function, which is given by

$$G_{n}^{(0)}(1,\cdots n;n'\cdots 1') = \begin{vmatrix} G_{1}^{(0)}(1,1') & G_{1}^{(0)}(1,2') & \cdots & G_{1}^{(0)}(1,n') \\ G_{1}^{(0)}(2,1') & G_{1}^{(0)}(2,2') & \cdots & G_{1}^{(0)}(2,n') \\ \cdots & \cdots & \cdots & \cdots \\ G_{1}^{(0)}(n,1') & G_{1}^{(0)}(n,2') & \cdots & G_{1}^{(0)}(n,n') \end{vmatrix}$$
(7.56)

The result (7.56) is *Wick's theorem* at finite temperature. It forms the basis for the diagrammatic expansion of the Green function given by (7.51).

7.4.1 Feynman rules

The Feynman rules for the contribution to the Green function to a given order in the interaction are obtained in the same manner as the zero-temperature rules of chapter 6. The conservation of frequency at each vertex follows from the expansion in Fourier series and subsequent integration over τ . In analogy to (6.88) we obtain

$$\int_{0}^{\beta\hbar} d\tau_1 e^{-i(\omega_{n_1} - \omega_{n_2} + \omega_{n_3})\tau_1} = \beta\hbar\delta_{\omega_{n_1},\omega_{n_2} - \omega_{n_3}}.$$
 (7.57)

• Draw all topologically different diagrams with n interaction lines and 2n + 1 oriented free-particle Green functions $G^{(0)}$.

- Associate an oriented 'four-momentum' (\mathbf{k}, ω_n) with each interaction line and conserve four-momentum at each vertex.
- Associate the factor

$$G^{(0)}(\mathbf{k},\omega_n) = \frac{1}{i\omega_n - \xi_k/\hbar} \delta_{\sigma,\sigma'}$$
(7.58)

with each particle line, $\xi_k = \hbar^2 k^2/2m - \mu$ being the free-particle (kinetic) energy minus the chemical potential μ .

- Associate $V_{\mathbf{q}}$ with each interaction line.
- Sum over spin and frequency and integrate over momentum variables.
- Multiply by

$$\frac{1}{(-\beta\hbar^2)^n}(-1)^F \frac{1}{(2\pi)^{3n}}.$$
(7.59)

• Interpret

$$\sim k, \omega_n \quad \vec{k}, \omega_n$$

as $e^{i\omega_n\eta}G^{(0)}(\mathbf{k},\omega_n)$.

We define the irreducible self-energy $\Sigma(\mathbf{k}, \omega_n)$ as the sum of all those contributions to the self-energy which cannot be cut into two pieces by the cutting of a single line. One therefore has

$$G(\mathbf{k},\omega_n) = G^{(0)}(\mathbf{k},\omega_n) + G^{(0)}(\mathbf{k},\omega_n)\Sigma(\mathbf{k},\omega_n)G(\mathbf{k},\omega_n),$$
(7.60)

as may be seen by iteration. The equation (7.60) is the Dyson equation. It may also be written in the form

$$G(\mathbf{k},\omega_n)^{-1} = G^{(0)}(\mathbf{k},\omega_n)^{-1} - \Sigma(\mathbf{k},\omega_n), \qquad (7.61)$$

as in the case of zero temperature.

7.5 Retarded and advanced Green functions

It is often useful to consider *retarded* or *advanced* Green functions rather than time-ordered ones such as (7.11). The retarded Green function corresponding to (7.11) is (we suppress spin labels)

$$G^{\text{ret}}(\mathbf{k},t) = -i\Theta(t) < (c_{\mathbf{k}}(t)c_{\mathbf{k}}^{\dagger}(0) + c_{\mathbf{k}}^{\dagger}(0)c_{\mathbf{k}}(t)) >,$$
(7.62)

where the field operators now depend on real time t according to the Heisenberg equation of motion,

$$c_{\mathbf{k}}(t) = e^{iKt/\hbar} c_{\mathbf{k}}(0) e^{-iKt/\hbar}.$$
(7.63)

As usual $\Theta(t)$ is 1 if t > 0, and zero if t < 0. The thermal average involves as before the grand canonical ensemble, cf. (7.5). The advanced function is similarly defined by

$$G^{\mathrm{adv}}(\mathbf{k},t) = i\Theta(-t) < (c_{\mathbf{k}}(t)c_{\mathbf{k}}^{\dagger}(0) + c_{\mathbf{k}}^{\dagger}(0)c_{\mathbf{k}}(t)) > .$$
(7.64)

The connection between these different Green functions may be elucidated by introducing a *spectral representation*. This is achieved by inserting into the expression for G a unit operator $\hat{1}$ defined by

$$\hat{1} = \sum_{m} |m\rangle \langle m|. \tag{7.65}$$

Here $|m\rangle$ denotes a complete set of states¹, which are eigenstates for K,

$$K|m\rangle = E_m|m\rangle. \tag{7.66}$$

Since

$$\langle n|c_{\mathbf{k}}(t)|m\rangle = e^{i(E_n - E_m)t/\hbar} \langle n|c_{\mathbf{k}}(0)|m\rangle$$
(7.67)

we obtain

$$G^{\text{ret}}(\mathbf{k},t) = -i\Theta(t)e^{\beta\Omega}\sum_{n,m} e^{-\beta E_n} (e^{i(E_n - E_m)t/\hbar} |\langle n|c_{\mathbf{k}}(0)|n\rangle|^2 + e^{-i(E_n - E_m)t/\hbar} |\langle m|c_{\mathbf{k}}(0)|n\rangle|^2).$$
(7.68)

By interchanging the summation variables n and m in the second term we obtain

$$G^{\text{ret}}(\mathbf{k},t) = -i\Theta(t)e^{\beta\Omega}\sum_{n,m} (e^{-\beta E_n} + e^{-\beta E_m})e^{i(E_n - E_m)t/\hbar} |\langle n|c_{\mathbf{k}}(0)|m\rangle|^2$$
(7.69)

with the Fourier-transform

$$G^{\text{ret}}(\mathbf{k},\omega) = -ie^{\beta\Omega} \sum_{n,m} \int_{0}^{\infty} dt e^{i(E_{n}-E_{m})t/\hbar + i\omega t - \eta t}$$

$$(e^{-\beta E_{n}} + e^{-\beta E_{m}})|\langle n|c_{\mathbf{k}}(0)|m\rangle|^{2}$$

$$= e^{\beta\Omega} \sum_{n,m} (e^{-\beta E_{n}} + e^{-\beta E_{m}})$$

$$|\langle n|c_{\mathbf{k}}(0)|m\rangle|^{2} \frac{1}{\omega + (E_{n}-E_{m})/\hbar + i\eta}.$$
(7.70)

¹Note that the set includes states with differing total number of particles, as is necessary for a quantity such as $\langle m|c_k(0)|n\rangle$ to be non-zero.

Green functions at finite temperature

In defining the Fourier-transform we have multiplied the integrand by $\exp(-\eta t)$, where η is a positive infinitesimal in order to ensure convergence at large times. The result of this is that the Fourier-transform becomes an analytic function of ω in the upper half of the complex ω -plane. This analyticity in the upper half plane is the characteristic of retarded functions, which are used for describing the causal response to external disturbances. Similarly, the advanced functions are analytic in the lower half of the complex ω -plane.

Now let us compare the expression (7.70) with the corresponding one for the tau-ordered Green function

$$G(\mathbf{k},\tau) = - \langle T_{\tau} \{ c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^{\dagger}(0) \} \rangle .$$
(7.71)

By inserting the unit operator in the same fashion as before we obtain for $\tau > 0$ that

$$G(\mathbf{k},\tau) = -e^{\beta\Omega} \sum_{n,m} e^{-\beta E_n} e^{(E_n - E_m)\tau/\hbar} |\langle n|c_{\mathbf{k}}(0)|m\rangle|^2.$$
(7.72)

The Fourier-coefficient in the Fourier-series expansion is

$$G(\mathbf{k}, \omega_n) = \int_0^{\beta\hbar} d\tau e^{i\omega_n \tau} G(\mathbf{k}, \tau)$$

= $e^{\beta\Omega} \sum_{n,m} (e^{-\beta E_n} + e^{-\beta E_m})$
 $|\langle n|c_{\mathbf{k}}(0)|m \rangle|^2 \frac{1}{i\omega_n + (E_n - E_m)/\hbar}.$ (7.73)

From this we conclude that the expression for the retarded Green function may be obtained from the tau-ordered one by replacing $i\omega_n$ with $\omega + i\eta$. This procedure is called *analytic continuation*. It implies that the retarded Green function may be obtained as a function of the continuous, real frequency variable ω from the knowledge of the Matsubara Green function on the discrete set of points $i\omega_n$ on the imaginary axis in the complex frequency plane. Similarly, the advanced Green function is obtained by replacing $i\omega_n$ with $\omega - i\eta$. From this it follows that the imaginary part of G^{ret} is equal to minus the imaginary part of the advanced one G^{adv} , while their real parts are equal to each other. One defines the so-called spectral density $A(\mathbf{k}, \omega)$ as

$$A(\mathbf{k},\omega) = \frac{1}{i} (G^{\mathrm{adv}}(\mathbf{k},\omega) - G^{\mathrm{ret}}(\mathbf{k},\omega)).$$
(7.74)

By taking the imaginary parts of the retarded and advanced Green functions with the help of the identity

$$\frac{1}{x+i\eta} = \frac{P}{x} - i\pi\delta(x),\tag{7.75}$$

we obtain the explicit expression for the spectral density

$$A(\mathbf{k},\omega) = 2\pi e^{\beta\Omega} \sum_{n,m} (e^{-\beta E_n} + e^{-\beta E_m}) |\langle n|c_{\mathbf{k}}(0)|m\rangle|^2 \delta(\hbar\omega + E_n - E_m).$$
(7.76)

By integrating the spectral density (7.76) over frequency one obtains that

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(\mathbf{k}, \omega) = e^{\beta\Omega} \sum_{n,m} (e^{-\beta E_n} + e^{-\beta E_m}) |\langle n|c_{\mathbf{k}}(0)|m\rangle|^2$$
$$= e^{\beta\Omega} \sum_{n,m} e^{-\beta E_n} (\langle n|c_{\mathbf{k}}(0)|m\rangle \langle m|c_{\mathbf{k}}^{\dagger}(0)|n\rangle + \langle n|c_{\mathbf{k}}^{\dagger}(0)|m\rangle \langle m|c_{\mathbf{k}}(0)|n\rangle).$$
(7.77)

The use of the commutation rule $c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}} + c_{\mathbf{k}}c_{\mathbf{k}}^{\dagger} = 1$ then leads to the sum-rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(\mathbf{k}, \omega) = 1.$$
 (7.78)

The spectral density has another important property, namely that

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(\mathbf{k}, \omega) \frac{1}{e^{\beta \hbar \omega} + 1} = \langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \rangle \equiv n_{\mathbf{k}}.$$
 (7.79)

This is demonstrated by writing out the expression for the mean occupation number, $n_{\mathbf{k}}$,

$$n_{\mathbf{k}} = e^{\beta\Omega} \operatorname{Tr}(e^{-\beta K} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}})$$

$$= e^{\beta\Omega} \sum_{n,m} \langle m | e^{-\beta K} c_{\mathbf{k}}^{\dagger}(0) | n \rangle \langle n | c_{\mathbf{k}}(0) | m \rangle$$

$$= e^{\beta\Omega} \sum_{n,m} e^{-\beta E_{m}} \langle m | c_{\mathbf{k}}^{\dagger}(0) | n \rangle \langle n | c_{\mathbf{k}}(0) | m \rangle.$$
(7.80)

The use of the identity

$$(e^{-\beta E_n} + e^{-\beta E_m})\delta(\hbar\omega + E_n - E_m) = e^{-\beta E_m}(e^{\beta\hbar\omega} + 1)\delta(\hbar\omega + E_n - E_m)$$
(7.81)

in (7.76) then proves the property (7.79). For non-interacting particles, $A(\mathbf{k}, \omega)$ is given by the delta-function

$$A(\mathbf{k},\omega) = 2\pi\delta(\omega - (\epsilon_k - \mu)/\hbar). \tag{7.82}$$

When this is inserted into the sum-rule (7.79), $n_{\mathbf{k}}$ becomes equal to the Fermi-function,

$$n_{\mathbf{k}} = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)}+1},\tag{7.83}$$

as one would expect.



Figure 7.1: Contour for the evaluation of Matsubara sum.

7.6 Matsubara sums

In this last subsection we shall discuss the technique involved in summing over the discrete Matsubara frequencies. The Hartree-Fock contribution to the selfenergy is

$$\Sigma_{\mathbf{H}-\mathbf{F}}(\mathbf{k},\omega_{n}) = \frac{-1}{\hbar^{2}\beta} \frac{1}{(2\pi)^{3}} \int d\mathbf{k}' \sum_{n'} (2V_{\mathbf{0}} - V_{\mathbf{k'}-\mathbf{k}}) G^{(0)}(\mathbf{k}',\omega_{n'}) e^{i\omega_{n'}\eta}.$$
 (7.84)

Since the Fourier-transform of the interaction is frequency-independent, the summation over Matsubara frequencies reduces to the calculation of the sum F(a) given by

$$F(a) = \sum_{n} e^{i\omega_n \eta} \frac{1}{i\omega_n - a},$$
(7.85)

where a depends on the momentum variables but not on n. Such a sum may be carried out by converting it to a contour integral involving a function f(z), which is defined such that it has simple, first-order poles (with unit residue) at the Matsubara-frequencies ω_n :

$$f(z) = -\frac{\beta\hbar}{e^{\beta\hbar z} + 1}.$$
(7.86)

The function f is clearly infinite when $z = i\omega_n = i\pi(2n+1)/\beta\hbar$ and has unit residue.

We thus consider the contour integral

$$I_C = -\frac{1}{2\pi i} \int_C dz e^{z\eta} \frac{1}{z-a} \frac{\beta\hbar}{e^{\beta\hbar z}+1}.$$
 (7.87)

If we choose the contour C as indicated in Fig. 7.1, the contour-integral I_C is zero, since the contributions from the arcs vanish for Rez < 0 because of

 $\exp(\eta z)$ and for $\operatorname{Re} z > 0$ because of $(\exp(\beta \hbar z) + 1)^{-1}$. The two parts of the contour named C_1 and C_2 together yield the sum F(a). Therefore the integral around the pole at z = a along the part of the contour named C_3 must yield -F(a). Thus we have

$$F(a) = \frac{1}{2\pi i} \int_{C_3} dz e^{z\eta} \frac{1}{z-a} \frac{\beta\hbar}{e^{\beta\hbar z}+1} = \frac{\beta\hbar}{e^{\beta\hbar a}+1}.$$
 (7.88)

Now, since $a = \epsilon_k - \mu$ we recover the Fermi distribution function n_k and the Hartree-Fock expression for the self-energy becomes

$$\hbar \Sigma_{\rm H-F}(\mathbf{k}) = \frac{1}{(2\pi)^3} \int d\mathbf{k}' (2V_0 - V_{\mathbf{k}'-\mathbf{k}}) n_{\mathbf{k}'}.$$
 (7.89)

At T = 0 this reduces to our previous result from Chapter 6.

8 Electron-electron interaction

The electron gas has played a very important role in the development of manybody theory¹. In the present chapter we employ the random-phase approximation (RPA) to obtain the dielectric function and the ground state energy of the electron gas. The random-phase approximation is valid for a high-density electron gas. By means of diagrammatic perturbation theory it is possible to go beyond RPA and include more terms in the perturbation series. One should note, however, that it has not proved fruitful to extend RPA by simply going to higher order in the parameter r_s , as defined in (3.8), and $\ln r_s$. Such an expansion only converges when $r_s < 1$, while in metals r_s ranges between 2 and 6. It has therefore been necessary to devise approximation schemes that do not represent an expansion in a small parameter but which nevertheless serve as a useful basis for the description of the properties of conduction electrons in the range of metallic densities.

Our starting point is the Hamiltonian of a homogeneous electron gas,

$$H = H_0 + H' \tag{8.1}$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(8.2)

represents the kinetic energy, while

$$H' = \frac{1}{2V} \sum_{\mathbf{q}\neq 0, \mathbf{k}, \mathbf{k}', \sigma, \sigma'} V(q) c^{\dagger}_{\mathbf{k}+\mathbf{q}, \sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}, \sigma'} c_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}$$
(8.3)

is the interaction between the electrons with

$$V(q) = \frac{4\pi e_0^2}{q^2}.$$
 (8.4)

The restriction on the q-sum arises because the electrons are immersed in a positive background of charge due to the lattice ions, as explained in Chapter 2.

8.1 The random-phase approximation

In Section 6.5.1 we have obtained G in the Hartree-Fock approximation by determining the irreducible self-energy $\Sigma(\mathbf{k},\omega)$ in the approximation where only the diagram shown in Fig. 8.1 (a) is included, the Hartree-term being absent

¹A collection of reprints covering the important developments in the fifties may be found in D. Pines: The Many Body Problem, Benjamin 1962.



Figure 8.1: Terms in the irreducible self-energy

due to the existence of the positive background. It is natural to proceed by considering second-order contributions to $\Sigma(\mathbf{k},\omega)$ such as the diagram shown in Fig. 8.1 (b). Due to the occurrence of two interaction lines carrying the same momentum, this term gives a divergent contribution to the ground-state energy for the same reason that the use of second-order perturbation theory led to a divergence, as demonstrated in Chapter 3. Moreover, third-order and fourth-order terms such as those exhibited in Fig. 8.1 c) and d) yield increasingly strong divergences, since they contain $1/q^6$ and $1/q^8$, respectively. The solution to the problem is to sum all such divergent terms, which results in a finite answer. This constitutes the random-phase approximation.

Let us define an effective interaction $V_{\text{eff}}(\mathbf{q},\omega)$, which is equal to the sum of V(q) and the infinity of terms obtained by inserting the *polarization bubble* $\Pi^{(0)}(\mathbf{q},\omega)$ in the manner illustrated in Fig. 8.1 (b-d). Thus $V_{\text{eff}}(\mathbf{q},\omega)$ represents a geometric series,

$$V_{\rm eff}(\mathbf{q},\omega) = V(q) + V(q)\Pi^{(0)}V(q) + V(q)\Pi^{(0)}V(q)\Pi^{(0)}V(q)\cdots.$$
(8.5)

This infinite series is readily summed with the result

$$V_{\text{eff}}(\mathbf{q},\omega) = \frac{V(q)}{1 - V(q)\Pi^{(0)}(\mathbf{q},\omega)},\tag{8.6}$$

where $\Pi^{(0)}(\mathbf{q},\omega)$ is the polarization bubble indicated in the diagram of Fig. 8.1 (b). According to the Feynman rules, the polarization bubble is

$$\Pi^{(0)}(\mathbf{q},q_0) = -2\frac{i}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}_0}{2\pi} G^{(0)}(\mathbf{k},k_0) G^{(0)}(\mathbf{q}+\mathbf{k},q_0+k_0).$$
(8.7)

The factor of 2 is due to the summation over spin, while the minus-sign comes from the presence of the closed fermion loop. The factor of i/\hbar originates in the fact that we have separated out V(q) in the definition of $\Pi^{(0)}$, cf. (6.94) and the denominator of (8.6). As we shall see, this polarization bubble determines the dielectric function of the electron gas within the RPA, and we shall therefore need to know it as a function of q and q_0 .

We now use the expression (8.7) together with the free-particle Green function $G^{(0)}$ to determine $\Pi^{(0)}$ as a function of wave-vector **q** and frequency q_0 . The free-particle propagator $G^{(0)}(\mathbf{k}, \omega)$ is given by

$$G^{(0)}(\mathbf{k},\omega) = \frac{1-n_{\mathbf{k}}}{\omega-\omega_{\mathbf{k}}+i\eta} + \frac{n_{\mathbf{k}}}{\omega-\omega_{\mathbf{k}}-i\eta},$$
(8.8)

where

$$\omega_{\mathbf{k}} = \frac{\hbar k^2}{2m}.\tag{8.9}$$

Thus we obtain

$$\Pi^{(0)}(\mathbf{q}, q_0) = -2\frac{i}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{dk_0}{2\pi} \\ \left(\frac{1-n_{\mathbf{k}}}{k_0 - \omega_{\mathbf{k}} + i\eta} + \frac{n_{\mathbf{k}}}{k_0 - \omega_{\mathbf{k}} - i\eta}\right) \\ \left(\frac{1-n_{\mathbf{k}+\mathbf{q}}}{k_0 + q_0 - \omega_{\mathbf{k}+\mathbf{q}} + i\eta} + \frac{n_{\mathbf{k}+\mathbf{q}}}{k_0 + q_0 - \omega_{\mathbf{k}+\mathbf{q}} - i\eta}\right). \quad (8.10)$$

It is a simple matter to carry out the integration over frequency, using the theorem of residues. The result is

$$\Pi^{(0)}(\mathbf{q}, q_0) = \frac{2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} \left(\frac{n_{\mathbf{k}}(1 - n_{\mathbf{k}+\mathbf{q}})}{\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}} + q_0 + i\eta} + \frac{n_{\mathbf{k}+\mathbf{q}}(1 - n_{\mathbf{k}})}{\omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}} - q_0 + i\eta} \right).$$
(8.11)

Note that $\Pi^{(0)}$ only depends on the length of **q** for reasons of symmetry. Therefore one has

$$\Pi^{(0)}(\mathbf{q}, q_0) = \Pi^{(0)}(-\mathbf{q}, q_0).$$
(8.12)

Before we consider the general dependence of (8.11) on q and q_0 , we shall exhibit its static limit $q_0 = 0$. In this limit the two terms in (8.11) may combined as follows

$$\Pi^{(0)}(\mathbf{q},0) = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{n_{\mathbf{k}+\mathbf{q}/2} - n_{\mathbf{k}-\mathbf{q}/2}}{\epsilon_{\mathbf{k}+\mathbf{q}/2} - \epsilon_{\mathbf{k}-\mathbf{q}/2}}.$$
(8.13)

To obtain this expression we have introduced the new variable $\mathbf{k}' = \mathbf{k} + \mathbf{q}/2$ and subsequently replaced \mathbf{k}' by \mathbf{k} . Next we take the long-wavelength limit $q \to 0$ of (8.13). By expanding the differences in the numerator and the denominator in powers of q one obtains in the limit $q \to 0$

$$\Pi^{(0)}(0,0) = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial n_{\mathbf{k}}}{\partial \epsilon_k} = -2N(0), \qquad (8.14)$$

where $2N(0) = mk_{\rm F}/\pi^2\hbar^2$ equals the density of states per unit energy and volume at the Fermi energy. The long-wavelength limit yields (minus) the density of states at the Fermi energy, because the derivative of $n_{\rm k}$ with respect to energy equals (minus) a delta-function situated at the Fermi energy.

In the static, long-wavelength limit we thus obtain from (8.6) a screened interaction V_{eff} given by

$$V_{\rm eff}(q) = \frac{V(q)}{1 + k_s^2/q^2} = \frac{4\pi e_0^2}{q^2 + k_s^2},\tag{8.15}$$

where $k_s^2 = 8N(0)\pi e_0^2 = 4k_F/\pi a_0$, a_0 being the Bohr radius. The Fourier-transform of this interaction is the screened Coulomb-interaction

$$V_{\rm eff}(r) = \frac{e_0^2}{r} e^{-k_* r}.$$
 (8.16)

Note that this interaction has the same form as the Yukawa-potential used in nuclear physics. The range a of the interaction is $a = k_s^{-1}$. In metals k_F and a_0^{-1} are comparable, and a is therefore approximately equal to the mean interelectronic distance.

8.2 The dielectric function

The difference between V and V_{eff} is that the latter is screened,

$$V_{\text{eff}}(q,\omega) = \frac{V(q)}{\epsilon(q,\omega)},\tag{8.17}$$

where the dielectric function ϵ is

$$\epsilon(q, q_0) = 1 - \frac{4\pi e_0^2}{q^2} \Pi^{(0)}(q, q_0), \qquad (8.18)$$

in terms of the function $\Pi^{(0)}(q, q_0)$ given by (8.11). Since there is no preferred direction in momentum space, $\Pi^{(0)}$ only depends on the length of **q** and on q_0 .

By carrying out the integration over k and the angle between k and q we may determine the real and imaginary part of the dielectric function. The result is conveniently expressed in the dimensionless variables

$$x = \frac{q}{2k_{\rm F}}$$
, $x_0 = \frac{\hbar q_0}{4\epsilon_{\rm F}}$. (8.19)

In order to determine the dielectric function we must carry out the integrals over \mathbf{k} in the expression (8.11). Before doing that we write the expression in the form

$$\Pi^{(0)}(\mathbf{q}, q_0) = \frac{2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} n_{\mathbf{k}} (1 - n_{\mathbf{k}+\mathbf{q}}) (\frac{1}{\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}} + q_0 + i\eta} + \frac{1}{\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}} - q_0 + i\eta}), \qquad (8.20)$$

which is obtained by exchanging the variables \mathbf{k} and $\mathbf{k} + \mathbf{q}$ in the second term of (8.11) while making use of (8.12). We note from (8.20) that $\Pi^{(0)}$ is an even function of the frequency variable q_0 . The real part of $\Pi^{(0)}$ is seen to be given by

$$\operatorname{ReII}^{(0)}(\mathbf{q}, q_0) = \frac{2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} n_{\mathbf{k}} (1 - n_{\mathbf{k}+\mathbf{q}}) \frac{2(\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}})}{(\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}})^2 - q_0^2}.$$
 (8.21)

The term in (8.21) containing the product $n_{\mathbf{k}}n_{\mathbf{k}+\mathbf{q}}$ yields a vanishing contribution, since it changes sign upon the interchange of \mathbf{k} and $\mathbf{k} + \mathbf{q}$. Consequently we have

$$\operatorname{ReII}^{(0)}(\mathbf{q}, q_{0}) = \frac{2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^{3}} n_{\mathbf{k}} \frac{2(\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}})}{(\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}})^{2} - q_{0}^{2}}$$
$$= \frac{2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^{3}} n_{\mathbf{k}} (\frac{1}{\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}} + q_{0}}$$
$$+ \frac{1}{\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{q}} - q_{0}}). \tag{8.22}$$

It is convenient to introduce the dimensionless variables given in (8.19) together with

$$y = \frac{k}{k_{\rm F}}.\tag{8.23}$$

Then we obtain

$$\operatorname{Re}\Pi^{(0)}(\mathbf{q}, q_0) = N(0) \int_{-1}^{1} \frac{d(\cos\theta)}{2} \int_{0}^{1} dyy^2 \left(\frac{1}{x_0 - x^2 - yx\cos\theta} - \frac{1}{x_0 + x^2 + yx\cos\theta}\right), \quad (8.24)$$

where we have used that $\hbar(q_0 + \omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}}) = 4\epsilon_{\mathbf{F}}(x_0 + x^2 + yx\cos\theta)$. Now the remaining integrals are elementary and yield

$$\operatorname{ReII}^{(0)}(\mathbf{q}, q_0) = -2N(0)\left(\frac{1}{2} + \frac{1}{8x}\left[\left\{1 - \left(\frac{x_0}{x} - x\right)^2\right\}\ln\frac{|x - x_0 + x^2|}{|x + x_0 - x^2|} + \left\{1 - \left(\frac{x_0}{x} + x\right)^2\right\}\ln\frac{|x + x_0 + x^2|}{|x - x_0 - x^2|}\right]\right).$$

$$(8.25)$$

The imaginary part becomes

$$Im\Pi^{(0)}(\mathbf{q}, q_0) = -N(0)\pi \int_{-1}^{1} \frac{d(\cos\theta)}{2} \int_{0}^{1} dyy^2$$

$$\Theta(x^2 + xy\cos\theta - \frac{1}{4}(1 - y^2))$$

$$(\delta(x_0 - x^2 - yx\cos\theta) + \delta(x_0 + x^2 + yx\cos\theta)).(8.26)$$

This integral is readily worked out by considering separately the regions x > 1and x < 1. Since the imaginary part is even in x_0 , it is sufficient to consider it for $x_0 > 0$. In this case the argument of the second delta-function, $\delta(x_0 + x^2 + yx \cos \theta)$, is never equal to zero, because of the constraint (expressed by the Θ -function) that $|\mathbf{k} + \mathbf{q}| > k_F$. Consequently we may leave it out and focus on the contribution of the first delta-function, $\delta(x_0 - x^2 - yx \cos \theta)$.

First we treat the region x > 1. In this case the argument of the Θ -function is always positive, since 0 < y < 1. We distinguish two cases, a) $x_0 < x^2$ and b) $x_0 > x^2$. In case a) the lower limit y_{\min} of the y-integration is obtained by setting $\cos \theta = -1$ in the delta-function, and is therefore $y_{\min} = (x^2 - x_0)/x$. Since y_{\min} must be less than 1 in order to get a non-zero contribution, we deduce that $(x^2 - x_0)/x < 1$ or $x_0 > x^2 - x$. In case b) the lower limit y_{\min} of the y-integration is obtained by setting $\cos \theta = +1$ in the delta-function, and is therefore $y_{\min} = (x_0 - x^2)/x$. Since y_{\min} must be less than 1, we obtain the condition $x_0 < x^2 + x$.

Provided x > 1, the imaginary part thus becomes

Im
$$\Pi^{(0)}(\mathbf{q}, q_0) = -N(0)\frac{\pi}{4x}\{1 - (\frac{x_0}{x} - x)^2\}$$
 for $x^2 - x < x_0 < x^2 + x$. (8.27)

The other region, x < 1, may be treated in a similar fashion. The results are exhibited in the expression (8.30) below.

The resulting dielectric function ϵ then becomes $(q_0 \ge 0)$

$$\epsilon(q, q_0) = 1 + \frac{k_s^2}{q^2} F(x, x_0), \qquad (8.28)$$

where

$$\operatorname{Re} F = \frac{1}{2} + \frac{1}{8x} \left[\left\{ 1 - \left(\frac{x_0}{x} - x\right)^2 \right\} \ln \frac{|x - x_0 + x^2|}{|x + x_0 - x^2|} + \left\{ 1 - \left(\frac{x_0}{x} + x\right)^2 \right\} \ln \frac{|x + x_0 + x^2|}{|x - x_0 - x^2|} \right],$$
(8.29)

while

Im
$$F = \frac{\pi}{8x} \{1 - (\frac{x_0}{x} - x)^2\}$$
 for $|x - x^2| < x_0 < x + x^2$

$$= \frac{\pi x_0}{2x} \text{ for } x_0 < x - x^2$$

= 0 otherwise. (8.30)

Note that the real part of the dielectric function in the static limit $(q_0 = 0)$ has a singular slope at $q = 2k_F$. This is reflected experimentally in metals in the Kohn anomaly of their phonon spectra or in the Friedel oscillations of the conduction electron density surrounding a charged impurity. In the static long-wavelength limit Re $F \rightarrow 1$, and one recovers the Thomas-Fermi approximation for the screening.

Now let us consider the limit of high frequencies ω , with q tending to zero, while ω remains finite. In this case we find from (8.29) the familiar result

$$\epsilon(q,\omega) \simeq 1 - \frac{\omega_p^2}{\omega^2} \tag{8.31}$$

where ω_p is the plasma frequency given by

$$\omega_p^2 = \frac{4\pi n e_0^2}{m} = \frac{n e^2}{m \epsilon_0}.$$
(8.32)

When $\epsilon(q,\omega)$ vanishes it becomes possible for longitudinal electromagnetic waves to propagate, with wavevector parallel to the electric field (cf. *Transport Phenomena* Section 1.15.3). These are the plasma oscillations or *plasmons*. Their dispersion is found by calculating the real part of F from (8.29) to fourth order in q, with the result

$$\epsilon \simeq 1 - \frac{\omega_p^2}{\omega^2} \left(1 + \frac{3v_F^2 q^2}{5\omega^2}\right). \tag{8.33}$$

This vanishes for

$$\omega^2 \simeq \omega_p^2 + \frac{3}{5} v_F^2 q^2, \qquad (8.34)$$

where $v_{\rm F} = \hbar k_{\rm F}/m$ is the Fermi velocity. As long as the curve given by (8.34) does not enter the *particle-hole continuum*, where the imaginary part of the dielectric function ϵ is non-zero, cf. (8.30), the plasmon is undamped. At finite temperature the plasmon is damped at any non-zero value of q. In the following subsection we investigate the dielectric function at finite temperatures.

8.2.1 Finite temperatures

At finite temperatures the polarization bubble $\Pi^{(0)}$ is given by

$$\Pi^{(0)}(\mathbf{q},\omega_n) = \frac{2}{\hbar^2 \beta} \sum_{n'} \int \frac{d\mathbf{k}}{(2\pi)^3} G^{(0)}(\mathbf{k},\omega_{n'}) G^{(0)}(\mathbf{q}+\mathbf{k},\omega_n+\omega_{n'}). \quad (8.35)$$

We insert the appropriate expressions for the Green functions and obtain

$$\Pi^{(0)}(\mathbf{q},\omega_n) = \frac{2}{\hbar^2 \beta} \sum_{\mathbf{n}'} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{i\omega_{\mathbf{n}'} - (\epsilon_k - \mu)/\hbar} \frac{1}{i(\omega_n + \omega_{\mathbf{n}'}) - (\epsilon_{\mathbf{q}+\mathbf{k}} - \mu)/\hbar}$$
(8.36)

The integrand is seen to vary as $|\omega_{n'}|^{-2}$ for large $|\omega_{n'}|$. This implies that any contribution from the arcs in a subsequent contour integration vanishes, and we are therefore allowed to insert the factor $\exp(i\eta\omega_{n'})$ at will. Thereby it becomes possible to exploit the result (7.87) directly, using

$$\frac{1}{i\omega_{n'} - (\epsilon_{k} - \mu)/\hbar} \frac{1}{i(\omega_{n} + \omega_{n'}) - (\epsilon_{\mathbf{q}+\mathbf{k}} - \mu)/\hbar} = (\frac{1}{i\omega_{n'} - (\epsilon_{k} - \mu)/\hbar} - \frac{1}{i(\omega_{n} + \omega_{n'}) - (\epsilon_{\mathbf{q}+\mathbf{k}} - \mu)/\hbar})\frac{1}{i\omega_{n} - (\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{k})/\hbar} (8.37)$$

The final result is thus

$$\Pi^{(0)}(\mathbf{q},\omega_n) = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{n_k - n_{\mathbf{k}+\mathbf{q}}}{i\hbar\omega_n - \epsilon_{\mathbf{q}+\mathbf{k}} + \epsilon_k}.$$
(8.38)

This is the temperature-dependent result for the polarization bubble in the random-phase approximation. After analytic continuation $i\omega_n \rightarrow \omega + i\eta$, its long-wavelength limit $(q \rightarrow 0)$ yields the same dielectric function, which we previously obtained from the Boltzmann equation, cf. Transport Phenomena.

8.2.2 Lower dimensions

The RPA-result for the screening may also be generalized to other dimensions: In the static limit we get

$$\Pi^{(0)}(\mathbf{q},0) = -2 \int \frac{d^d k}{(2\pi)^d} \frac{f_{\mathbf{k}+\mathbf{q}/2} - f_{\mathbf{k}-\mathbf{q}/2}}{\epsilon_{\mathbf{k}-\mathbf{q}/2} - \epsilon_{\mathbf{k}+\mathbf{q}/2}}$$
$$= 2 \int \frac{d^d k}{(2\pi)^d} \frac{f(\epsilon_{\mathbf{k}+1}) - f(\epsilon_{\mathbf{k}-1})}{\hbar^2 \mathbf{k} \cdot \mathbf{q}/m}$$
(8.39)

where $f(\epsilon)$ denotes the equilibrium Fermi function, and

$$\epsilon_{k\pm} = \frac{\hbar^2 (k^2 \pm \mathbf{k} \cdot \mathbf{q} + q^2/4)}{2m}.$$
(8.40)

It is convenient to write the difference of the Fermi functions as a definite integral over a variable λ ,

$$f(\epsilon_{k+}) - f(\epsilon_{k-}) = \int_{-1}^{1} d\lambda \frac{\partial f(\hbar^2(k^2 + \lambda \mathbf{k} \cdot \mathbf{q} + q^2/4)/2m)}{\partial \lambda}, \qquad (8.41)$$



Figure 8.2: $\Pi^{(0)}(q,0)$ in 1, 2 and 3 dimensions as function of $q/2k_{\rm F}$

since this allows one to write (8.39) in terms of the derivative with respect to $\lambda \mathbf{k} \cdot \mathbf{q}$ according to

$$\Pi^{(0)}(\mathbf{q},0) = \int \frac{d^d \mathbf{k}}{(2\pi)^d} \int_{-1}^1 d\lambda \frac{\partial f(\hbar^2(\mathbf{k}^2 + \lambda \mathbf{k} \cdot \mathbf{q} + q^2/4)/2m)}{\partial(\hbar^2 \mathbf{k} \cdot \mathbf{q}\lambda/2m)}.$$
 (8.42)

By introducing the variable $\mathbf{k}' = \mathbf{k} + \lambda \mathbf{q}/2$ we obtain

$$\Pi^{(0)}(q,0) = \int \frac{d^d k'}{(2\pi)^d} \int_{-1}^1 d\lambda f'(\hbar^2 (k'^2 + q^2(1-\lambda^2)/4)/2m), \qquad (8.43)$$

where f' is the derivative of the Fermi function. At zero temperature we have

$$f' = -\delta(\epsilon - \epsilon_{\rm F}). \tag{8.44}$$

The density of states $g(\epsilon)$ for both spin directions in d dimensions is given by

$$g(\epsilon) = g(\epsilon_{\rm F}) \left(\frac{\epsilon}{\epsilon_{\rm F}}\right)^{(d-2)/2},\tag{8.45}$$

where $g(\epsilon_{\rm F})$ is the density of states for both spin directions at the Fermi energy. At zero temperature we therefore have

$$\Pi^{(0)}(q,0) = -\frac{1}{2} \int_0^\infty d\epsilon g(\epsilon) \int_{-1}^1 d\lambda \delta(\epsilon + \frac{\hbar^2 q^2 (1-\lambda^2)}{8m} - \epsilon_{\rm F}) = -g(\epsilon_{\rm F}) \int_{\lambda_{\rm min}}^1 d\lambda (1 - (1-\lambda^2) x^2)^{(d-2)/2}, \qquad (8.46)$$

where we have introduced the natural dimensionless variable $x = q/2k_{\rm F}$, while $\lambda_{\rm min}$ is 0 for x < 1 and $\sqrt{1 - x^{-2}}$ for x > 1. The remaining steps are elementary. Note that $-\Pi^{(0)}(q,0)/g(\epsilon_{\rm F})$ in two dimensions equals $1 - \lambda_{\rm min}$, because the density of states is independent of energy.

In Fig. 8.2 we sketch the q-dependence of $\Pi^{(0)}(q,0)$ in 1, 2 and 3 dimensions. In a later problem we shall see how the divergence at $2k_{\rm F}$ in one dimension is reflected in the *Peierls instability* occurring in one-dimensional conductors.

8.3 The ground-state energy

In Chapter 6 we showed that the total energy in the ground state could be obtained from the expectation value

$$E - E_0 = \int_0^1 \frac{d\lambda}{\lambda} \langle \Psi(\lambda) | \lambda H' | \Psi(\lambda) \rangle.$$
(8.47)

where

$$H' = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d\mathbf{x}_1 \int d\mathbf{x}_2 \psi_{\sigma_1}^{\dagger}(\mathbf{x}_1) \psi_{\sigma_2}^{\dagger}(\mathbf{x}_2) V(\mathbf{x}_1 - \mathbf{x}_2) \psi_{\sigma_2}(\mathbf{x}_2) \psi_{\sigma_1}(\mathbf{x}_1).$$
(8.48)

We shall now use this formula to calculate the correlation energy $E_{\rm corr}$, which is defined as the total energy E minus the sum of the kinetic energy $E_{\rm kin}^0$ of the noninteracting system and Hartree-Fock contribution $E_{\rm HF}$,

$$E_{\rm corr} = E - E_{\rm kin}^0 - E_{\rm HF}.$$
 (8.49)

By definition, then, the correlation energy vanishes in the Hartree-Fock approximation. We shall show how the correlation energy is determined within the RPA, where we keep only the most divergent diagrams. It is convenient to formulate the calculation in terms of density-fluctuation propagators, which we introduce in the following subsection.

8.3.1 The density-fluctuation propagator

The density operator is

$$\rho(\mathbf{x}) = \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{x}) \psi_{\sigma}(\mathbf{x}).$$
(8.50)

Here the field operators ψ and ψ^{\dagger} are given by

$$\psi_{\sigma} = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k},\sigma} \tag{8.51}$$

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and its hermitian conjugate. For simplicity we consider a unit volume, corresponding to $\sum_{\mathbf{q}} \cdots = \int d\mathbf{q}/(2\pi)^3 \cdots$. In Fourier-components the density operator thus becomes

$$\rho(\mathbf{x}) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}\rho(\mathbf{q}); \ \rho(\mathbf{q}) = \int d\mathbf{x} e^{-i\mathbf{q}\cdot\mathbf{x}}\rho(\mathbf{x}), \tag{8.52}$$

where

$$\rho(\mathbf{q}) = \sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma}.$$
(8.53)

It is readily seen from (2.23) by moving $c_{\mathbf{k},\sigma}$ next to $c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}$ that the interaction energy H' may be written as

$$H' = \frac{1}{2} \sum_{\mathbf{q}(\neq 0)} V(q)(\rho(\mathbf{q})\rho(-\mathbf{q}) - N)$$
(8.54)

where N is the number of particles. Since $[\rho(\mathbf{q}), \rho(-\mathbf{q})] = 0$ it follows that $\rho(\mathbf{q})$ commutes with the interaction energy.

In the following we consider only spatially homogeneous systems, where the ground-state expectation value $\langle \rho(\mathbf{x}) \rangle$ of the density is a constant, *n*, equal to the number of particles per unit volume,

$$\langle \rho(\mathbf{x}) \rangle = n. \tag{8.55}$$

The density fluctuation operator $\tilde{\rho}$ is defined as

$$\tilde{\rho}(\mathbf{x}) = \rho(\mathbf{x}) - n \tag{8.56}$$

and has consequently its ground-state expectation value equal to zero. The corresponding Heisenberg operator is denoted by $\tilde{\rho}(\mathbf{x}, t)$. The density-fluctuation propagator $D(\mathbf{x}, t; \mathbf{x}', t')$ is a time-ordered correlation function, which is defined in analogy with the single-particle Green function (6.1),

$$D(\mathbf{x}, t; \mathbf{x}', t') = -i < T\{\tilde{\rho}(\mathbf{x}, t)\tilde{\rho}(\mathbf{x}', t')\} >$$
(8.57)

in terms of a time-ordered product of density-fluctuation operators in the Heisenberg picture. In a translationally invariant system, the density fluctuation operator only depends on the difference variables $\mathbf{x} - \mathbf{x}'$ and t - t'.

By using the commutation rules for the operators ψ and ψ^{\dagger} we see that the expectation value $\langle H' \rangle$ of the interaction energy in general may be written as

$$\langle H' \rangle = \frac{1}{2} \int d\mathbf{x}_1 \int d\mathbf{x}_2 V(\mathbf{x}_1 - \mathbf{x}_2) \langle \rho(\mathbf{x}_1) \rho(\mathbf{x}_2) \rangle - n\delta(\mathbf{x}_1 - \mathbf{x}_2))$$

$$= \frac{1}{2} \int d\mathbf{x}_1 \int d\mathbf{x}_2 V(\mathbf{x}_1 - \mathbf{x}_2)$$

$$\langle \tilde{\rho}(\mathbf{x}_1) \tilde{\rho}(\mathbf{x}_2) \rangle + n^2 - n\delta(\mathbf{x}_1 - \mathbf{x}_2)).$$

$$(8.58)$$



Figure 8.3: Density-fluctuation propagators

The result of the Hartree-Fock approximation is recovered from (8.58) by taking the expectation value in the ground state of the non-interacting system, since we have shown in Chapter 4 that the ground-state energy of a homogeneous electron gas in the Hartree-Fock approximation may be obtained by treating the interaction energy as a perturbation to first order. Consequently the correlation energy is given in terms of the difference between $\langle H' \rangle$ and $\langle H' \rangle_0$, the latter denoting the expectation value of H' in the ground state of the noninteracting system. It is convenient to introduce the Fourier-transform of the density-fluctuation propagator,

$$D(\mathbf{q},\omega) = \int d(\mathbf{x}-\mathbf{x}') \int d(t-t') e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} e^{i\omega(t-t')} D(\mathbf{x}-\mathbf{x}',t-t').$$
(8.59)

Then we get the final formula for the correlation energy, expressed in terms of the Fourier-transform of the density-fluctuation propagator,

$$E_{\rm corr} = \frac{i}{2} \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d\mathbf{q}}{(2\pi)^3} \int \frac{d\omega}{2\pi} \lambda V(\mathbf{q}) (D^\lambda(\mathbf{q},\omega) - D^0(\mathbf{q},\omega)).$$
(8.60)

This formula is exact. A knowledge of the density-fluctuation propagator $D(\mathbf{q}, \omega)$ thus allows one to determine the ground-state energy of the homogeneous electron gas.

8.3.2 The correlation energy

In order to calculate the correlation energy one is forced to make approximations to D. Let us first consider $D^{(0)}$, the density-fluctuation propagator of the noninteracting system. As we have seen in Problem 41, $D^{(0)}(\mathbf{q},\omega)$ is given by

$$D^{(0)}(\mathbf{q},\omega) = -2i \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}_0}{2\pi} G^{(0)}(\mathbf{k}+\mathbf{q},\mathbf{k}_0+\omega) G^{(0)}(\mathbf{k},\mathbf{k}_0).$$
(8.61)

This is diagrammatically illustrated in Fig. 8.3 (a). In the RPA, we approximate D by the sum illustrated in Fig. 8.3 (b), which is a geometric series. We note that $D^{(0)} = \hbar \Pi^{(0)}$ and obtain

$$E_{\rm corr} = \frac{1}{2}i\hbar \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d\mathbf{q}}{(2\pi)^3} \int \frac{d\omega}{2\pi} [\lambda V(q)\Pi^{(0)}(q,\omega)]^2 \frac{1}{1 - \lambda V(q)\Pi^{(0)}(q,\omega)}.$$
(8.62)

We shall now carry out the integrations over \mathbf{q}, ω and λ and use the previously found weight function (3.27) to show that this expression in the limit of small r_s reproduces the result (3.29) for the correlation energy. Since the leading $\ln r_s$ -contribution arises from the region of small wave-vectors and frequencies we may approximate the denominator as $1 - V(q)\Pi^{(0)} \simeq 1 + k_s^2/q^2$, which effectively screens one of the two interaction matrix elements V(q). Carrying out the integration over frequencies by means of the residue theorem we obtain

$$E_{\text{corr}} = -4 \int_{0}^{1} \frac{d\lambda}{\lambda} \int \frac{d\mathbf{q}}{(2\pi)^{3}} \int \frac{d\mathbf{k}}{(2\pi)^{3}} \int \frac{d\mathbf{p}}{(2\pi)^{3}} \\ \cdot (1 - n_{\mathbf{k}}) n_{\mathbf{k}+\mathbf{q}} (1 - n_{\mathbf{p}+\mathbf{q}}) n_{\mathbf{p}} (\lambda V(q))^{2} \\ \cdot \frac{1}{\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{k}+\mathbf{q}}} \frac{1}{1 + k_{s}^{2}/q^{2}}.$$
(8.63)

Evidently, we obtain the same weight function I(q) as in (3.27) when the integrals over **k** and **p** are carried out, since the integrand (apart from its additional q-dependence) is the same in the two cases. With $\tilde{q} = q/k_{\rm F}$ we therefore get

$$E_{\rm corr} = -\frac{m\epsilon_0^4}{\hbar^2} \frac{k_{\rm F}^3}{\pi^2} 2 \int_0^1 d\lambda \lambda \int_0^\infty d\tilde{q} I(\tilde{q}) \frac{1}{\tilde{q}^2 + \lambda k_s^2/k_{\rm F}^2}.$$
 (8.64)

The dominant contribution from the lower limit in (8.64) is obtained by using the result (3.27), $I(\tilde{q}) = 2(1-\ln 2)\tilde{q}/3\pi^2$. With $k_{\rm F}^3 = 3\pi^2 N$ (we are considering a unit volume) and utilizing $k_s^2/k_{\rm F}^2 \propto r_s$ together with

$$\int_{0}^{1} d\lambda \lambda \int_{0}^{\infty} d\tilde{q} I(\tilde{q}) \frac{1}{\tilde{q}^{2} + \lambda k_{s}^{2}/k_{\mathrm{F}}^{2}} \simeq -\frac{1}{6\pi^{2}} (1 - \ln 2) \ln r_{s}, \qquad (8.65)$$

we finally get that

$$E_{\rm corr} = N \frac{1}{\pi^2} (1 - \ln 2) \frac{m e_0^4}{\hbar^2} \ln r, \qquad (8.66)$$

in agreement with (3.29).

9 Electron-phonon interaction

The interaction between electrons and phonons determines many of the most important properties of solids. The temperature-dependence of the electrical resistivity of metals is largely due to electron-phonon scattering, while the transition to the superconducting state (in conventional superconductors) is due to the attractive interaction between electrons, mediated by their mutual exchange of phonons. From the point of view of many-body theory, the electron-phonon interaction is in some ways simpler than the Coulomb repulsion between the electrons, due to the smallness of the ratio between the maximum phonon energy and the Fermi energy. This allows one to neglect diagrams containing vertex corrections, as shown first by Migdal (1958).

When an ion moves, the bulk of the electrons follow its motion adiabatically, because there are no available states into which an electron deep inside the Fermi sea may scatter. This tends to maintain local charge neutrality and results in a screening of the long-range electron-phonon interaction. The few electrons that may undergo scattering due to the electron-phonon interaction lie within an energy shell of the order of (\hbar times) a typical phonon frequency.

In the present chapter we first determine the characteristic magnitude of phonon energies from the sound velocity in metals and show that they are of order $(m/M)^{1/2}$ times the Fermi energy, m being the electron mass and M the ion mass. Then we discuss the electron-phonon coupling and obtain its dependence on momentum transfer within a simple model. The following sections deal with the influence of the phonons on the effective mass and life-time of electron states near the Fermi energy. For simplicity, we first treat the electron-phonon coupling within ordinary second-order perturbation theory. Subsequently we introduce phonon propagators and discuss the Feynman rules. The mass enhancement is obtained by calculating the electron self-energy to lowest order in the electron-phonon coupling.

9.1 Sound in metals

First let us review the calculation of sound velocities in classical gases on the basis of ordinary hydrodynamics. The conservation of mass is expressed by the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0, \qquad (9.1)$$

where ρ is the mass density and $\mathbf{j} = \rho \mathbf{v}$ is the mass current density. We have introduced a velocity field $\mathbf{v} = \mathbf{v}(\mathbf{r}, t)$, which specifies the local drift velocity. According to Newton's second law the time derivative of \mathbf{j} is determined by the pressure gradient ∇p ,

$$\frac{\partial \mathbf{j}}{\partial t} = -\nabla p. \tag{9.2}$$

We have neglected friction, which leads to damping of the sound, as well as nonlinear terms in the equation of motion. By taking the derivative of (9.1) with respect to time we obtain

$$\frac{\partial^2 \rho}{\partial t^2} = \nabla^2 p. \tag{9.3}$$

Since the equation (9.3) involves both pressure and density, we must now relate small changes Δp in the pressure p to small changes $\Delta \rho$ in the mass density ρ . Let us first assume that the propagation of sound occurs isothermally, thereby allowing us to use the equation of state

$$p = \frac{\rho}{M} kT, \tag{9.4}$$

where M is the (average) mass of an air molecule. Since $\Delta p = (\partial p / \partial \rho)_T \Delta \rho$, it follows from (9.3) and (9.4) that the sound velocity s is given by

$$s^2 = \left(\frac{\partial p}{\partial \rho}\right)_T = \frac{kT}{M}.$$
(9.5)

Under usual circumstances the propagation of sound does not take place isothermally (at constant temperature), but adiabatically (at constant entropy). As a result (9.5) should be multiplied by the ratio C_p/C_V between the heat capacity at constant pressure and at constant volume. The resulting expression for the sound velocity, $s = (C_p kT/C_V M)^{1/2}$, is in very good agreement with measured sound velocities in gases.

Let us now turn to the determination of sound velocities in metals. At the relatively low frequencies and long wavelengths characterizing sound it is possible to regard the metal as a continuum and use the equations (9.1) and (9.2) leading to (9.3). The connection between pressure and volume is not, however, given by (9.4), which holds for an ideal classical gas. In order to determine the pressure as a function of volume we identify the ground-state energy E_0 in our simple model with the internal energy U at T = 0 K. Thus

$$U = \frac{3}{5} N \epsilon_{\rm F} \propto V^{-2/3}. \tag{9.6}$$

As a consequence the pressure becomes proportional to $V^{-5/3}$, since it is given by

$$p = -\frac{\partial U}{\partial V} = \frac{2U}{3V} = \frac{2}{5}nkT_{\rm F},\tag{9.7}$$

which shows that the equation of state at T = 0 is obtained by replacing the temperature in (9.4) with the Fermi temperature $T_{\rm F}$, apart from a numerical factor.

The mass density ρ is given to a good approximation by

$$\rho = n_{\rm ion} M, \tag{9.8}$$

where M is the mass of an ion in the crystal lattice, while n_{ion} is the ion density. We assume that there are z conduction electrons per ion, which implies that n_{ion} is equal to n/z. Consequently the sound velocity is given by

$$s^2 = \frac{\partial p}{\partial \rho} = \frac{z}{3} \frac{m}{M} v_{\rm F}^2, \tag{9.9}$$

where $v_{\rm F} = \hbar k_{\rm F}/m$ is the Fermi velocity.

This result is in qualitative agreement with measurements of sound velocities in simple metals such as Al, Na and Cu. One finds for these three metals that the value calculated according to (9.9) is 9.1, 3.0 and 2.7 km/s, respectively, while the measured longitudinal sound velocities are 6.8, 3.1 and 4.7 km/s.

Note that it is the compressibility of the electron gas which enters the sound velocity in this simple model. The physical reason for this is that the motion of the ions and the electrons is not independent. The electrons follow the motion of the ions in order to neutralize their charges locally. As a consequence the electrons are compressed and expanded, resulting in pressure oscillations which are determined locally by changes in the energy of the electron gas due to changes in its density.

The expression (9.9) for the sound velocity may be used to estimate the maximum phonon frequency ω_{max} . Neglecting dispersion and using that the phonon wave-vector is about 1/a at the Brillouin-zone boundary, where a is the interatomic distance (cf. (5.35)), we obtain

$$\omega_{\rm max} \simeq sa^{-1} \simeq \sqrt{m/M} v_{\rm F} a^{-1}. \tag{9.10}$$

In most metals the interatomic distance a is comparable to the wavelength for an electron at the Fermi surface, $a^{-1} \simeq k_{\rm F}$. Consequently we have

$$\hbar\omega_{\rm max} \simeq \sqrt{m/M}\epsilon_{\rm F},$$
 (9.11)

which shows that typical phonon energies in metals are about one hundredth of the Fermi energy, m/M being about 10^{-4} or less.

9.2 The electron-phonon coupling

We shall show that the electron-phonon interaction has the general form

$$H_{\rm el-ph} = \sum_{\mathbf{k}\mathbf{k}'\sigma\mathbf{q}\alpha} g(\mathbf{k},\mathbf{k}',\mathbf{q},\alpha) c^{\dagger}_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma} (b_{\mathbf{q}\alpha} + b^{\dagger}_{-\mathbf{q}\alpha}).$$
(9.12)

and determine g in a simple model.

The potential energy, due to the ions of the lattice, of an electron at position \mathbf{r} is given by

$$H_{\rm el-ion} = \sum_{i} U(\mathbf{r} - \mathbf{R}_{i}), \qquad (9.13)$$

where \mathbf{R}_i denotes the position of the *i*th ion. It is assumed that the unit cell of the crystal contains only one atom. The potential $U(\mathbf{r})$ is taken to be a Coulomb potential given by

$$U(r) = -\frac{ze^2}{4\pi\epsilon_0 r},\tag{9.14}$$

corresponding to an ion of charge ze. The electron-phonon interaction is caused by the ions oscillating around their equilibrium position. We therefore expand the potential energy (9.13) to first order in the difference $\delta \mathbf{R}_i$ between the actual position \mathbf{R}_i and the equilibrium position \mathbf{R}_i^0 ,

$$\delta \mathbf{R}_i = \mathbf{R}_i - \mathbf{R}_i^0, \tag{9.15}$$

according to

$$\sum_{i} U(\mathbf{r} - \mathbf{R}_{i}) \simeq \sum_{i} U(\mathbf{r} - \mathbf{R}_{i}^{0}) - \sum_{i} \delta \mathbf{R}_{i} \cdot \frac{\partial}{\partial \mathbf{r}} U(\mathbf{r} - \mathbf{R}_{i}^{0}).$$
(9.16)

The phonon operators are introduced as in Section 5.2.2 by a straightforward generalization to three dimensions. Thus we write

$$\delta \mathbf{R}_{i} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}\alpha} Q_{\mathbf{q}\alpha} \bar{\mathbf{e}}_{\mathbf{q}\alpha} \epsilon^{i\mathbf{q}\cdot\mathbf{R}_{i}^{0}}, \qquad (9.17)$$

where N is the total number of atoms, and express Q in terms of creation and annihilation operators, b and b^{\dagger} by inverting the equations corresponding to (5.48-49),

$$Q_{\mathbf{q}\alpha} = \frac{\sqrt{\hbar}}{\sqrt{2M\omega_{\mathbf{q}\alpha}}} (b_{\mathbf{q}\alpha} + b_{-\mathbf{q}\alpha}^{\dagger}). \tag{9.18}$$

Since the electron-ion interaction is a one-body operator as regards the electrons, the electron-phonon Hamiltonian must have the general form

$$H_{\rm el-ph} = \sum_{\mathbf{k}\sigma\mathbf{k}'\sigma'} c^{\dagger}_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} \langle \mathbf{k}'\sigma' | \hat{O} | \mathbf{k}\sigma \rangle, \qquad (9.19)$$

where the operator O is

$$\bar{O} = -\sum_{i} \delta \mathbf{R}_{i} \cdot \frac{\partial}{\partial \mathbf{r}} U(\mathbf{r} - \mathbf{R}_{i}^{0}).$$
(9.20)

Since the electron-ion interaction does not change the spin quantum number σ of the electron, we have that $\sigma' = \sigma$.

Now we evaluate the matrix-element in (9.19) for the case when the electrons are described by plane waves $\exp i\mathbf{k} \cdot \mathbf{r}/V^{1/2}$. We multiply and divide by $\exp i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_i^0$ in order to introduce $\mathbf{r} - \mathbf{R}_i^0$ in the exponent. Furthermore we use that the gradient of -1/r is \mathbf{r}/r^3 , which according to Appendix A has a Fourier-transform given by $-4\pi i \mathbf{q}/q^2$. We sum over lattice points *i*, utilizing that

$$\sum_{i} e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q})\cdot\mathbf{R}_{i}^{0}} = N\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}+\mathbf{G}}, \qquad (9.21)$$

where G is a reciprocal lattice vector¹.

We shall assume that $\mathbf{G} = 0$ is the only reciprocal lattice vector, which satisfies (9.21). In a real metal, processes with $\mathbf{G} \neq 0$ (the socalled *Umklapp* processes) are in fact important, but here we neglect them along with band-structure effects.

When these results are put together, we obtain the following expression for the coupling function $g_{\mathbf{q}}^{0}$ (the superscript 0 means that we have not taken screening into account),

$$g_{\mathbf{q}}^{0} = \frac{ie^{2}z}{\epsilon_{0}g^{2}V} \frac{\sqrt{N\hbar}}{\sqrt{2M\omega_{\mathbf{q}}}} \mathbf{q} \cdot \hat{e}_{\mathbf{q}}.$$
(9.22)

For simplicity we assume that the polarization vectors $\hat{e}_{\mathbf{q}}$ are either parallel or perpendicular to \mathbf{q} . Then (9.22) implies that the electrons only couple to longitudinal phonons, and we may therefore leave out the sum over polarization vectors labelled by the index α . This assumption is not true in real metals, since the phonons in general are neither longitudinal nor transverse, except along symmetry directions. We shall also assume that the phonon spectrum is isotropic, $\omega_{\mathbf{q}} = \omega_{q}$.

It should be noted that (9.22) diverges when q tends to zero. This is due to our neglect of the screening properties of the electron gas. In the longwavelength limit $(q \rightarrow 0)$ the dielectric function according to (8.14) is given by $\epsilon = 1 + k_s^2/q^2$. If we assume the validity of this expression for the dielectric function at larger q as well (which of course constitutes an approximation) we get $g_q = g_q^0/\epsilon$. After taking the square of the modulus of $g_q = g_q^0/\epsilon$ and letting q tend to zero we obtain the long-wavelength limit of the coupling function $g(\mathbf{k}, \mathbf{k}', \alpha) = g_{\mathbf{k}'-\mathbf{k}}$,

$$|g_q|^2 = \lambda \frac{\hbar \omega_q}{2N(0)V}$$
 for $q \to 0.$ (9.23)

Here λ is a constant of order unity, while $\omega_q = sq$ is the longitudinal phonon frequency. As usual we have denoted by N(0) the density of states at the Fermi

¹The set of reciprocal lattice vectors satisfy the condition $\mathbf{G} \cdot \mathbf{R}_{i}^{0} = 2\pi p$, where p is an integer.

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surface per unit volume and per spin. In the calculations that follow we shall consider a unit volume, and the normalization volume V appearing in (9.23) may therefore be replaced by unity.

Since $Nz/V = n = k_F^3/3\pi^2$, the dimensionless parameter λ occurring in (9.23) is

$$\lambda = \frac{z}{6} \frac{\hbar^2 k_{\rm F}^2}{mMs^2},\tag{9.24}$$

when the phonon frequencies are given by the long-wavelength limit $\omega_q = sq$. If the sound velocity s given by (9.9) is inserted into (9.24), the result is seen to be $\lambda = 1/2$.

In the following we shall use the simple long-wavelength form (9.23), even though it is not quantitatively accurate, but we shall also show how the electron-phonon self-energy is obtained without making specific assumptions of the form of the electron-phonon coupling.

9.3 Perturbation treatment

As an introduction to the use of the Green function method we shall first employ ordinary second-order perturbation theory to determine the effect of the electron-phonon interaction on the single-electron energies. The validity of second-order perturbation theory depends on the electron-phonon coupling being weak in the sense $\lambda \ll 1$. In subsequent sections we shall see how the use of Green functions allows one to generalize these results to the case where the electron-phonon interaction is strong.

Let us determine the energy E_p of a state with non-zero momentum $\hbar p$ by adding a particle with momentum $\hbar p$. First we determine the ground-state energy E_0^N of a system with N electrons, to second order in the interaction (9.12). It is

$$E_0^N = \sum_{\mathbf{k}\sigma} \epsilon_k n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'\sigma} \frac{|g_{\mathbf{k}'-\mathbf{k}}|^2 n_{\mathbf{k}'\sigma} (1-n_{\mathbf{k}\sigma})}{\epsilon_{k'} - \epsilon_k - \hbar \omega_{\mathbf{k}'-\mathbf{k}}}.$$
(9.25)

Here $n_{\mathbf{k}\sigma} = 1$ for $k < k_{\mathrm{F}}$, while $n_{\mathbf{k}\sigma} = 0$ for $k > k_{\mathrm{F}}$. There is no contribution to first order in the interaction, since the coupling function $g_{\mathbf{k}'-\mathbf{k}}$ is zero for $\mathbf{k}' = \mathbf{k}$. In order to determine the energy of an excited state of the (N + 1)particle system, we imagine adding a particle to the system in such a manner that the momentum is $\hbar \mathbf{p}$. Then the energy difference $E_p = E_p^{N+1} - E_0^N$ between the two states is

$$E_p = \epsilon_p + \sum_{\mathbf{k}} \frac{|g_{\mathbf{p}-\mathbf{k}}|^2 (1-n_{\mathbf{k}})}{\epsilon_p - \epsilon_k - \hbar \omega_{\mathbf{p}-\mathbf{k}}} - \sum_{\mathbf{k}'} \frac{|g_{\mathbf{k}'-\mathbf{p}}|^2 n_{\mathbf{k}'}}{\epsilon_{k'} - \epsilon_p - \hbar \omega_{\mathbf{k}'-\mathbf{p}}}.$$
 (9.26)

The second term in (9.26) arises because the sum over the occupied states (the k'-sum in (9.25)) must include p, while the last term in (9.26) enters because

the sum over the empty states (the k-sum in (9.25)) must exclude **p**. Note that the last term in (9.26) arises because there is a term in E_0^N which is not in E_p^{N+1} , since the state **p** is filled in the unperturbed (N + 1)-particle state.

The effective mass may be calculated by taking the derivative of E_k with respect to k (we relabel the variable p in (9.26) as k). Since the matrix-element $g_{\mathbf{k}'-\mathbf{k}}$ only depends weakly on k, it is sufficient to consider the k-dependence arising from the occurrence of ϵ_k in the denominator. One gets

$$E_k - \mu = \xi_k (1 - \lambda) \tag{9.27}$$

where

$$\xi_k = \epsilon_k - \mu \tag{9.28}$$

and

$$\bar{\lambda} = -N(0)V \int \frac{d\Omega}{4\pi} |g_{\mathbf{k}-\mathbf{k}'}|^2 \int_0^\infty d\xi_{\mathbf{k}'} \frac{\partial}{\partial\xi_k} \left(\frac{1}{\xi_k - \xi_{\mathbf{k}'} - \hbar\omega_{\mathbf{k}'-\mathbf{k}}} - \frac{1}{\xi_k + \xi_{\mathbf{k}'} + \hbar\omega_{\mathbf{k}'-\mathbf{k}}}\right)|_{\xi_k=0} \quad (9.29)$$

with $d\Omega = 2\pi d(\cos \theta_{kk'})$, where $\theta_{kk'}$ denotes the angle between $\mathbf{k'}$ and \mathbf{k} . Note that we have changed the integration variable $\xi_{k'}$ in the second term into $-\xi_{k'}$. The integral may be carried out by noting that the same terms are generated by taking derivatives with respect to $\xi_{k'}$ and then taking the limit $\xi_k \rightarrow 0$. The result is

$$\bar{\lambda} = N(0)V \int \frac{d\Omega}{4\pi} |g_{\mathbf{k}-\mathbf{k}'}|^2 \int_0^\infty d\xi'_k \frac{\partial}{\partial \xi_{k'}} \left(\frac{1}{-\xi_{k'} - \hbar\omega_{\mathbf{k}'-\mathbf{k}}} - \frac{1}{\xi_{k'} + \hbar\omega_{\mathbf{k}'-\mathbf{k}}}\right),\tag{9.30}$$

which results in the simple expression

$$\bar{\lambda} = 2N(0)V \int \frac{d\Omega}{4\pi} \frac{|g_{\mathbf{k}-\mathbf{k}'}|^2}{\hbar\omega_{\mathbf{k}'-\mathbf{k}}}.$$
(9.31)

The effective mass m^* is defined by the equation

$$\frac{1}{m^*} = \frac{1}{\hbar^2 k} \frac{\partial E_k}{\partial k}|_{k=k_{\rm F}},\tag{9.32}$$

and we consequently obtain that

$$\frac{m}{m^*} = 1 - \bar{\lambda}. \tag{9.33}$$

We have implicitly assumed that $\overline{\lambda} \ll 1$. In the following subsections we shall demonstrate how the use of Green function methods allows us to extend
this result of perturbation theory to higher orders in $\overline{\lambda}$. As we shall see, the result (9.27) will be changed into

$$E_{k} - \mu = \xi_{k} (1 + \bar{\lambda})^{-1} \tag{9.34}$$

with $\bar{\lambda}$ given by (9.31), corresponding to $m^* = m(1 + \bar{\lambda})$. By contrast, the perturbation theory result (9.33) yields $m^* = m/(1 - \bar{\lambda})$, provided $\bar{\lambda} \ll 1$.

A specific calculation of $\overline{\lambda}$ for a given metal requires one to know the form of the electron-phonon coupling function $g_{\mathbf{q}}$. The use of the simple long-wavelength expression (9.23) evidently results in $\overline{\lambda} = \lambda$.

9.4 Phonon Green functions

Phonon propagators are defined in close analogy with fermion propagators. For the single harmonic oscillator, the operator $b+b^{\dagger}$ is proportional to the position operator x. The transition to collective coordinates introduces $(b_{q\alpha} + b^{\dagger}_{-q\alpha})$, cf. (9.18) and Section 5.2.2. We thus define the field operators

$$\phi(\mathbf{q},\tau) = e^{H\tau/\hbar} (b_{\mathbf{q}} + b_{-\mathbf{q}}^{\dagger}) e^{-H\tau/\hbar}, \qquad (9.35)$$

with H being the Hamiltonian (for convenience we have suppressed the polarization index α).

The phonon Green function D is defined by

$$D(\mathbf{q},\tau) = - \langle T_{\tau} \{ \phi(\mathbf{q},\tau) \phi(-\mathbf{q},0) \} \rangle .$$
(9.36)

Since ϕ is a Bose field, the operator T_{τ} is defined as in (7.7) without the factor of $(-1)^p$. The Green function possesses the following symmetry property within the domain $-\hbar\beta < \tau < \hbar\beta$,

$$D(\mathbf{q},\tau) = D(\mathbf{q},\tau + \hbar\beta). \tag{9.37}$$

In order to prove (9.37) we assume that $0 > \tau > -\hbar\beta$. Then

$$\exp(-\beta\Omega)D(\mathbf{q},\tau) = -\operatorname{Tr}\left(\phi(-\mathbf{q},0)e^{H\tau/\hbar}\phi(\mathbf{q},0)e^{-H\tau/\hbar}e^{-\beta H}\right).$$
 (9.38)

Likewise we have

$$\exp(-\beta\Omega)D(\mathbf{q},\tau+\hbar\beta) = -\operatorname{Tr}\left(e^{H\tau/\hbar}e^{\beta H}\phi(\mathbf{q},0)e^{-\beta H}e^{-H\tau/\hbar}\phi(-\mathbf{q},0)e^{-\beta H}\right).$$
(9.39)

Using the cyclic invariance of the trace, the right hand side of (9.38) is seen to be equal to the right hand side of (9.39), resulting in (9.37).

The Fourier-expansion is thus

$$D(\mathbf{q},\tau) = \frac{1}{\beta\hbar} \sum_{n} e^{-i\omega_{n}\tau} D(\mathbf{q},\omega_{n}), \qquad (9.40)$$

where the Matsubara frequencies ω_n are given by

$$\omega_n = 2n \frac{\pi}{\beta \hbar}, \quad n = 0, \pm 1, \pm 2, \pm 3 \cdots.$$
(9.41)

The symmetry property (9.37) together with the relation $\exp(-i\omega_n\beta\hbar) = 1$ allows one to write the Fourier-coefficients $D(\mathbf{q},\omega_n)$ as

$$D(\mathbf{q},\omega_n) = \int_0^{\hbar\beta} d\tau e^{i\omega_n\tau} D(\mathbf{q},\tau).$$
(9.42)

9.4.1 Green functions for free phonons

The Hamiltonian for free phonons is

$$H = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} (b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \frac{1}{2}), \qquad (9.43)$$

cf. (5.51) (we suppress the polarization index α). Since $b_{\mathbf{q}}(\tau)$ satisfies the equation of motion

$$-\hbar \frac{\partial}{\partial \tau} b_{\mathbf{q}} = [b_{\mathbf{q}}(\tau), H] = \hbar \omega_{\mathbf{q}} b_{\mathbf{q}}(\tau), \qquad (9.44)$$

it develops in time according to

$$b_{\mathbf{q}}(\tau) = e^{-\omega_{\mathbf{q}}\tau} b_{\mathbf{q}}(0). \tag{9.45}$$

Likewise

$$-\hbar \frac{\partial}{\partial \tau} b_{\mathbf{q}}^{\dagger} = [b_{\mathbf{q}}^{\dagger}(\tau), H] = -\hbar \omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger}(\tau), \qquad (9.46)$$

which yields

$$b_{\mathbf{q}}^{\dagger}(\tau) = e^{\omega_{\mathbf{q}}\tau} b_{\mathbf{q}}^{\dagger}(0). \tag{9.47}$$

The Green function is therefore given for $\tau > 0$ as

$$D^{(0)}(\mathbf{q},\tau) = - \langle (b_{\mathbf{q}}e^{-\omega_{\mathbf{q}}\tau} + b^{\dagger}_{-\mathbf{q}}e^{\omega_{\mathbf{q}}\tau})(b_{-\mathbf{q}} + b^{\dagger}_{\mathbf{q}}) \rangle_{0}, \qquad (9.48)$$

provided that $\omega_{-\mathbf{q}} = \omega_{\mathbf{q}}$. Now we have

$$< b_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} >_{0} = 1 + N_{\mathbf{q}} \tag{9.49}$$

Figure 9.1: Electron-phonon vertex

and

$$< b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} >_{0} = N_{\mathbf{q}}, \tag{9.50}$$

where N_{q} is the Planck function

$$N_{\mathbf{q}} = \frac{1}{e^{\hbar\omega_{\mathbf{q}}\beta} - 1}.\tag{9.51}$$

The Fourier-transform is seen to be

$$D^{(0)}(\mathbf{q},\omega_n) = \int_0^{\hbar\beta} d\tau e^{i\omega_n\tau} D^{(0)}(\mathbf{q},\tau) = -\frac{1}{i\omega_n + \omega_\mathbf{q}} + \frac{1}{i\omega_n - \omega_\mathbf{q}},\qquad(9.52)$$

where the Matsubara frequencies ω_n assume the values given by (9.41).

9.5 Feynman rules

The derivation of the Feynman rules proceeds in analogy with Chapter 6. The main difference is that the Coulomb interaction lines are replaced by phonon propagators.

The following rules apply to the calculation of the self-energy.

- Draw all topologically different diagrams containing electron and p phonon lines, with vertices as illustrated in Fig. 9.1.
- Associate an oriented 'four-momentum' (\mathbf{k}, ω_n) with each interaction line and conserve four-momentum at each vertex.
- Associate the factor

$$G^{(0)}(\mathbf{k},\omega_n) = \frac{1}{i\omega_n - \xi_k/\hbar} \delta_{\sigma,\sigma'}$$
(9.53)

with each electron line, $\xi_k = \hbar^2 k^2 / 2m - \mu$ being the free-particle (kinetic) energy minus the chemical potential μ .



Figure 9.2: Electron self-energy diagram

• Associate with each phonon line

$$|g_{\mathbf{k}-\mathbf{k}'}|^2 D^{(0)}(\mathbf{q},\omega_n), \qquad (9.54)$$

where the phonon propagator is given by

$$D^{(0)}(\mathbf{q},\omega_n) = -\frac{1}{i\omega_n + \omega_\mathbf{q}} + \frac{1}{i\omega_n - \omega_\mathbf{q}},\tag{9.55}$$

while g is the electron-phonon coupling function.

- Sum over spin, frequency and momentum variables.
- Multiply by

$$\frac{1}{(-\beta\hbar^2)^p}(-1)^F,$$
(9.56)

where F is the number of closed fermion loops.

9.6 The electron self-energy

We shall now calculate the electron self-energy given by the lowest-order diagram exhibited in Fig. 9.2. According to the Feynman rules it is

$$\hbar\Sigma(\mathbf{k},\omega_n) = -\frac{V}{\beta\hbar^2} \int \frac{d\mathbf{q}}{(2\pi)^3} \sum_m |g_\mathbf{q}|^2 G^{(0)}(\mathbf{k}+\mathbf{q},\omega_n+\omega_m) D^{(0)}(\mathbf{q},\omega_m).$$
(9.57)

First we carry out the summation over the Matsubara frequency ω_m with the result

$$-\frac{1}{\beta\hbar^2}\sum_{m}G^{(0)}(\mathbf{k}+\mathbf{q},\omega_n+\omega_m)D^{(0)}(\mathbf{q},\omega_m) = \frac{N_{\mathbf{q}}+1-f_{\mathbf{k}+\mathbf{q}}}{i\hbar\omega_n-\xi_{\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}}} + \frac{N_{\mathbf{q}}+f_{\mathbf{k}+\mathbf{q}}}{i\hbar\omega_n-\xi_{\mathbf{k}+\mathbf{q}}+\hbar\omega_{\mathbf{q}}}.$$
(9.58)



Figure 9.3: Contour in the complex plane

Here f denotes the Fermi distribution.

The sum is calculated as follows. Consider the expression

$$Q = \frac{1}{\beta} \sum_{m} \frac{2\omega_q}{\omega_m^2 + \omega_q^2} \frac{1}{i\omega_n + i\omega_m - \xi_{k'}/\hbar}.$$
(9.59)

Now we have the identity

$$0 = \int_C \frac{dz}{2\pi i} f(z) \frac{1}{e^{z\hbar\beta} - 1}$$
(9.60)

with

$$f(z) = \frac{2\omega_q}{z^2 - \omega_q^2} \frac{1}{i\omega_n + z - \xi_{k'}/\hbar},$$
(9.61)

since the integration contour is chosen as shown in Fig. 9.3. The sum is determined by noting that it is given by (minus) the sum of the residues at $z = 2\pi i m/\hbar\beta$ and hence may be identified with the sum of the other residues at $z = \pm \omega_q$ and $z = \xi_{k'}/\hbar - i\omega_n$. Note that the latter residue involves the factor $\exp(-i\omega_n\hbar\beta)$, which is equal to -1 and hence introduces the Fermi-function $1/(1 + \exp\beta\xi_{k'})$.

After analytic continuation to the real axis, $i\hbar\omega_n \to E + i\eta$, the self-energy then becomes

$$\hbar\Sigma(\mathbf{k}, E/\hbar) = V \int \frac{d\mathbf{k}'}{(2\pi)^3} |g_{\mathbf{k}'-\mathbf{k}}|^2 \left(\frac{N_{\mathbf{k}'-\mathbf{k}}+1-f_{\mathbf{k}'}}{E-\xi_{\mathbf{k}'}-\hbar\omega_{\mathbf{k}'-\mathbf{k}}+i\eta} + \frac{N_{\mathbf{k}'-\mathbf{k}}+f_{\mathbf{k}'}}{E-\xi_{\mathbf{k}'}+\hbar\omega_{\mathbf{k}'-\mathbf{k}}+i\eta}\right).$$
(9.62)

We set $k \simeq k_{\rm F}$, since we are interested in the effect of the electron-phonon interaction on states near the Fermi-surface. In doing the integration over \mathbf{k}' we may set the density of states equal to its value at the Fermi surface. The reason is that only states \mathbf{k}' with $k' \simeq k_{\rm F}$ contribute, due to the smallness of

the maximum phonon energy compared to the Fermi energy. Setting $\mathbf{k}' - \mathbf{k}$ equal to q, we write the integration over \mathbf{k}' as

$$\int \frac{d\mathbf{k}'}{(2\pi)^3} \cdots = N(0) \frac{1}{2} \int_{-1}^{1} d(\cos \theta_{\mathbf{k}'\mathbf{k}}) \int_{-\infty}^{\infty} d\xi' \cdots$$
$$= N(0) \int_{0}^{2\mathbf{k}_{\mathrm{F}}} \frac{qdq}{2\mathbf{k}_{\mathrm{F}}^2} \int_{-\infty}^{\infty} d\xi' \cdots, \qquad (9.63)$$

where

$$N(0) = \frac{mk_{\rm F}}{2\pi^2\hbar^2} \tag{9.64}$$

is the density of states at the Fermi energy.

We define

$$\alpha^2 F(\omega) = N(0) V \int_0^{2k_{\rm F}} \frac{q dq}{2\hbar k_{\rm F}^2} |g_q|^2 \delta(\omega - \omega_q)$$
(9.65)

and separate Σ in real and imaginary parts according to

$$\Sigma = \Sigma_1 + i\Sigma_2. \tag{9.66}$$

Since

$$1 + N(\omega_q) - f(\xi') = \frac{1}{2} \left(\coth \frac{\beta \hbar \omega_q}{2} + \tanh \frac{\beta \xi'}{2} \right)$$
(9.67)

and

$$N(\omega_q) + f(\xi') = \frac{1}{2} \left(\coth \frac{\beta \hbar \omega_q}{2} - \tanh \frac{\beta \xi'}{2} \right), \tag{9.68}$$

the dependence of Σ_1 on the frequency variable E/\hbar is given by

$$\Sigma_{1}(E) = \int_{0}^{\infty} d\omega \alpha^{2} F(\omega)$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} d\xi' (\tanh \frac{\beta \xi'}{2} \{ \frac{1}{E - \xi' - \hbar \omega} - \frac{1}{E - \xi' + \hbar \omega} \}$$

$$+ \operatorname{coth} \frac{\beta \hbar \omega}{2} \{ \frac{1}{E - \xi' - \hbar \omega} + \frac{1}{E - \xi' + \hbar \omega} \})$$

$$= -\int_{0}^{\infty} d\omega \alpha^{2} F(\omega) \frac{1}{2} \int_{-\infty}^{\infty} dE' \frac{1}{E' + \hbar \omega}$$

$$(\tanh \frac{(E + E')\beta}{2} + \tanh \frac{(E - E')\beta}{2}). \qquad (9.69)$$

The second equality is obtained by exploiting that the coth-term yields zero when integrated over ξ' , as may be seen by introducing the integration variable $E' = E - \xi'$ and noting that the integrand is an odd function of E'.

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Figure 9.4: Real part $\hbar \Sigma_1$ of the self-energy

It is seen from (9.69) that the real part of the self-energy is odd in E, $\Sigma_1(E) = -\Sigma_1(-E)$. At T = 0 K we get

$$\Sigma_{1}(E) = -\int_{0}^{\infty} d\omega \alpha^{2} F(\omega) \int_{-E}^{E} dE' \frac{1}{E' + \hbar\omega}$$
$$= -\int_{0}^{\infty} d\omega \alpha^{2} F(\omega) \ln \frac{|\hbar\omega + E|}{|\hbar\omega - E|}.$$
(9.70)

In the following we assume that the phonon frequencies ω_q are given as $\omega_q = sq$ for $\omega < \omega_D$, where $\omega_D = 2sk_F$ is a characteristic frequency of the order of the Debye frequency. Furthermore, we shall use the model form (9.23) for all wavevectors corresponding to $0 < \omega_q < \omega_D$. When (9.23) is inserted into (9.65), one therefore obtains that

$$\alpha^2 F(\omega) = \lambda \frac{\omega^2}{\omega_D^2} \quad \text{for} \quad \omega < \omega_D$$
 (9.71)

and

$$\alpha^2 F(\omega) = 0 \quad \text{for} \quad \omega > \omega_D. \tag{9.72}$$

As we shall see below, the mass-renormalization is generally given by a definite frequency moment of the function $\alpha^2 F(\omega)$ defined in (9.65), regardless of its specific form. For the simple model form given by (9.6) and (9.72) the result is 7/

$$\hbar\Sigma_1(E) = -E \int_0^\infty d\omega \alpha^2 F(\omega) \frac{2}{\omega} = -\lambda E \quad \text{for} \quad E \ll \hbar\omega_D \tag{9.73}$$

and

$$\hbar\Sigma_1(E) = -\int_0^\infty d\omega \alpha^2 F(\omega) \frac{2\hbar^2 \omega}{E} = -\lambda \frac{(\hbar\omega_D)^2}{2E} \quad \text{for} \quad E \gg \hbar\omega_D \quad (9.74)$$

The real part of the self-energy is sketched as a function of E on Fig. 9.4.

When we use the low-energy limit of Σ_1 given by (9.73) in the electron Green function, its denominator is seen to be $E - \hbar \Sigma_1(E) - \xi \simeq E(1+\lambda) - \xi$,

and the pole is therefore given by $E = \xi/(1 + \lambda)$. The effective mass thus becomes

$$m^* = m(1+\lambda). \tag{9.75}$$

If we use a more general form for the electron-phonon coupling than (9.23) we obtain (9.75) with λ replaced by $\overline{\lambda}$ given by

$$\bar{\lambda} = \int_0^\infty d\omega \alpha^2 F(\omega) \frac{2}{\omega}, \qquad (9.76)$$

as may be seen from the low-energy expansion (9.73). The function $\alpha^2 F(\omega)$ is here given by (9.65). By tunneling experiments it is possible to measure directly the frequency dependence of $\alpha^2 F$, which in metals has much more structure as a function of frequency than the simple model form given by (9.6) and (9.72).

The electron-phonon interaction is thus seen to have a significant effect on electron states lying near the Fermi surface. The mass-renormalization results in an increase by the factor $(1 + \bar{\lambda})$ of the low-temperature specific heat, in agreement with what is observed in metals. In Section 1.3.1 we saw that the observed enhancement factor was 1.38 in aluminium. If we calculate λ from (9.24), using the measured sound velocity of aluminium, we find that $\lambda = 0.9$, corresponding to an enhancement factor of 1.9. This result, however, is based on the assumption that the electron-phonon coupling function g may be identified with its long-wavelength limit (9.23). In reality the electron-ion pseudopotential (which we implicitly have taken to be independent of q) is reduced relative to its long-wavelength limit, when q becomes comparable to $k_{\rm F}$. If this effect is taken into account in (9.65), one finds from (9.76) that the enhancement factor $(1+\bar{\lambda})$ is 1.4 for aluminium, in agreement with experiment.

The spin susceptibility, however, is essentially unaffected by the interaction between electrons and phonons, because the electron-phonon interaction (unlike the Coulomb interaction) effectively only involves states near the Fermi surface within an energy shell of a thickness equal to the Debye energy. When the interaction between the electrons is screened in the Thomas-Fermi approximation (the long-wavelength limit of the random phase approximation), one obtains as we have seen in Section 4.3.2 an increase of the spin susceptibility by 34%. The corresponding effect due to the phonons is reduced by the ratio of the Debye energy to the Fermi energy and is therefore entirely negligible.

10 Superconductivity

The phenomenon of superconductivity was discovered experimentally early in this century, but it took more than 40 years before the theory was developed. The basic clue to the understanding of superconductivity was given in 1956 by Cooper, who showed that the Fermi sea of electrons is unstable with regard to the formation of bound pairs with zero total momentum and spin, provided there exists an attractive interaction between electrons near the Fermi surface. These Cooper pairs formed the starting point for the theory of superconductivity due to Bardeen, Cooper and Schrieffer (1957). The BCS-model keeps only that part of the many-body interaction Hamiltonian, which connects pairs of electrons with total momentum and total spin equal to zero. This simplified Hamiltonian may be diagonalized by means of a canonical transformation, as described in Section 5.4. The resulting energy spectrum exhibits a gap, which depends on temperature. The BCS theory was astonishingly successful in explaining essential all the important features of superconductivity that had been observed prior to 1957. Furthermore, it provided a general framework for the further development of the theory of superconductivity, including the prediction and subsequent observation of the Josephson effects, which involve tunneling of Cooper pairs (Josephson 1962).

In the present chapter we shall derive the basic equations of superconductivity by use of temperature Green functions. The resulting *Gorkov equations* (Gorkov 1958) are more general than the original BCS-model in that they may be applied to spatially inhomogeneous situations, where boundaries or external magnetic fields play an important role. The Gorkov equations may also be generalized to take into account the retarded nature of the attractive interaction between electrons due to the exchange of phonons, leading to a description of *strong-coupling* superconductivity.

10.1 The Gorkov equations

The Gorkov formulation of the theory of superconductivity starts with the following model Hamiltonian

$$H = \int d\mathbf{x} \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{x}) (-\frac{\hbar^2}{2m} \nabla^2) \psi_{\sigma}(\mathbf{x}) + \frac{g}{2} \int d\mathbf{x} \sum_{\sigma\sigma'} \psi_{\sigma'}^{\dagger}(\mathbf{x}) \psi_{\sigma'}^{\dagger}(\mathbf{x}) \psi_{\sigma'}(\mathbf{x}) \psi_{\sigma}(\mathbf{x}),$$
(10.1)

where it has been assumed that the interaction $V(\mathbf{x}, \mathbf{x}')$ has zero range,

$$V(\mathbf{x}, \mathbf{x}') = g\delta(\mathbf{x} - \mathbf{x}'), \qquad (10.2)$$

and therefore involves opposite-spin particles ($\sigma' = -\sigma$) only. The constant g is negative for attractive interaction, positive for repulsive interaction.

In the Schrödinger picture the operators $\psi(\mathbf{x})$ satisfy the usual anticommutation rules

$$\{\psi_{\sigma}(\mathbf{x}), \psi_{\sigma'}^{\dagger}(\mathbf{x}')\} = \delta_{\sigma\sigma'}\delta(\mathbf{x} - \mathbf{x}')$$
(10.3)

and

$$\{\psi_{\sigma}(\mathbf{x}),\psi_{\sigma'}(\mathbf{x}')\}=\{\psi_{\sigma}^{\dagger}(\mathbf{x}),\psi_{\sigma'}^{\dagger}(\mathbf{x}')\}=0.$$
(10.4)

The grand-canonical Hamiltonian is $K = H - \mu N$, where N is the particle number operator. The BCS-model is equivalent to replacing K by the effective grand-canonical Hamiltonian K_{eff} , where

$$K_{\text{eff}} = \int d\mathbf{x} \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{x}) (-\frac{\hbar^2}{2m} \nabla^2 - \mu) \psi_{\sigma}(\mathbf{x}) + g \int d\mathbf{x} (<\psi_{\downarrow}^{\dagger}(\mathbf{x}) \psi_{\uparrow}^{\dagger}(\mathbf{x}) > \psi_{\uparrow}(\mathbf{x}) \psi_{\downarrow}(\mathbf{x}) + \psi_{\downarrow}^{\dagger}(\mathbf{x}) \psi_{\uparrow}^{\dagger}(\mathbf{x}) < \psi_{\uparrow}(\mathbf{x}) \psi_{\downarrow}(\mathbf{x}) >).$$
(10.5)

Here the thermal average involves the effective grand-canonical Hamiltonian,

$$<\psi_{\downarrow}^{\dagger}(\mathbf{x})\psi_{\uparrow}^{\dagger}(\mathbf{x})>=\frac{\mathrm{Tr}(e^{-\beta K_{\mathrm{eff}}}\psi_{\downarrow}^{\dagger}(\mathbf{x})\psi_{\uparrow}^{\dagger}(\mathbf{x}))}{\mathrm{Tr}e^{-\beta K_{\mathrm{eff}}}}.$$
(10.6)

Since the number operator N does not commute with the Hamiltonian K_{eff} , this average is nonvanishing.

The equations of motion for the Heisenberg operators

$$\psi(\mathbf{x},\tau) = e^{K_{\text{eff}}\tau/\hbar}\psi(\mathbf{x})e^{-K_{\text{eff}}\tau/\hbar}$$
(10.7)

and

$$\psi^{\dagger}(\mathbf{x},\tau) = e^{K_{\text{eff}}\tau/\hbar}\psi^{\dagger}(\mathbf{x})e^{-K_{\text{eff}}\tau/\hbar}$$
(10.8)

are

$$\hbar \frac{\partial}{\partial \tau} \psi_{\uparrow}(\mathbf{x},\tau) = -(-\frac{\hbar^2}{2m} \nabla^2 - \mu) \psi_{\uparrow}(\mathbf{x},\tau) + g < \psi_{\uparrow}(\mathbf{x}) \psi_{\downarrow}(\mathbf{x}) > \psi_{\downarrow}^{\dagger}(\mathbf{x},\tau) \quad (10.9)$$

and

$$\hbar \frac{\partial}{\partial \tau} \psi_{\downarrow}^{\dagger}(\mathbf{x},\tau) = \left(-\frac{\hbar^2}{2m} \nabla^2 - \mu\right) \psi_{\downarrow}^{\dagger}(\mathbf{x},\tau) + g < \psi_{\downarrow}^{\dagger}(\mathbf{x}) \psi_{\uparrow}^{\dagger}(\mathbf{x}) > \psi_{\uparrow}(\mathbf{x},\tau).$$
(10.10)

With the help of these equations one finds that the Green function G defined by

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = - \langle T_{\tau}\{\psi_{\uparrow}(\mathbf{x},\tau)\psi_{\uparrow}^{\dagger}(\mathbf{x}',\tau')\}\rangle$$
(10.11)

satisfies

$$\begin{split} \hbar \frac{\partial}{\partial \tau} G(\mathbf{x}, \tau; \mathbf{x}', \tau') &= -\hbar \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') - (-\frac{\hbar^2}{2m} \nabla^2 - \mu) G(\mathbf{x}, \tau; \mathbf{x}', \tau') \\ &- g < \psi_{\uparrow}(\mathbf{x}) \psi_{\downarrow}(\mathbf{x}) > < T_{\tau} \{ \psi_{\downarrow}^{\dagger}(\mathbf{x}, \tau) \psi_{\uparrow}^{\dagger}(\mathbf{x}', \tau') \} > (10.12) \end{split}$$

We note that the equation of motion for the Green function involves a new type of *anomalous* Green function, defined by

$$F(\mathbf{x},\tau;\mathbf{x}',\tau') = - \langle T_{\tau} \{ \psi_{\uparrow}(\mathbf{x},\tau) \psi_{\downarrow}(\mathbf{x}',\tau') \} \rangle .$$
(10.13)

In addition we introduce the function F^{\dagger} by

$$F^{\dagger}(\mathbf{x},\tau;\mathbf{x}',\tau') = - \langle T_{\tau}\{\psi^{\dagger}_{\downarrow}(\mathbf{x},\tau)\psi^{\dagger}_{\uparrow}(\mathbf{x}',\tau')\} \rangle .$$
(10.14)

The function F^{\dagger} is not the Hermitian conjugate of F.

An important role is played by the gap parameter Δ , which is defined by

$$\Delta(\mathbf{x}) \equiv -gF(\mathbf{x}, \tau + 0^+; \mathbf{x}, \tau) = g < \psi_{\uparrow}(\mathbf{x})\psi_{\downarrow}(\mathbf{x}) > .$$
(10.15)

The equation of motion satisfied by G may then be written as

$$(-\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu)G(\mathbf{x},\tau;\mathbf{x}',\tau') + \Delta(\mathbf{x})F^{\dagger}(\mathbf{x},\tau;\mathbf{x}',\tau') = \\ \hbar\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau') \qquad (10.16)$$

Correspondingly we find

$$(-\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu)F(\mathbf{x},\tau;\mathbf{x}',\tau') - \Delta(\mathbf{x})G(\mathbf{x}',\tau';\mathbf{x},\tau) = 0 \qquad (10.17)$$

and

$$\left(\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla_{\tau}^2 + \mu\right)F^{\dagger}(\mathbf{x},\tau;\mathbf{x}',\tau') - \Delta^{*}(\mathbf{x})G(\mathbf{x},\tau;\mathbf{x}',\tau') = 0, \quad (10.18)$$

which are the Gorkov equations. In the presence of a magnetic field described by the vector potential \mathbf{A} the equations (10.16) and (10.17) are modified according to

$$\frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\nabla + e\mathbf{A} \tag{10.19}$$

where e is the magnitude of the electron charge, while in (10.18) one has

$$\frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\nabla - e\mathbf{A}.$$
(10.20)

These changes are due to the corresponding change in the first term of (10.1), which becomes

$$\frac{1}{2m} \int d\mathbf{x} \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{x}) (\frac{\hbar}{i} \nabla + e\mathbf{A})^2 \psi_{\sigma}(\mathbf{x}).$$
(10.21)

In the presence of a vector potential, with the proper boundary conditions added, the Gorkov equations are in general difficult to solve. A considerable simplification may be achieved for slow spatial variations (on the scale of the Fermi wavelength) by integrating out the magnitude of the momentum, i. e. integrating out the normal-state energy variable ξ_k defined by

$$\xi_k = \frac{\hbar^2 k^2}{2m} - \mu. \tag{10.22}$$

This results in the so-called *quasi-classical* approximation, which has been used to solve a great variety of important problems, including ones involving nonequilibrium phenomena, but we shall not develop this approximation scheme here.

In the following we consider the Gorkov equations under the simplifying condition that the system is spatially uniform. This implies that the gap parameter $\Delta(\mathbf{x})$ is a constant in space, $\Delta(\mathbf{x}) = \Delta$. First we shall recover the results of the BCS-theory. Since the Hamiltonian is time-independent and the system is assumed to be spatially uniform, we may expand the Green functions in the Fourier-series

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{1}{\hbar\beta} \int \frac{d\mathbf{k}}{(2\pi)^3} \sum_{n} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} e^{-i\omega_n(\tau-\tau')} G(\mathbf{k},\omega_n)$$
(10.23)

and

$$F^{\dagger}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{1}{\hbar\beta} \int \frac{d\mathbf{k}}{(2\pi)^3} \sum_{n} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} e^{-i\omega_{n}(\tau-\tau')} F^{\dagger}(\mathbf{k},\omega_{n}). \quad (10.24)$$

Then (10.16) becomes

$$(i\hbar\omega_n - \xi_k)G(\mathbf{k},\omega_n) + \Delta F^{\dagger}(\mathbf{k},\omega_n) = \hbar, \qquad (10.25)$$

while (10.18) is

$$(-i\hbar\omega_n - \xi_k)F^{\dagger}(\mathbf{k},\omega_n) - \Delta^* G(\mathbf{k},\omega_n) = 0.$$
(10.26)

The gap parameter Δ is given by the self-consistency equation

$$\Delta^* = -g \frac{1}{\hbar\beta} \int \frac{d\mathbf{k}}{(2\pi)^3} \sum_n e^{-i\omega_n \eta} F^{\dagger}(\mathbf{k}, \omega_n).$$
(10.27)

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Figure 10.1: The temperature-dependent energy gap $\Delta(T)$

The solution to the equations (10.25) and (10.26) are seen to be

$$G(\mathbf{k},\omega_n) = -\hbar \frac{i\hbar\omega_n + \xi_k}{(\hbar\omega_n)^2 + \xi_k^2 + |\Delta|^2}$$
(10.28)

and

$$F^{\dagger}(\mathbf{k},\omega_n) = \hbar \frac{\Delta^*}{(\hbar\omega_n)^2 + \xi_k^2 + |\Delta|^2},$$
(10.29)

where ξ_k is defined in (10.22). When the magnetic field is zero, we may choose Δ to be real, implying that

$$F^{\dagger}(\mathbf{k},\omega_n) = F(\mathbf{k},\omega_n). \tag{10.30}$$

The coherence factors u and v occurring in the BCS-theory (cf. Section 5.4) may be used to write the Green functions in the form

$$G(\mathbf{k},\omega_n) = \frac{u_k^2}{i\omega_n - (E_k/\hbar)} + \frac{v_k^2}{i\omega_n + (E_k/\hbar)}$$
(10.31)

together with

$$F^{\dagger}(\mathbf{k},\omega_n) = F(\mathbf{k},\omega_n) = -\frac{u_k v_k}{i\omega_n - (E_k/\hbar)} + \frac{u_k v_k}{i\omega_n + (E_k/\hbar)},$$
(10.32)

where

$$E_k^2 = \Delta^2 + \xi_k^2. \tag{10.33}$$

Furthermore we have

$$u_k^2 + v_k^2 = 1, (10.34)$$

and

$$u_k v_k = \frac{\Delta}{2E_k}.\tag{10.35}$$

We need to determine Δ from the self-consistency equation (10.27). When F^{\dagger} is inserted, it becomes

$$\Delta = -\frac{g}{\beta} \int \frac{d\mathbf{k}}{(2\pi)^3} \sum_{n} \frac{\Delta}{(\hbar\omega_n)^2 + \xi_k^2 + \Delta^2}$$
(10.36)

We may carry out the frequency sum, in the manner of Chapter 7, by inserting (10.32) into the expression for Δ and use $uv = \Delta/2E$. The result is the BCS gap-equation

$$\Delta = -g \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\Delta}{2E_k} \tanh(\beta E_k/2).$$
(10.37)

Note that $\tanh(\beta E_k/2)$ tends to 1 in the limit of zero temperature. In this limit (10.37) is identical to (5.70), since the ground-state average $\langle c_{\mathbf{k}',\uparrow}^{\dagger}c_{-\mathbf{k}',\downarrow}^{\dagger} \rangle$ is seen to be equal to $\Delta/2E_k$ as a consequence of the Bogoliubov-transformation (5.14) and (10.35).

The solution to the gap equation may be expressed in terms of the dimensionless coupling constant λ , which we define by

$$\lambda = -gN(0). \tag{10.38}$$

Then the gap equation (10.37) may be written as

$$\Delta = \lambda \int_0^{\hbar\omega_D} d\xi_k \frac{\Delta}{(\Delta^2 + \xi_k^2)^{1/2}} \tanh(\beta E_k/2).$$
(10.39)

At zero temperature we obtain from carrying out the integral over ξ that

$$\Delta = \Delta(0) = 2\hbar\omega_D e^{-1/\lambda},\tag{10.40}$$

provided $\hbar\omega_D \gg \Delta(0)$. The transition temperature T_c is determined as the highest temperature for which (10.39) has a solution. It must therefore satisfy

$$1 = \lambda \int_0^{\hbar\omega_D} d\xi_k \frac{1}{\xi_k} \tanh(\xi_k/2kT_c), \qquad (10.41)$$

which yields

$$kT_c = \frac{2e^{\gamma}}{\pi} \hbar \omega_D e^{-1/\lambda}, \qquad (10.42)$$

provided $\hbar\omega_D \gg kT_c$. Here $\gamma = 0.577 \cdots$ is the Euler constant.

According to (10.40) and (10.42) the ratio between the zero-temperature gap and kT_c is a universal constant,

$$\frac{\Delta(0)}{kT_c} = 1.76. \tag{10.43}$$

This important result of the BCS-theory is in good agreement with experiment for many different superconducting materials, with widely different values of $\Delta(0)$ and T_c . The deviations observed in strong-coupling superconductors such as Pb or Hg may be explained by taking into account the retarded nature of the interaction responsible for superconductivity.

Near the transition temperature T_c one finds from (10.36) that

$$\Delta \simeq 3.06 k T_c (1 - T/T_c)^{1/2}. \tag{10.44}$$

This temperature dependence is in agreement with that obtained from Landau's theory of second-order phase transitions, as we shall see below.

10.2 Ginzburg-Landau theory

Near the transition temperature T_c it is possible to perform an expansion in the parameter Δ/kT_c , since Δ goes continuously to zero in the manner characteristic of a second-order transition. In addition an expansion in gradients or "slowness of variation" is carried out. This allows one to reduce the Gorkov equations for superconductors to the Ginzburg-Landau equations, which are coupled equations for the Ginzburg-Landau 'wavefunction' $\Psi(\mathbf{x})$ and the vector potential $\mathbf{A}(\mathbf{x})$. One finds that $\Psi(\mathbf{x})$ is related to the gap-parameter $\Delta(\mathbf{x})$ by

$$\Psi(\mathbf{x}) = \left(\frac{7\zeta(3)n}{8\pi^2(kT_c)^2}\right)^{1/2} \Delta(\mathbf{x})$$
(10.45)

with n being the number density of electrons in the normal state. The resulting equation for Ψ obtained by the expansion of the Gorkov equations is reminiscent of the Schrödinger equation, with the addition of a non-linear (cubic) term,

$$\frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - e^* \mathbf{A}\right)^2 \Psi(\mathbf{x}) + a \Psi(\mathbf{x}) + b \Psi(\mathbf{x}) |\Psi(\mathbf{x})|^2 = 0.$$
(10.46)

Here, the effective mass m^* is

$$m^* = 2m \tag{10.47}$$

while the effective charge e^* is

$$e^* = -2e, (10.48)$$

reflecting the presence of Cooper pairs in the condensed state. The constants a and b are found to be

$$a = -\frac{6\pi^2 (kT_c)^2}{7\zeta(3)\epsilon_{\rm F}} (1 - \frac{T}{T_c})$$
(10.49)

while

$$b = \frac{6\pi^2 (kT_c)^2}{7\zeta(3)\epsilon_{\rm F} n}.$$
 (10.50)

We have introduced the Fermi energy $\epsilon_{\rm F} = \hbar^2 k_{\rm F}^2/2m$. It is related to the density of states N(0) through $N(0) = 3n/4\epsilon_{\rm F}$. Under spatially homogeneous conditions one finds from (10.46) that

$$|\Psi|^2 = -\frac{a}{b} = n(1 - \frac{T}{T_c}). \tag{10.51}$$

When Ψ is expressed in terms of Δ this becomes

$$|\Delta|^2 = \frac{8\pi^2 (kT_c)^2}{7\zeta(3)} (1 - \frac{T}{T_c}).$$
(10.52)

The other Ginzburg-Landau equation besides (10.46) relates the supercurrent density j to the vector potential and the gradient of Ψ according to

$$\mathbf{j} = e^* \frac{\hbar}{2m^* i} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) - \frac{(e^*)^2}{m^*} |\Psi|^2 \mathbf{A}.$$
(10.53)

The two Ginzburg-Landau equations must be supplemented by boundary conditions on Ψ and the vector potential. These boundary conditions will be discussed below, where we indicate how the Ginzburg-Landau equations are derived phenomenologically within the context of the general theory of secondorder phase transitions.

10.2.1 Second-order phase transitions

The Ginzburg-Landau equations (10.46) and (10.53) were derived by Ginzburg and Landau¹ well before the advent of the microscopic theory due to Bardeen, Cooper and Schrieffer. The parameters occurring in the equations therefore had to be fixed by comparison to experiment. The starting point was Landau's general theory of second-order phase transitions. According to this theory², the difference in free energy between the normal state and the 'condensed' state (here the superconducting state) may be written as a series expansion in the magnitude of an order parameter. In the present case the order parameter is the quantity Ψ , which was introduced above on the basis of the microscopic theory. While the assumption of the existence of such a series expansion may seem natural, it does in fact imply that the system is well described by a mean field. The mean-field assumption is generally an excellent one for superconductors but it breaks down for many other physical systems, yielding critical exponents

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¹V. L. Ginzburg and L. D. Landau, Zh. Eksp. Teor. Fiz. 20, 1064, 1950.

²Landau and Lifshitz: Statistical Physics, vol I.

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Figure 10.2: The free energy difference $\Delta G = G_s - G_n$ as a function of $|\Psi|^2$ under spatially homogeneous conditions

that differ from the mean-field values mentioned below. Spatial variations are taken into account by a gradient expansion, which limits the validity of Ginzburg-Landau theory to slow spatial variations.

According to the Ginzburg-Landau theory, the difference in the Gibbs freeenergy density G_s in the superconducting state and the corresponding freeenergy density in the normal state, G_n , may be written as

$$G_s - G_n = a|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{2m^*}|(\frac{\hbar}{i}\nabla - e^*\mathbf{A})\Psi|^2 + \frac{1}{2\mu_0}B^2 - \mathbf{B}\cdot\mathbf{H}_{\text{ext}}.$$
 (10.54)

The absence of terms linear and cubic in Ψ follows from the fact that G_s must be unchanged under a change of phase of the order parameter. Such changes are associated with gauge transformations. The order parameter Ψ itself is not invariant under gauge transformations. This is the broken symmetry of the superconducting state. Its analogue in the case of ferromagnetism is the breaking of the rotational symmetry associated with the magnetic moment of the ordered state pointing in a definite direction. The gradient term was written in a form reminiscent of the kinetic energy of quantum mechanics. When comparing their theory to experiment Ginzburg and Landau took m^* to be equal to the electron mass. The last terms in (10.54) are due to the magnetic induction, $\mathbf{B} = \nabla \times \mathbf{A}$, with \mathbf{H}_{ext} being the externally controlled field strength. In Fig. 10.2 we illustrate the dependence of the free energy difference on $|\psi|^2$ in two cases, a) $T > T_c$ and b) $T < T_c$ under spatially homogeneous conditions.

The Ginzburg-Landau equations result from varying (10.54) with respect to Ψ^* and **A**, with the following boundary condition at the surface,

$$\dot{\mathbf{n}} \cdot (\frac{\hbar}{i} \nabla - e^* \mathbf{A}) \Psi = 0, \qquad (10.55)$$

n being the surface normal, and

$$\hat{\mathbf{n}} \times (\mathbf{B} - \mu_0 \mathbf{H}_{\text{ext}}) = 0. \tag{10.56}$$

These boundary conditions ensure the vanishing of the surface terms arising from the variation of the functional (10.54) with respect to Ψ and \mathbf{A} . Physically, (10.55) ensures that no current is leaving the sample at the boundary, while (10.56) expresses that the tangential component of the magnetic field is continuous across the metal surface.

In the following we shall give a few examples of simple solutions to the Ginzburg-Landau equations. These examples introduce the two important characteristic lengths, the coherence length $\xi(T)$ and the penetration depth $\lambda(T)$.

10.2.2 Characteristic lengths

Let us first consider a situation without an magnetic field, and furthermore assume that the order parameter only varies in the x-direction. Then (10.46) becomes

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}\Psi(x) + a\Psi(x) + b\Psi(x)|\Psi(x)|^2 = 0.$$
(10.57)

In order to study solutions of this equation one may introduce the dimensionless length variable \tilde{x} by

$$\tilde{x} = \frac{x}{\xi},\tag{10.58}$$

where

$$\xi^2 = \xi^2(T) = \frac{\hbar^2}{2m^*|a|}.$$
(10.59)

The length $\xi(T)$ is the temperature-dependent coherence length. It follows from (10.49) and (10.59) that $\xi(T)$ is proportional to $(1 - T/T_c)^{-1/2}$ and thus becomes larger as the critical temperature is approached from below. This is the general behavior of the coherence length within Landau's theory of secondorder phase transitions. The temperature dependence is due to the fact that a is proportional to $(1 - T/T_c)$, which is also responsible for the $(1 - T/T_c)^{1/2}$ dependence of $|\Psi|$ or $|\Delta|$ in the homogeneous case, cf. (10.44) and (10.52). In the theory of critical phenomena such exponents characterizing the temperature dependence of the coherence length and the order parameter are called critical exponents. In general one writes

$$|\Psi| \propto (T_c - T)^{\beta} \tag{10.60}$$

and

$$\xi \propto (T_c - T)^{-\nu}$$
. (10.61)

The fact that β and ν both are 1/2 reflects that the BCS-theory is a meanfield theory. In the case of superconductivity the mean-field description yields excellent results except in a very small temperature region in the immediate vicinity of the transition temperature.

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The penetration depth of a magnetic field may be obtained by combining the Ginzburg-Landau equation without the gradient-term,

$$\mathbf{j} = -\frac{(e^*)^2}{m^*} |\Psi|^2 \mathbf{A},$$
(10.62)

with the Maxwell equation $\tilde{\mu}_0^{\prime} \nabla \times \mathbf{B} = \mathbf{j}$. By taking the rotation of (10.62), assuming Ψ to be spatially uniform, we obtain

$$\nabla^2 \mathbf{B} = \frac{\mu_0(e^*)^2}{m^*} |\Psi|^2 \mathbf{B} = \frac{1}{\lambda^2} \mathbf{B}, \qquad (10.63)$$

where the characteristic length λ is given by

$$\lambda^{2} = \frac{m^{*}}{\mu_{0}(e^{*})^{2}|\Psi|^{2}} = \frac{m^{*}b}{\mu_{0}(e^{*})^{2}|a|}.$$
(10.64)

We shall now determine the critical magnetic field for the nucleation of the superconducting state in terms of the parameters of the Ginzburg-Landau theory.

Let us assume that the magnetic field in the normal state is given by the vector potential

$$\mathbf{A} = B(0, x, 0). \tag{10.65}$$

Since we shall determine the critical value of B for the nucleation of the superconducting state we may use the vector potential (10.65) in the first Ginzburg-Landau equation (10.46) and neglect the non-linear term. The equation then becomes identical to the eigenvalue equation for a particle moving in a harmonic-oscillator potential,

$$\frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - e^* \mathbf{A}\right)^2 \Psi(\mathbf{x}) = -a \Psi(\mathbf{x}).$$
(10.66)

If we assume that Ψ only depends on x, the operator on the left-hand side of (10.66) is

$$\frac{1}{2m^*}(-\hbar^2\frac{d^2}{dx^2} + (e^*B)^2x^2), \qquad (10.67)$$

which is the Hamiltonian for a harmonic oscillator with the smallest eigenvalue equal to $\hbar |e^*|B/2m^*$. The nucleation of the superconducting state sets in, when this eigenvalue is equal to |a|. The upper critical field B_{c2} (commonly called H_{c2}) is thus given by the equation

$$\frac{\hbar|e^*|B_{c2}}{2m^*} = |a|. \tag{10.68}$$

When the values of the parameters are inserted in (10.68), the upper critical field becomes

$$B_{c2} = \frac{12\pi^2 (kT_c)^2 m}{7\zeta(3)\epsilon_{\rm F} e\hbar} (1 - \frac{T}{T_c}).$$
(10.69)

The quantity

$$\xi_0 = \frac{\hbar v_{\rm F}}{kT_c} \tag{10.70}$$

is a characteristic length, of magnitude 100 to 10000 Å for typical superconductors. Apart from a numerical constant, the magnetic field B_{c2} is seen to be equal to $h/e\xi_0^2$ times the temperature dependent factor $1 - T/T_c$.

10.2.3 The Josephson effects

Finally, we shall briefly mention the special effects associated with the weak coupling between two superconductors that are spatially separated. The effects were predicted theoretically by Josephson, and subsequently verified in great detail by experiments. The Josephson effect is the most direct demonstration of the existence of two conjugate variables, the phase of the order parameter and the number of Cooper pairs.

Josephson considered two superconductors separated by a thin insulating barrier and found, on the basis of a Green function calculation, that a supercurrent I could flow across the barrier in the absence of any voltage difference. When the order parameters in the two superconductors are written in terms of their magnitude f and phase ϕ

$$\Psi_1 = f_1 e^{i\phi_1} \tag{10.71}$$

and

$$\Psi_2 = f_2 e^{i\phi_2},\tag{10.72}$$

the supercurrent was given by the simple expression

$$I = I_0 \sin \phi, \tag{10.73}$$

with ϕ being the phase difference between the two superconductors,

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$$\phi = \phi_1 - \phi_2. \tag{10.74}$$

The zero-temperature value of I_0 was found to be

$$I_0 = \frac{\pi \sigma_0 \Delta}{2e}.\tag{10.75}$$

Here σ_0 is the normal-state tunnel conductance, which in the normal state of the metal determines the current I_n across the junction to be

$$I_n = \sigma_0 V, \tag{10.76}$$

with V being the applied voltage. The Josephson effect implies that a supercurrent may flow even when V = 0. At finite voltages the phase difference ϕ acquires a time dependence according to

$$\hbar \frac{\partial \phi}{\partial t} = 2eV. \tag{10.77}$$

Like (10.73) this equation reflects the conjugate relation between the number of Cooper pairs and the phase, as may be seen from the simple Hamiltonian description based on

$$H = -E_0 \cos \phi - 2enV \tag{10.78}$$

together with the Hamilton equations of motion

$$\hbar\dot{\phi} = -\frac{\partial H}{\partial n} = 2eV \tag{10.79}$$

and

$$\hbar \dot{n} = \frac{\partial H}{\partial \phi} = E_0 \sin \phi. \tag{10.80}$$

The Josephson tunneling current may be calculated as a function of temperature by the Green function method, starting from the BCS Hamiltonian for two superconducting metals with the addition of a tunneling Hamiltonian describing the effect of the tunneling barrier. The result is

$$I_0 = \frac{\pi \sigma_0 \Delta}{2e} \tanh(\Delta/2kT), \qquad (10.81)$$

where Δ is the temperature-dependent gap shown in Fig. 10.1. Near the transition temperature, the Josephson current therefore vanishes as $T_c - T$, since the gap itself is proportional to $(T_c - T)^{1/2}$.

11 Electrical conductivity

In this final chapter we show how the methods of diagrammatic perturbation theory may be applied to the determination of transport coefficients such as electrical conductivity. We shall derive the Drude formula for the frequencydependent conductivity and show how the summation of a particular class of diagrams describes the effect of *weak localization*, which is observed in the magnetoresistance of two-dimensional electron systems.

The chapter is organized as follows: First we derive the general formulae of linear response theory. Subsequently the current operator is identified and used for expressing the conductivity in terms of a retarded current-current correlation function. The latter is calculated by diagrammatic perturbation theory, taking into account the influence of impurity scattering on the electron Green function. We determine the electron self-energy by using the Born approximation and averaging over the positions of randomly located impurities. Following that, the Drude formula for the frequency-dependent conductivity is derived. The concluding section treats the effects of weak localization by summing up the contribution to the conductivity due to the class of maximally crossed diagrams.

11.1 Linear response

Many physical problems involve a linear response to an external disturbance. Perhaps the best known example is Ohm's law, which states that the current density j is linear in the applied electric field E, or $j = \sigma E$. Another example is the spin magnetization of an electron gas in the presence of an external field. In the following we derive a general expression for the change in a physical quantity due to an external disturbance, treating separately the zero-temperature and finite-temperature case.

11.1.1 Zero temperature

Let us consider a general physical system described by the time-independent Hamiltonian H. The Schrödinger equation has the form

$$i\hbar\frac{\partial\Psi_S}{\partial t} = H\Psi_S,\tag{11.1}$$

where ψ_S denotes the Schrödinger wave function. The transition to the Heisenberg picture is accomplished by the unitary transformation

$$\Psi_H = e^{iHt/\hbar} \Psi_S, \tag{11.2}$$

while the operator A_S in the Schrödinger picture becomes

$$A_H = e^{iHt/\hbar} A_S e^{-iHt/\hbar}.$$
 (11.3)

The operator A_H satisfies the equation of motion

$$i\hbar\frac{dA_H}{dt} = [A_H, H],\tag{11.4}$$

provided A_s has no explicit dependence on time.

We now consider an external disturbance characterized by an additional time-dependent term H'(t) in the Hamiltonian. The disturbance is switched on at a definite time $t = t_0$. From this moment on, the system develops according to the Schrödinger equation

$$i\hbar \frac{\partial \Psi_S}{\partial t} = (H + H'(t))\Psi_S. \qquad (11.5)$$

It is convenient to describe the time development of the wave function in terms of the operator U(t), which is defined according to

$$\Psi_{S}(t) = e^{-iHt/\hbar} U(t) \Psi_{S}(0).$$
(11.6)

In the absence of the external disturbance, corresponding to H' = 0, the operator U equals 1 at all times. We shall now solve for U to lowest order in H', with the boundary condition that U(t) = 1 for $t < t_0$. By differentiating (11.6) with respect to time we find that the operator U must satisfy the equation

$$i\hbar\frac{\partial U}{\partial t} = e^{iHt/\hbar}H'(t)e^{-iHt/\hbar}U = H'_H U, \qquad (11.7)$$

where we have introduced the Heisenberg operator H'_H . The equation (11.7) may now be solved by iteration,

$$U(t) = 1 + \frac{1}{i\hbar} \int_{t_0}^t dt' H'_H(t') + \cdots .$$
(11.8)

Since we only want to consider terms linear in H', there is no need to carry the expansion in (11.8) any further.

Having obtained the operator U to first order in H' we now proceed to consider the linear response of the ground-state expectation value of an operator O. If we consider changes in density due to an external field, we take O to be the density operator. Alternatively, O is the current operator if we are interested in the change in current due to an external field. We seek to determine the change $\delta < O >$ in the expectation value < O > given by

$$\delta < O >= < O >_{H'} - < O >_0, \tag{11.9}$$

where the subscript 0 indicates that the expectation value is determined in the absence of the external disturbance. Since

$$\Psi_S(t) = e^{-iHt/\hbar} (1 + \frac{1}{i\hbar} \int_{t_0}^t dt' H'_H(t')) \Psi_S(0)$$
(11.10)

to first order in H', we obtain

$$=\langle 0|(1+\frac{i}{\hbar}\int_{t_0}^t dt' H'_H(t'))e^{iHt/\hbar}O_S e^{-iHt/\hbar}(1-\frac{i}{\hbar}\int_{t_0}^t dt' H'_H(t'))|0\rangle,$$
(11.11)

where $|0\rangle = |\Psi_S(0)\rangle$ denotes the ground state of the system with Hamiltonian H.

Consequently we have

$$\delta < O >= \frac{i}{\hbar} \int_{t_0}^t dt' \langle 0 | [H'_H(t'), O_H(t)] | 0 \rangle.$$
 (11.12)

Let us consider an example where H' is given by

$$H'_{H} = \int d\mathbf{x}(-e)\rho_{H}(\mathbf{x},t)\phi_{\text{ext}}(\mathbf{x},t), \qquad (11.13)$$

where $\phi_{\text{ext}}(\mathbf{x}, t)$ is an external scalar potential, which couples to the charge -e of the particles, while $\rho_H(\mathbf{x}, t)$ is the Heisenberg operator for the particle density introduced in (8.49). In this case (11.12) shows that the linear response involves a retarded density-density correlation function.

Similarly, the spin magnetization induced by an external magnetic field introduces the generalized spin susceptibility as a retarded spin density-spin density correlation function.

11.1.2 Finite temperature

The linear response theory discussed in the preceding section is readily extended to finite temperatures. The expression (11.12) for the change in the ground-state expectation value may be generalized to any matrix element involving the exact eigenstates of the operator $K = H - \mu N$ introduced in Chapter 7. Consequently it also applies to the diagonal matrix elements $\langle m | \int_{t_0}^t dt' [H'_H(t'), O_H(t)] | m \rangle$, which enter the statistical average. Thus we obtain the finite-temperature generalization of (11.12),

$$\delta < O >= \frac{i}{\hbar} \int_{t_0}^t dt' \operatorname{Tr}(e^{-\beta K}[H'_H(t'), O_H(t)]) e^{\beta \Omega}, \qquad (11.14)$$

where

$$e^{-\beta\Omega} = \mathrm{Tr}e^{-\beta K}.$$
 (11.15)

Let us assume that the Hamiltonian H' has the form

$$H' = \int d\mathbf{x} O(\mathbf{x}, t) \phi_{\text{ext}}(\mathbf{x}, t). \qquad (11.16)$$

Then

$$\delta < O >= -\frac{i}{\hbar} \int d\mathbf{x}' \int_{t_0}^t dt' < [O_H(\mathbf{x}, t), O_H(\mathbf{x}', t')] > \phi_{\text{ext}}(\mathbf{x}', t'). \quad (11.17)$$

We now let t_0 tend to minus infinity. Introducing the retarded correlation function $D^{\text{ret}}(1, 1')$ by the definition

$$iD^{\rm ret}(1,1') = \langle [O_H(1), O_H(1')] \rangle \Theta(t-t'),$$
 (11.18)

where 1 and 1' refer to the space-time points \mathbf{x}, t and \mathbf{x}', t' , respectively, we are able to write the final result in the simple form

$$\delta < O(1) >= \frac{1}{\hbar} \int d1' D^{\text{ret}}(1, 1') \phi_{\text{ext}}(1'), \qquad (11.19)$$

where the integration over the time variable t' extends from minus infinity to plus infinity.

The quantity of physical interest is thus a retarded correlation function. In the case where an external probe couples to the density or the current density, the operator O_H is bilinear in the field operators. To obtain the correlation function at finite temperatures within the Matsubara approach one must therefore consider a two-particle Green function, which is calculated by diagrammatic perturbation theory, using free-particle Green functions as building blocks. When the Fourier coefficients of the appropriate two-particle Green function have been obtained as function of the Matsubara frequencies, the method of analytic continuation is employed for determining the retarded correlation function, in precise analogy to the way in which the retarded (oneparticle) Green function is obtained from the tau-ordered one, as demonstrated in Section 7.5, cf. (7.73) and (7.70). An example of the use of this procedure is given in Section 11.4 below, where the frequency-dependent conductivity is related to a particular case of a two-particle Matsubara Green function.

11.2 The current operator

The quantum mechanical expression for the electric current density \mathbf{j} associated with a particle of charge -e and mass m moving in a magnetic field described by the vector potential \mathbf{A} , is

$$\mathbf{j} = (-e)\frac{\hbar}{2mi}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) - \frac{e^2}{m}\mathbf{A}|\Psi|^2.$$
(11.20)

Note that this current expression is gauge-invariant, since the gauge transformation obtained by adding the term $\nabla \chi$ to the vector potential **A** changes the wavefunction Ψ to $\Psi \exp(-ei\chi/\hbar)$, where χ is an arbitrary function of the coordinates. The expression (11.20) is the mean value of the current in the state Ψ for a single particle. We shall now write down the current-density operator for a system of N particles, each with charge -e and mass m.

The electric current density may be obtained from the quantum mechanical expression (11.20) after replacing the wavefunction Ψ by the annihilation operator ψ (and Ψ^* by its hermitian conjugate ψ^{\dagger}). This results in the secondquantized form of the current-density operator \mathbf{j}_{op}

$$\mathbf{j}_{\rm op} = (-e)\frac{\hbar}{2mi}(\psi^{\dagger}\nabla\psi - \psi\nabla\psi^{\dagger}) - \frac{e^2}{m}\mathbf{A}\psi^{\dagger}\psi.$$
(11.21)

The expectation value \mathbf{j} of this operator may then be written in terms of the Green function

$$G_{\sigma\sigma'}(\mathbf{x},\tau;\mathbf{x}',\tau') = G(\mathbf{x},\tau;\mathbf{x}',\tau')\delta_{\sigma\sigma'}$$
(11.22)

according to

$$\mathbf{j} = (-e)\frac{\hbar}{mi}(\frac{\partial}{\partial \mathbf{x}} - \frac{\partial}{\partial \mathbf{x}'})G(\mathbf{x}, \tau; \mathbf{x}', \tau')_{\mathbf{x}' \to \mathbf{x}, \tau' \to \tau + \eta} - \frac{ne^2}{m}\mathbf{A}, \qquad (11.23)$$

where η denotes a positive infinitesimal.

It is often useful to write the current operator in terms of operators that add and remove a particle in a definite momentum state $\hbar k$. Thus we introduce

$$\psi_{\sigma}(\mathbf{x}) = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k},\sigma}$$
(11.24)

into (11.21) and obtain the Fourier-expansion

$$\mathbf{j}_{\rm op}(\mathbf{x}) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \mathbf{j}_{\rm op}(\mathbf{q})$$
(11.25)

where $\mathbf{j}_{op}(\mathbf{q})$ is given by

$$\mathbf{j}_{\rm op}(\mathbf{q}) = (-e)\frac{\hbar}{m} \sum_{\mathbf{k},\sigma} (\mathbf{k} + \frac{\mathbf{q}}{2}) c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q},\sigma}.$$
(11.26)

In the presence of an external vector potential \mathbf{A} the perturbing Hamiltonian H' is

$$H' = -\int d\mathbf{x} \, \mathbf{j} \cdot \mathbf{A}. \tag{11.27}$$

In the remainder of this chapter we consider the uniform case where the electrical field is homogeneous in space. The electric field \mathbf{E} is described in terms of a time-dependent vector potential \mathbf{A} according to

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t}.\tag{11.28}$$

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For a vector potential, which oscillates in time according to

$$\mathbf{A} = \mathbf{A}_0 e^{-i\omega t} \tag{11.29}$$

we thus get

$$\mathbf{A} = \frac{1}{i\omega} \mathbf{E}.\tag{11.30}$$

The final expression for the conductivity within linear response then becomes

$$j_{\alpha} = \sigma_{\alpha\beta} E_{\beta}, \tag{11.31}$$

where we sum over repeated indices, with the conductivity tensor $\sigma_{\alpha\beta}$ being given by

$$\sigma_{\alpha\beta} = \frac{1}{\omega} \int_{-\infty}^{t} dt' e^{i\omega(t-t')} < [j_{\alpha}(t), j_{\beta}(t')] > -\frac{ne^2}{mi\omega} \delta_{\alpha\beta}.$$
(11.32)

Here the current-density operator is obtained by setting q = 0 in (11.26) and dividing by the volume V,

$$j_{\alpha} = (-e) \frac{\hbar}{mV} \sum_{\mathbf{k},\sigma} k_{\alpha} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}, \qquad (11.33)$$

Before we proceed to the evaluation of (11.32) we shall consider the electron Green function in the presence of randomly located impurities.

11.3 Electron-impurity interaction

The Hamitonian for a single electron interacting with impurities, which occupy fixed positions in a lattice, is

$$H = H_0 + H_1 = \frac{\mathbf{p}^2}{2m} + \sum_i V(\mathbf{r} - \mathbf{R}_i).$$
(11.34)

Here the sum extends over the position vectors \mathbf{R}_i of the N_{imp} impurities.

In the language of second quantization the two terms of this Hamiltonian are written in the form

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(11.35)

and

$$H_1 = \sum_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} \langle \mathbf{k}'\sigma' | U | \mathbf{k}\sigma \rangle c^{\dagger}_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}$$
(11.36)

where the matrix element of the electron-impurity interaction is given by

$$\langle \mathbf{k}' \sigma' | U | \mathbf{k} \sigma \rangle = \frac{1}{V} \int d\mathbf{r} e^{-i\mathbf{k}' \cdot \mathbf{r}} \sum_{i} V(\mathbf{r} - \mathbf{R}_{i}) e^{i\mathbf{k} \cdot \mathbf{r}}.$$
 (11.37)

The integral in (11.37) is calculated by shifting the integration variable to $\mathbf{r} - \mathbf{R}_i$ as a result of which one gets

$$H_1 = \frac{1}{V} \sum_{\mathbf{q}} \rho_{\text{imp}}(\mathbf{q}) V(-\mathbf{q}) \rho(\mathbf{q}).$$
(11.38)

Here $\rho(\mathbf{q})$ is the Fourier component of the density operator, given by

$$\rho(\mathbf{q}) = \sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} , \qquad (11.39)$$

while

$$\rho_{\rm imp}(\mathbf{q}) = \sum_{i} e^{i\mathbf{q}\cdot\mathbf{R}_{i}},\tag{11.40}$$

and $V(\mathbf{q})$ is the Fourier-transform of $V(\mathbf{r})$,

$$V(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{r}). \tag{11.41}$$

11.3.1 The electron self-energy

The electron-impurity interaction may be treated by diagrammatic perturbation theory just like the electron-electron or the electron-phonon interaction. We shall only consider the self-energy to second order in the interaction matrix element $V(\mathbf{q})$. When expanding the S-matrix one generates terms containing products $\rho_{imp}(\mathbf{q}_1)\rho_{imp}(\mathbf{q}_2)\cdots$. Since we do not know the location of the impurities, we assume that they are randomly located in space and average each term in the self-energy over the positions of the impurities. The total number of impurities is called N_{imp} , and their density is thus

$$n_{\rm imp} = \frac{N_{\rm imp}}{V}.$$
 (11.42)

The average $\langle \rangle_{imp}$ of the first order term yields

$$< \rho_{\rm imp}(\mathbf{q}) >_{\rm imp} = < \sum_{i} e^{i\mathbf{q}\cdot\mathbf{R}_{i}} >_{\rm imp}.$$
 (11.43)

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Since the impurities are randomly located, we only get a contribution when q = 0, in which case each of the N_{imp} terms equals unity,

$$<\sum_{i} \epsilon^{i\mathbf{q}\cdot\mathbf{R}_{i}} >_{imp} = N_{imp} \delta_{\mathbf{q},\mathbf{0}}.$$
 (11.44)

In second order we obtain

$$<\sum_{ij} e^{i\mathbf{q}_{1}\cdot\mathbf{R}_{i}} e^{i\mathbf{q}_{2}\cdot\mathbf{R}_{j}} >_{imp} = N_{imp}\delta_{\mathbf{q}_{1}+\mathbf{q}_{2},\mathbf{0}} + N_{imp}(N_{imp}-1)\delta_{\mathbf{q}_{1},\mathbf{0}}\delta_{\mathbf{q}_{2},\mathbf{0}}, (11.45)$$

which is seen by separating the sum over i, j into two, the first of which having i = j, the second $i \neq j$.

Let us consider the contributions $\Sigma^{(n)}$ to the self-energy to order n in the interaction matrix element $V(\mathbf{q})$. First we treat the case n = 1. The self-energy is then given by

$$\hbar \Sigma^{(1)} = \frac{N_{\rm imp}}{V} \sum_{\mathbf{q}} \delta_{\mathbf{q},0} V(-\mathbf{q}) = \frac{N_{\rm imp} V(0)}{V}.$$
 (11.46)

This lowest-order term is evidently real, since V(0) according to (11.41) is the integral over all space of $V(\mathbf{r})$. It contributes just a constant, which shifts the single-particle energies by the same amount (alternatively we may absorb the shift in the chemical potential).

In second order we get the term which is illustrated diagrammatically in Fig. 11.1. In order to ease the analytic continuation later on, we write the Fourier coefficients as functions of the (purely imaginary) variable $i\omega_n$.

$$\begin{split} \hbar \Sigma^{(2)}(\mathbf{k}, i\omega_n) &= \frac{N_{\rm imp}}{V^2} \sum_{\mathbf{q}_1 \mathbf{q}_2} \delta_{\mathbf{q}_1 + \mathbf{q}_2, \mathbf{0}} V(-\mathbf{q}_1) V(-\mathbf{q}_2) G^{(0)}(\mathbf{k} + \mathbf{q}_1, i\omega_n) \\ &= \frac{N_{\rm imp}}{V^2} \sum_{\mathbf{q}_1} V(-\mathbf{q}_1) V(\mathbf{q}_1) G^{(0)}(\mathbf{k} + \mathbf{q}_1, i\omega_n). \end{split}$$
(11.47)

After insertion of the electron (temperature) Green function this becomes

$$\hbar\Sigma^{(2)}(\mathbf{k}, i\omega_n) = \frac{N_{\rm imp}}{V} \int \frac{d\mathbf{k}'}{(2\pi)^3} V(\mathbf{k} - \mathbf{k}') V(\mathbf{k}' - \mathbf{k}) \frac{1}{i\hbar\omega_n - \xi_{\mathbf{k}'}},\qquad(11.48)$$

which is analytically continued to the real axis according to $i\omega_n \to \omega + i\eta$. By carrying out the integration over $\xi_{k'}$ we then find that the imaginary part of Σ for $k \simeq k_{\rm F}$ is independent of ω and given by

Im
$$\Sigma = \frac{\pi}{\hbar} n_{\rm imp} N(0) \int_{-1}^{1} \frac{d(\cos \theta)}{2} |V(\theta)|^2.$$
 (11.49)

Here $N(0) = mk_{\rm F}/2\pi^2\hbar^2$ is the density of states per spin at the Fermi energy, while $V(\theta)$ is the matrix element $V(\mathbf{k}' - \mathbf{k})$ evaluated for $\mathbf{k} = \mathbf{k}' = \mathbf{k}_{\rm F}$, as a function of the angle θ between \mathbf{k} and \mathbf{k}' . Apart from a constant shift, which we absorb in the chemical potential, the retarded electron Green function may accordingly be written as

$$G^{\rm ret} = \frac{1}{\omega - \xi_k/\hbar + i/2\tau},\tag{11.50}$$

where τ is given by

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} n_{\rm imp} N(0) \int_{-1}^{1} \frac{d(\cos\theta)}{2} |V(2k_{\rm F}\sin\theta/2)|^2.$$
(11.51)

If V is a constant, independent of θ , this result is equivalent to (2.1.14) in *Transport Phenomena*, which may be obtained from (2.1.9), where the term involving $\cos \theta$ integrates to zero. In this case $1/\tau$ becomes

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} n_{\rm imp} N(0) |V(0)|^2.$$
(11.52)

Note that this expression has the correct dimension of inverse time, since the number density of impurities n_{imp} and the density of states N(0) both are inversely proportional to the volume, while V(0) has the dimension of energy times volume. If V(0) is set equal to 1/2N(0), which is the long wavelength limit of the (Thomas-Fermi) screened Coulomb interaction, we recover from (11.52) the result (2.1.14) given in *Transport Phenomena*. In the following subsection we shall determine the frequency-dependent conductivity σ in an approximation, which yields $\sigma = ne^2 \tau/(1 - i\omega\tau)$. While this looks similar to the result of solving the Boltzmann equation, there is an important difference: the time τ given by (11.51) is not the transport time, since the factor $(1 - \cos \theta)$ is missing from the integrand. As we mention below, it is possible to identify the class of diagrams which produces the $\cos \theta$ term, but we shall not consider it in any detail.

11.4 The Drude formula

In the previous section we obtained the electron Green function, with the selfenergy evaluated in the lowest Born approximation. Now we proceed to calculate the current-current correlation function, using finite-temperature Green functions. Thus we consider the τ -ordered quantity $\Pi_{\alpha\beta}(\tau)$, which is defined as

$$\Pi_{\alpha\beta}(\tau) = -\langle T_{\tau}(j_{\alpha}(\tau)j_{\beta}(0)) \rangle, \qquad (11.53)$$

where $\langle \rangle$ as usual means the thermal average defined in (7.5). According to (11.32) the conductivity $\sigma_{\alpha\beta}(\omega)$ associated with a definite frequency ω is obtained from $\Pi_{\alpha\beta}(i\omega_n)$ as

$$\sigma_{\alpha\beta} = \frac{i}{\omega} \Pi_{\alpha\beta} (i\omega_n \to \omega + i\eta) - \frac{ne^2}{i\omega m} \delta_{\alpha\beta}.$$
(11.54)

The conductivity tensor $\sigma_{\alpha\beta}$ is diagonal,

$$\sigma_{\alpha\beta}(\omega) = \sigma(\omega)\delta_{\alpha\beta}, \qquad (11.55)$$

and we may therefore obtain $\sigma(\omega)$ by taking the trace of (11.54) and dividing by the dimension d,

$$\sigma(\omega) = \frac{i}{\omega d} \Pi_{\alpha\alpha} (i\omega_n \to \omega + i\eta) - \frac{n\epsilon^2}{i\omega m}.$$
 (11.56)

We evaluate $\Pi_{\alpha\alpha}(\tau)$ by inserting the $\mathbf{q} = \mathbf{0}$ limit of the current operator given in (11.33), resulting in

$$\Pi_{\alpha\alpha}(\tau) = -\frac{e^2\hbar^2}{m^2} \sum_{\mathbf{k},\sigma,\mathbf{k}',\sigma'} \mathbf{k} \cdot \mathbf{k}' < T_{\tau}(c^{\dagger}_{\mathbf{k},\sigma}(\tau)c_{\mathbf{k},\sigma}(\tau)c^{\dagger}_{\mathbf{k}',\sigma'}(0)c_{\mathbf{k}',\sigma'}(0)) > .$$
(11.57)

The terms in (11.57) which involve pairing of the two operators carrying the same wave vector \mathbf{k} vanish by symmetry, due to the integration over \mathbf{k} and \mathbf{k}' . After carrying out the Fourier-transformation and the summation over spin we therefore get

$$\Pi_{\alpha\alpha}(i\omega_n) = -2\frac{e^2\hbar^2}{m^2V^2} \sum_{n'} \sum_{\mathbf{k},\mathbf{k}'} \mathbf{k} \cdot \mathbf{k}' < G(\mathbf{k},\mathbf{k}',i\omega_n+i\omega_{n'})G(\mathbf{k}',\mathbf{k},i\omega_{n'}) >_{\text{imp}}.$$
(11.58)

Note that the Green functions depend on two momenta, due to the absence of translational invariance. We have indicated explicitly the average $\langle \cdots \rangle_{imp}$ over the positions of the impurities.



Figure 11.2: Cuts in the complex z-plane

The sum over Matsubara frequencies is carried out as usual by introducing the Fermi function n(z) given by

$$n(z) = \frac{1}{e^{\beta \hbar z} + 1}.$$
 (11.59)

The analytic structure of $G(\mathbf{k}', \mathbf{k}, z) \equiv G_{k'k}(z)$ and $G_{kk'}(z + i\omega_n)$ occurring in (11.58) is such that they possess a cut along the lines $z = \tilde{\omega}$ and $z = \tilde{\omega} - i\omega_n$, respectively. Here $\tilde{\omega}$ is real and varies between $-\infty$ and ∞ (see Fig. 11.2). When deforming the contour as indicated in Fig. 11.2 we therefore integrate just above and just below these two lines. Let us consider the quantity Q defined by

$$Q(i\omega_n) = \frac{1}{\beta\hbar} \sum_{n'} G(\mathbf{k}, \mathbf{k}', i\omega_n + i\omega_{n'}) G(\mathbf{k}', \mathbf{k}, i\omega_{n'}).$$
(11.60)

After introducing the Fermi function and deforming the contour we see that Q may be written as

$$Q(i\omega_n) = -\int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi i} n(\tilde{\omega}) [(G_{k'k}^{\text{ret}}(\tilde{\omega}+i\eta) - G_{k'k}^{\text{adv}}(\tilde{\omega}-i\eta))G_{kk'}(\tilde{\omega}+i\omega_n) + (G_{kk'}^{\text{ret}}(\tilde{\omega}+i\eta) - G_{kk'}^{\text{adv}}(\tilde{\omega}-i\eta))G_{k'k}(\tilde{\omega}-i\omega_n)].$$
(11.61)

Now we carry out the analytic continuation $i\omega_n \rightarrow \omega + i\eta$, obtaining the appropriate retarded and advanced Green functions,

$$Q(\omega) = -\int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi i} n(\tilde{\omega}) [(G_{k'k}^{\text{ret}}(\tilde{\omega}+i\eta) - G_{k'k}^{\text{adv}}(\tilde{\omega}-i\eta))G_{kk'}^{\text{ret}}(\tilde{\omega}+\omega+i\eta) + (G_{kk'}^{\text{ret}}(\tilde{\omega}+i\eta) - G_{kk'}^{\text{adv}}(\tilde{\omega}-i\eta))G_{k'k}^{\text{adv}}(\tilde{\omega}-\omega-i\eta)].$$
(11.62)



Figure 11.3: Vertex corrections

In the static limit we expect to recover the elementary formula $\sigma = ne^2 \tau/m$. However, the right hand side of (11.56) contains a term which diverges as ω^{-1} in the limit $\omega \to 0$. This divergence is cancelled against a similar term arising from the products of retarded ($G^{\text{ret}}G^{\text{ret}}$) and advanced ($G^{\text{adv}}G^{\text{adv}}$) Green functions in (11.62). The cancellation is verified by using the Green functions for the noninteracting system in these two terms, while the higher-order diagrams yield a vanishing contribution. Thus the final conductivity formula becomes

$$\sigma(\omega) = \frac{2e^{2}\hbar^{2}}{m^{2}dV^{2}} \sum_{\mathbf{k}\mathbf{k}'} \mathbf{k} \cdot \mathbf{k}' \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} [n(\tilde{\omega}) < G_{k'k}^{adv}(\tilde{\omega} - i\eta))G_{kk'}^{ret}(\tilde{\omega} + \omega + i\eta) >_{imp} - n(\tilde{\omega} + \omega) < G_{kk'}^{ret}(\tilde{\omega} + \omega + i\eta)G_{k'k}^{adv}(\tilde{\omega} - i\eta) >_{imp}], \quad (11.63)$$

which may be written as

$$\sigma(\omega) = \frac{2e^{2}\hbar^{2}}{m^{2}dV^{2}} \sum_{\mathbf{k}\mathbf{k}'} \mathbf{k} \cdot \mathbf{k}' \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{n(\tilde{\omega}) - n(\tilde{\omega} + \omega)}{\omega} < G_{\mathbf{k}'\mathbf{k}}^{\mathrm{adv}}(\tilde{\omega} - i\eta) G_{\mathbf{k}\mathbf{k}'}^{\mathrm{ret}}(\tilde{\omega} + \omega + i\eta) >_{\mathrm{imp}}.$$
(11.64)

The formula (11.64) forms the starting point for our calculation of the conductivity.

The Drude formula for the frequency-dependent conductivity is obtained by using

$$G_{k'k}^{\text{adv}}(\tilde{\omega}+\omega) = \frac{1}{\tilde{\omega}+\omega-\xi_k/\hbar - i/2\tau} \delta_{\mathbf{k},\mathbf{k}'}$$
(11.65)

and

$$G_{kk'}^{\text{ret}}(\tilde{\omega}) = \frac{1}{\tilde{\omega} - \xi_k/\hbar + i/2\tau} \delta_{\mathbf{k},\mathbf{k}'}, \qquad (11.66)$$

where τ is given by (11.51). Since we consider the limit in which $\hbar\omega$ is much less than the Fermi energy $\epsilon_{\rm F}$, the main contribution to the momentum integration



Figure 11.4: Maximally crossed diagram

in (11.64) comes from the region near the Fermi surface. By first performing the momentum integration and then the frequency integration we get

$$\sigma = \frac{\sigma_0}{1 - i\omega\tau},\tag{11.67}$$

where the static conductivity σ_0 is given by

$$\sigma_0 = \frac{ne^2\tau}{m}.\tag{11.68}$$

The time τ occurring in our result for the frequency-dependent conductivity is not the same as the transport relaxation time obtained from solving the Boltzmann equation. The reason is that we have neglected vertex corrections of the kind illustrated diagrammatically in Fig. 11.3. When the contribution from such vertex corrections is taken into account, one obtains the complete expression for τ given in (2.1.9) of *Transport Phenomena*. We leave it as a problem for the reader to calculate the magnitude of the static conductivity both with and without the $\cos \theta$ -term for a screened Coulomb-interaction, and compare the result to the measured resistivity for magnesium impurities in Cu, cf. (1.24) in Section 1.3.3.

There are of course many other diagrams than the ones discussed so far. In three dimensions one may show that these are negligible in the limit when the mean free path $l = v_{\rm F}\tau$, where $v_{\rm F} = \hbar k_{\rm F}/m$ is the Fermi velocity, is much greater than $1/k_{\rm F}$. In two dimensions, however, the situation is different, as we shall see in the following section.

11.5 Weak localization

There exists a certain class of diagrams, the so-called maximally crossed diagrams, which give the dominant contribution to the conductivity in two dimensions, leading to the phenomenon of *weak localization*, which has been confirmed in many experiments. Weak localization (in the context of electronic conduction) was discovered by Abrahams, Anderson, Licciardello and Ramakrishnan (1979) on the basis of a scaling analysis. The phenomenon was

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Figure 11.5: Diagrammatic illustration of the integral equation for the particlehole ladder

subsequently explored by Gorkov, Larkin and Khmel'nitskii (1979), who calculated the frequency-dependent conductivity in the manner described below.

In the following we shall show how the summation of a select class of diagrams gives rise to weak localization in two dimensions. It is evident from Fig. 11.4 that a maximally crossed diagram in the particle-hole channel becomes a ladder-type diagram in the particle-particle channel, when the hole line is twisted. The particle-particle impurity ladder is called the *Cooperon*, because of the importance of electron states with opposite momenta. The properties of the Cooperon are best appreciated by considering the diffusive behavior of the particle-hole impurity ladder at low frequencies and long wavelengths. We shall only treat the case where the electron-impurity matrix element $V(\mathbf{q})$ is a (real) constant, V(0), independent of θ .

The particle-hole ladder satisfies the integral equation illustrated in Fig. 11.5. The integral equation is solved with the aid of the function $\zeta(\mathbf{q}, \omega)$, which in d dimensions is given by the expression (for convenience, we consider a unit volume and set \hbar equal to 1)

$$\zeta(\mathbf{q},\omega) = V(0)^2 \int \frac{d\mathbf{k}}{(2\pi)^d} G^{\text{ret}}(\mathbf{k},\tilde{\omega}) G^{\text{adv}}(\mathbf{k}-\mathbf{q},\tilde{\omega}-\omega).$$
(11.69)

Using the expressions (11.66) and (11.65) for G and carrying out the integral over \mathbf{k} , we see that the result for $q \ll k_{\rm F}$ is given by

$$\zeta = \frac{i}{2ql} \ln \frac{ql + \omega\tau + i}{-ql + \omega\tau + i}, \qquad (11.70)$$

when d = 3. In general, for the dimension d = 1, 2 or 3 and in the limit $ql \ll 1$ and $\omega \tau \ll 1$, we get that

$$\zeta \simeq 1 + i\omega\tau - D\tau q^2 \tag{11.71}$$

in terms of the diffusion coefficient

$$D = \frac{1}{d} v_{\rm F}^2 \tau. \tag{11.72}$$



Figure 11.6: A particle-particle channel diagram



Figure 11.7: The diagram of Fig. 11.6, with time-reversed lower line

The particle-hole ladder is proportional to the geometric series $(1 - \zeta)^{-1}$, which in the limit of low frequencies and long wavelengths becomes

$$\frac{1}{1-\zeta} \simeq \frac{1}{\tau(-i\omega + Dq^2)}.$$
(11.73)

From this it is evident that the particle-hole propagator has a pole at

$$\omega = -iDq^2. \tag{11.74}$$

This diffusive pole is a direct consequence of the conservation of the number of particles. It is thus a general property of the system at low frequencies and long wavelengths.



Figure 11.8: Quantum correction to the conductivity
Now we proceed to consider the form of the particle-particle impurity ladder for small total momentum. By comparing Fig. 11.6 and Fig. 11.7 we see that the time-reversal of the lower line in Fig. 11.6 brings us to Fig. 11.7, the hole line having reversed momentum. If time-reversal invariance applies, these diagrams therefore give identical contributions. The form of the Cooperon for small total momentum, $|\mathbf{k}+\mathbf{k}'| l \ll 1$ and small energy transfer ω is therefore

$$C \simeq \frac{V(0)^2}{\tau(-i\omega + D(\mathbf{k} + \mathbf{k}')^2)} \quad \text{for } |\mathbf{k} + \mathbf{k}'| l \ll 1 \text{ and } \omega\tau \ll 1.$$
(11.75)

We therefore have the following contribution from the diagram shown in Fig. 11.8

$$\delta\sigma(\omega) = \frac{e^2}{\pi m^2 d} \sum_{\mathbf{k}\mathbf{k}'} \mathbf{k} \cdot \mathbf{k}' G^{\text{ret}}(\mathbf{k}) G^{\text{ret}}(\mathbf{k}') G^{\text{adv}}(\mathbf{k}) G^{\text{adv}}(\mathbf{k}') C_{\omega}(\mathbf{k} + \mathbf{k}'). \quad (11.76)$$

In (11.76) we have performed the integration over $\tilde{\omega}$, since the momentum integrations yield a $\tilde{\omega}$ -independent result, and furthermore used that $\omega \tau \ll 1$. The important contribution to $\delta \sigma$ comes from regions of integration where $\mathbf{k} + \mathbf{k}' \simeq \mathbf{0}$. We therefore introduce $\mathbf{Q} = \mathbf{k} + \mathbf{k}'$ and replace $\mathbf{k} \cdot \mathbf{k}'$ by $-k_{\mathrm{F}}^2$. Similarly we replace \mathbf{k}' in the Green functions G^{ret} and G^{adv} by $-\mathbf{k}$. Then we may turn the integral over \mathbf{k} into an integral over $\boldsymbol{\xi}$, and use the peaked character of the integrand at the Fermi surface to carry out the $\boldsymbol{\xi}$ -integration. The result for $\delta \sigma$ is

$$\frac{\delta\sigma}{\sigma_0} = -\frac{1}{\pi N_d(0)} \int \frac{d\mathbf{Q}}{(2\pi)^d} \frac{1}{-i\omega + DQ^2},\tag{11.77}$$

where $N_d(0)$ is the density of states per spin in d dimensions. In two dimensions (d=2) the integral is evaluated by cutting off the Q-integral at the upper limit l^{-1} . The result is

$$\delta\sigma(\omega) = \frac{\sigma_0}{\pi k_{\rm F} l} \ln \omega \tau. \tag{11.78}$$

Evidently this tends to minus infinity when ω goes to zero, indicating the occurrence of localization. The role of time-reversal invariance is seen to be crucial. If the latter is violated by the presence of a magnetic field or magnetic impurities, then the particle-particle and particle-hole diagrams are not equal, and the weak localization is correspondingly suppressed. The effects of weak localization are sensitive to variations in a magnetic field on a scale which is much smaller than that which determines the classical magnetoresistance effects described in *Transport Phenomena*.

12 Problems

Problems 1-27 refer to Transport Phenomena, while the remaining Problems 28-55 refer to the present text.

PROBLEM 1 We consider a two-dimensional conductor with a density of conduction electrons given by n = N/A. Here N is the total number of electrons, while A is the area of the conductor. The dispersion relation for the electrons, that is the connection between the energy ϵ and the wave vector $\mathbf{k} = (k_x, k_y)$ characterizing a given single-particle state, is given by

$$k = k_0(\epsilon), \tag{12.1}$$

where $k_0(\epsilon)$ is a monotonically increasing function of ϵ . For free electrons we have $k_0(\epsilon) = \sqrt{2m\epsilon}/\hbar$.

Express the length of the Fermi wave vector, $k_{\rm F}$, in terms of *n*. Show that the Fermi energy $\epsilon_{\rm F}$ and the Fermi velocity $v_{\rm F}$ are given by

$$k_0(\epsilon_{\rm F}) = k_{\rm F} \tag{12.2}$$

and

$$\frac{1}{\hbar k_0'(\epsilon_{\rm F})} = v_{\rm F},\tag{12.3}$$

where ' denotes the derivative with respect to ϵ . Find an expression for the density of states at the Fermi energy and determine the entropy to lowest order in $T/T_{\rm F}$.

Calculate the Fermi energy and the associated Fermi temperature for the case where the electron dispersion relation is quadratic, $\epsilon = \hbar^2 k^2/2m^*$ with $m^* = 0.067m_e$, appropriate to the two-dimensional gas in a GaAs/AlGaAs heterostructure. Here m_e is the electron mass, while the number density n is assumed to be $n = 10^{11}$ cm⁻².

PROBLEM 2 The derivation of the Boltzmann equation is discussed in general terms in *Transport Phenomena* (see, in particular, Sections 1.1 and 2.3). In this problem we shall derive the Boltzmann equation for the special case of a two-dimensional electron gas, but the general procedure is very similar. In the present case the Boltzmann equation becomes a continuity equation with source terms in the four-dimensional phase space of a single particle. The one-particle distribution function $f(x, y, k_x, k_y, t)$ is defined in such a manner that $f(x, y, k_x, k_y, t) dx dy dk_x dk_y/(2\pi)^2$ is the mean number of particles at time t in the phase-space element $dx dy dk_x dk_y$. If collision terms are neglected, the conservation of particle number is expressed by

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_{\mu}}(v_{\mu}f) = 0, \qquad (12.4)$$

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analogous to the usual continuity equation, where $v_{\mu} = (\dot{x}, \dot{y}, k_x, k_y)$ is a fourdimensional velocity, while $\partial/\partial x_{\mu} = (\partial/\partial x, \partial/\partial y, \partial/\partial k_x, \partial/\partial k_y)$. It states that the rate of increase of f in a given phase-space volume element is equal to the net number of particles which stream from outside to inside this phasespace volume element. The effect of collisions is not included in (12.4). Since collisions move particles from one region of phase space to another, we describe their effect by adding a source term $(\partial f/\partial t)_{coll}$ to the right hand side of (12.4), resulting in

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_{\mu}} (v_{\mu} f) = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}.$$
(12.5)

Since $\partial v_{\mu}/\partial x_{\mu} = 0$ the Boltzmann equation assumes the form (cf. Transport Phenomena, Sections 1.1 and 2.3)

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}, \qquad (12.6)$$

where

$$\mathbf{v} = \frac{\partial \epsilon(\mathbf{k})}{\hbar \partial \mathbf{k}} \tag{12.7}$$

and

$$\hbar \mathbf{k} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \tag{12.8}$$

It is assumed that the electric field is within the plane, while the magnetic field is perpendicular to the plane.

The collision integral is given by

$$\begin{aligned} (\frac{\partial f}{\partial t})_{\text{coll}} &= \int \frac{d\mathbf{k}'}{(2\pi)^2} [w(\mathbf{k},\mathbf{k}')f(\mathbf{k}')(1-f(\mathbf{k})) - w(\mathbf{k}',\mathbf{k})f(\mathbf{k})(1-f(\mathbf{k}'))] \\ &= -\int \frac{d\mathbf{k}'}{(2\pi)^2} w(\mathbf{k},\mathbf{k}')(f(\mathbf{k}) - f(\mathbf{k}')), (12.9) \end{aligned}$$

since we assume that the electrons are scattered against fixed impurities (cf. Transport Phenomena Section 2.1.1).

Show that (12.9) may be written as

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{1}{\tau} (f(\mathbf{k}) - f^0), \qquad (12.10)$$

where f^0 is the Fermi function

$$f^{0} = \frac{1}{e^{(\epsilon - \mu)/kT} + 1},$$
(12.11)

provided 1) that the angular dependence of the distribution function is determined by $\mathbf{k} \cdot \hat{\mathbf{e}}$, where $\hat{\mathbf{e}}$ is a unit vector along the direction of the external field

or temperature gradient, and 2) that $w(\mathbf{k}, \mathbf{k}')$ only depends on (cosine of) the angle θ between \mathbf{k} og \mathbf{k}' . Find an expression for τ in terms of $w(\mathbf{k}, \mathbf{k}')$.

In the following Problems 3 and 4 we treat τ as a constant and furthermore assume that the temperature T is much less than the Fermi temperature $T_{\rm F}$.

PROBLEM 3 Consider the two-dimensional conductor described in Problems 1 and 2. Find the frequency dependent conductivity associated with an electric field proportional to $\exp(-i\omega t)$ from (12.6) and (12.10), in the case $\mathbf{B} = 0$. Discuss the result in the limit $\omega \tau \gg 1$. Compare to the result of the Drude model.

PROBLEM 4 Determine for the two-dimensional conductor described in Problems 1 and 2 the components σ_{ij} of the conductivity tensor in a perpendicular magnetic field together with the resistivity tensor ρ_{ij} , where *i* and *j* each may be *x* or *y*. Discuss the significance of the result for the observation of the Hall effect.

PROBLEM 5 We consider a two-dimensional electron gas with an energy dispersion relation given by

$$\epsilon(\mathbf{k}) = a(k_x^2 + k_y^2) + b(k_x^4 + k_y^4), \qquad (12.12)$$

where a and b are positive constants. The group velocity $\mathbf{v} = (v_x, v_y)$ is given by the usual expression

$$\mathbf{v} = \frac{1}{\hbar} \frac{\partial \epsilon}{\partial \mathbf{k}}.$$
 (12.13)

We let the electric field E be directed along the *x*-axis, while the magnetic field points along the *z*-direction, perpendicular to the plane in which the electrons move.

The linearized Boltzmann equation is given (in the relaxation-time approximation) by

$$-eEv_x\frac{\partial f^0}{\partial \epsilon} - \frac{eB}{\hbar}(v_y\frac{\partial g}{\partial k_x} - v_x\frac{\partial g}{\partial k_y}) = -\frac{g}{\tau},\qquad(12.14)$$

where $g = f - f^0$.

Show that the solution to the Boltzmann equation in the limit of high magnetic fields, where the collision term on the right hand side may be neglected, has the form $g = k_y F(\epsilon)$ and determine the function F. Use this solution to find the current density j_y in the y-direction (help: use partial integration with respect to the variable k_y) and show that the electric field and the current density are related by $E = \rho_{xy} j_y$, where

$$\rho_{xy} = \frac{B}{ne},\tag{12.15}$$

n being the number density of the electrons.

PROBLEM 6 The present problem concerns the same physical system as in Problem 5. We shall, however, furthermore assume that the electrons in equilibrium are described by the classical distribution function

$$f^{0} = e^{\mu/kT} e^{-\epsilon/kT}$$
(12.16)

with μ being a negative constant. In the present problem we consider the Hall-effect in low magnetic fields and compare our result to that obtained in the high-field limit of Problem 5.

a. Determine $g = g_0$ and calculate the associated conductivity $\sigma_{xx,0}$ in zero magnetic field, to first order in the constant b. (Help: in doing integrals it is permissible to use the approximation

$$\int_0^\infty dx e^{-x^2 - \gamma x^4} \simeq \int_0^\infty dx e^{-x^2} (1 - \gamma x^4)$$
 (12.17)

for $\gamma \ll 1$.)

b. Show that to first order in magnetic field the solution to the Boltzmann equation (12.14) is given by $g = g_0 + g_1$, where

$$g_1 = \tau \frac{eB}{\hbar} (v_y \frac{\partial g_0}{\partial k_x} - v_x \frac{\partial g_0}{\partial k_y}).$$
(12.18)

c. Calculate $\sigma_{yx}(=j_y/E)$ from (12.18), to first order in b. Find the offdiagonal element of the resistivity tensor $\rho_{xy} \simeq \sigma_{yx}/\sigma_{xx,0}^2$ and show that the result is identical to (12.15). Do you expect this identity to hold to higher order in b?

PROBLEM 7 The Hamiltonian operator describing the motion of an electron (with charge -e) in a homogeneous magnetic field is obtained from the classical Hamiltonian by replacing the generalized momentum **p** with the operator $\hbar \nabla / i$. This results in a Hamiltonian which resembles that of a particle in a harmonic oscillator potential.

The Hamiltonian for an electron moving in a magnetic field is given by

$$\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} + e\mathbf{A})^2.$$
 (12.19)

We shall assume that the magnetic field is homogeneous and points in the zdirection, $\mathbf{B} = (0, 0, B)$. It is often convenient to choose the vector potential as

$$\mathbf{A} : B(0, x, 0), \tag{12.20}$$

which is called the Landau gauge. The gauge

$$\mathbf{A}': \frac{B}{2}(-y, x, 0) \tag{12.21}$$

is called the symmetric gauge.

Exercise. Verify that (12.20) and (12.21) both yield the same magnetic field directed along the z-axis,

$$\mathbf{B}: (0,0,B). \tag{12.22}$$

In the Landau gauge the components of the velocity operator $\hat{\mathbf{v}} \equiv (\hat{\mathbf{p}} + e\mathbf{A})/m$ are thus given by

$$\hat{v}_x = \frac{\hbar}{im} \frac{\partial}{\partial x}; \quad \hat{v}_y = \frac{\hbar}{im} \frac{\partial}{\partial y} + \frac{eB}{m} x; \quad \hat{v}_z = \frac{\hbar}{im} \frac{\partial}{\partial z}.$$
 (12.23)

In the following we neglect the motion in the z-direction, since we consider a two-dimensional electron gas. The result we obtain for the energy eigenvalues may be easily generalized to three dimensions by multiplying the wavefunction by $L^{-1/2} \exp ik_z z$ and adding $\hbar^2 k_z^2/2m$ to the energy, since the motion in the z-direction is unaffected by the magnetic field.

It may be seen from (12.23) that the x- and y-components of the velocity do not commute because of the presence of the magnetic field, since

$$[\hat{v}_x, \hat{v}_y] = \frac{\hbar\omega_c}{im},\tag{12.24}$$

where

$$\omega_c = \frac{eB}{m} \tag{12.25}$$

is the classical cyclotron frequency for the electron.

In analogy with the harmonic oscillator it is convenient to introduce operators by the definition

$$\hat{v}_{+} = \hat{v}_{x} + i\hat{v}_{y} \tag{12.26}$$

and

$$\hat{v}_{-} = \hat{v}_{x} - i\hat{v}_{y}. \tag{12.27}$$

These operators satisfy commutation relations similar to those of the creation and annihilation operators $(a^{\dagger} \text{ and } a)$ for the harmonic oscillator.

Exercise. Verify that

$$[\hat{v}_{-}, \hat{v}_{+}] = 2\frac{\hbar\omega_{c}}{m}$$
(12.28)

and compare with the commutation relations for the creation and annihilation operators $(a^{\dagger} \text{ and } a)$ of the one-dimensional harmonic oscillator.

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When v_z is neglected, the Hamiltonian (12.19) can be written as

$$\hat{H} = \frac{1}{2}m\hat{\mathbf{v}}^2 = \frac{1}{2}m\hat{v}_+\hat{v}_- + \frac{1}{2}im[\hat{v}_x, \hat{v}_y].$$
(12.29)

We define the number operator \hat{N} by

$$\hat{N} = \frac{m}{2\hbar\omega_c}\hat{v}_+\hat{v}_-,\qquad(12.30)$$

which allows the Hamiltonian (12.29) to be expressed in the form

$$\hat{H} = \hbar \omega_c (\hat{N} + \frac{1}{2}).$$
 (12.31)

The Hamiltonian has thus the same appearance as that of the harmonic oscillator, since the commutation relations for \hat{N} and the operators \hat{v}_{-} , \hat{v}_{+} correspond precisely to those of the harmonic oscillator. The energy eigenvalues are therefore

$$E_n = \hbar \omega_c (n + \frac{1}{2}), \qquad (12.32)$$

where $n = 0, 1, 2 \cdots$. These are the Landau levels characterizing the quantum-mechanical motion of an electron in a magnetic field.

Unlike that of the one-dimensional harmonic oscillator, the spectrum (12.32) is strongly degenerate, in the sense that there are many linearly-independent eigenstates belonging to a particular value of n. The reason for this degeneracy is that there exists another operator, which commutes with the Hamiltonian and therefore corresponds to a classical constant of the motion. When the vector potential is chosen as the Landau gauge (12.20), this operator is \hat{p}_y . We may therefore label these eigenstates with the eigenvalue k_y for \hat{p}_y/\hbar ,

$$|n,k_y\rangle, \tag{12.33}$$

but it should be noted, that the eigenvalues k_y do not enter the energy eigenvalues. They determine however the degree of degeneracy, which we now turn to consider.

An alternative method of deriving the energy spectrum (12.32) is to solve the Schrödinger equation for the wave function ψ_{n,k_y} , which depends on x and y. As we shall see, this also allows the degree of degeneracy of the levels to be determined. Since the operator \hat{p}_y commutes with the Hamiltonian, we seek a solution in the form

$$\psi_{n,k_y}(x,y) = e^{ik_y y} f(x), \qquad (12.34)$$

which is an eigenfunction of \hat{p}_y .

Exercise. Show, by inserting (12.34) into the Schrödinger equation, that the function f must satisfy

$$-\frac{\hbar^2}{2m}\frac{d^2f}{dx^2} + \frac{1}{2m}(\hbar k_y + eBx)^2 f = Ef.$$
(12.35)

The equation (12.35) has the same form as the Schrödinger equation for a harmonic oscillator with its minimum displaced by the amount x_0 along the *x*-axis, where

$$x_0 = -\frac{\hbar k_y}{eB}.\tag{12.36}$$

It is thus readily seen from the Schrödinger equation (12.35), that the effective force constant is $(eB)^2/m$ and the eigenvalues those given by (12.32).

The degree of degeneracy of a level with a given n is determined by the requirement that the minimum of the oscillator (12.36) lies within the area considered. The number of states belonging to the interval Δk_y is given by $L\Delta k_y/2\pi$, and the condition $0 < x_0 < L$ implies that

$$\Delta k_y = \frac{eBL}{\hbar}.\tag{12.37}$$

The number N_u of linearly-independent state vectors belonging to the label n, k_y is therefore given by¹

$$N_u = \frac{eBL^2}{h}.$$
 (12.38)

The result (12.38) for the degree of degeneracy N_u may be interpreted pictorially by considering h/e to be a quantum of flux. The degree of degeneracy is thus the number of flux quanta corresponding to the flux BL^2 of the magnetic field through the area L^2 .

PROBLEM 8 In the present problem we consider the motion of a single electron in a magnetic field, by using the symmetric gauge (12.21). It is convenient to express energies in units of $\hbar\omega_c$ and lengths in units of $(\hbar/eB)^{1/2}$, which is often referred to as the magnetic length. Correspondingly, we express angular momentum in units of \hbar .

a) Show that the Hamiltonian for an electron moving in two dimensions, with the choice of gauge (12.21), may be written as

$$H = -\frac{1}{2}p_{+}p_{-} + \frac{1}{8}zz^{*} + \frac{1}{2}L.$$
 (12.39)

¹The existence of the electron spin is neglected here.

Here z = x + iy and $z^* = x - iy$, while

$$p_{+} = \frac{\partial}{\partial x} + i \frac{\partial}{\partial y}; \quad p_{-} = \frac{\partial}{\partial x} - i \frac{\partial}{\partial y}; \quad (12.40)$$

whereas L is the operator for angular momentum (perpendicular to the xy-plane),

$$L = \frac{1}{i} \frac{\partial}{\partial \phi}.$$
 (12.41)

The angle ϕ is the usual azimuthal angle, defined by

$$x = r \cos \phi, \quad y = r \sin \phi.$$
 (12.42)

b) Verify that the states

$$|m\rangle = \frac{1}{(2^{m+1}\pi m!)^{1/2}} (z^*)^m e^{-zz^*/4}$$
(12.43)

are normalized eigenstates of H and L, with eigenvalues given by 1/2 and -m, respectively. Find $\langle m|r^2|m\rangle$ and compare to the motion in the classical limit.

PROBLEM 9 The previous problem dealt with a single electron moving in a magnetic field. We shall now discuss the motion of two electrons in a magnetic field and take into account their Coulomb repulsion. We use the same notation as in Problem 8.

It is convenient to introduce center-of-mass and relative coordinates by the transformation

$$\bar{z} = \frac{1}{2}(z_1 + z_2), \quad z_a = \frac{1}{\sqrt{2}}(z_1 - z_2).$$
 (12.44)

The relative coordinate z_a is expressed in polar coordinates according to

$$z_a = x_a + iy_a = r e^{i\phi}.$$
 (12.45)

The potential energy describing the Coulomb-interaction is thus

$$V(r) = \frac{e^2}{4\pi\epsilon_r\epsilon_0\sqrt{2}r}.$$
(12.46)

where ϵ_r is the relative permittivity and $r = (x_a^2 + y_a^2)^{1/2}$. Note the appearance of the factor $\sqrt{2}$ in the potential energy, which originates in the transformation (12.44).

For the two-dimensional electron systems in GaAs/AlGaAs heterostructures, the relative permittivity may be taken to be $\epsilon_r = 13$, while the effective mass entering the cyclotron frequency ω_c is 0.067 times the bare electron mass. a) Calculate and compare the two characteristic energies $e^2/4\pi\epsilon_r\epsilon_0 l$ and $\hbar\omega_c$, where *l* is the magnetic length, for a magnetic field B = 10 T, with the values of the effective mass and relative permittivity given above.

b) We shall describe the relative motion of the two electrons in the absence of interactions by a state-vector of the form

$$|m\rangle = \frac{1}{(2^{m+1}\pi m!)^{1/2}} (z_a^*)^m e^{-z_a z_a^*/4}.$$
 (12.47)

Explain why this is an eigenstate of the Hamiltonian of the relative motion in the *absence* of the Coulomb interaction, and determine the corresponding eigenvalue by transforming the original Hamiltonian by means of (12.44). We shall refer to the energy associated with the relative motion as the internal energy. Show that $|m\rangle$ is an eigenstate of the relative angular momentum with eigenvalue -m. Which values of m are permitted by the requirement of antisymmetry (the spin degree-of-freedom is neglected throughout)?

c) Use first-order perturbation theory to calculate the contribution of the Coulomb interaction to the internal energy, as a function of m. Employ the value B = 10 T in giving specific results for the two cases m = 3 and m = 5, appropriate to GaAs/AlGaAs heterostructures.

d) Show that

$$|m,n\rangle = \frac{1}{(2^{n+m+1}\pi m!n!)^{1/2}} e^{r^2/4} (p_-)^m (p_+)^n e^{-r^2/2}.$$
 (12.48)

is a normalized eigenstate of the Hamiltonian for a single electron, with the eigenvalue (n + 1/2) (we use the notation of Problem 8). Note: it is sufficient to show this for the case n = 1, since we shall use only the states belonging to n = 1 to calculate higher-order corrections to the energy obtained in c).

e) Show that $|m + 1, 1\rangle$ is an eigenstate of angular momentum with eigenvalue -m. Explain why it is sufficient to use the basis $|m, 0\rangle$ and $|m + 1, 1\rangle$ for calculating corrections to the energy, as long as we neglect states belonging to the higher-lying energies $5/2, 7/2 \cdots$, and determine the correction to the first-order result found under c) for the case m = 5.

PROBLEM 10 Collective modes like sound exist in both three- and twodimensional systems. In the following we shall determine the velocity and attenuation of sound in a two-dimensional monatomic gas of ³He-atoms. Except for question 6) below, we consider the classical limit where the Maxwell-Boltzmann distribution applies in equilibrium. The number density of atoms is n and the mass of an atom is denoted by m. The gas occupies an area A, the pressure (dimensionally a force per unit length) is denoted by p, while Tis the temperature. In making estimates, the number density of atoms may be taken to be $n = 10^{10}$ cm⁻². 1) Determine the (equilibrium) equation of state. Find the specific heat per particle at constant area and at constant pressure.

2) Write down (in analogy with Section 1.10 in Transport Phenomena) the hydrodynamical equations that describe the propagation of sound under adiabatic conditions. Determine the corresponding sound velocity and find its value at T = 10 K.

3) Use the results obtained in Section 1.7 to estimate the temperaturedependent viscosity of the two-dimensional gas, assuming an interatomic potential corresponding to that of hard disks with radius R = 10 Å. Estimate the size of the mean free path.

4) Estimate the attenuation length of sound at the frequency $\omega = 10^3 \text{ s}^{-1}$ and the temperature T = 10 K. (The attenuation length may be defined as the length over which the amplitude of the sound wave decreases by the factor 1/e).

5) Show how the sound attenuation and the sound velocity may be obtained from the Boltzmann equation, in analogy with Section 1.14.

6) Estimate the magnitude of the sound velocity at T = 0 K.

PROBLEM 11 We shall in the following discuss the screening properties of an electron gas, which is constricted to move in two dimensions. In order to generalize the result (1.15.13) in *Transport Phenomena* to two dimensions we first express it in terms of the Fourier-transform of the Coulomb-interaction, thereby anticipating the result of the RPA-approximation, which is illustrated diagrammatically in Fig. 1.12.

a) Show that the Fourier transform in three dimensions of the screened Coulomb interaction

$$V(r) = \frac{e_0^2}{r} e^{-k_s r},$$
 (12.49)

where $e_0^2 = e^2/4\pi\epsilon_0$, is given by

$$\tilde{V}(q) = \frac{4\pi e_0^2}{q^2 + k_s^2}.$$
(12.50)

Here k_s is a constant, which has the dimension of an inverse length. The Fourier-transform is defined by

$$\tilde{V}(\mathbf{q}) = \int \int \int dx dy dz e^{-i\mathbf{q}\cdot\mathbf{r}} V(r).$$
(12.51)

(Help: In order to evaluate $\tilde{V}(\mathbf{q})$ it is convenient to introduce polar coordinates with a polar axis along \mathbf{q} . From symmetry considerations it is clear that $\tilde{V}(\mathbf{q})$ can only depend on the magnitude of \mathbf{q} .)

b) Show that (1.15.13) may be written as

$$\epsilon = 1 + \tilde{V}(q)\chi(q,\omega), \qquad (12.52)$$

with $\tilde{V}(q) = 4\pi e_0^2/q^2$. Determine $\chi(q,\omega)$ in the limit where q tends to zero in i) the high-frequency regime and ii) the static limit.

c) Show that the Fourier transform in two dimensions of the Coulomb interaction

$$V(r) = \frac{e_0^2}{r},$$
 (12.53)

where $r^2 = x^2 + y^2$, is given by

$$\tilde{V}(q) = \frac{2\pi e_0^2}{q}.$$
 (12.54)

The Fourier-transform is defined by

$$\tilde{V}(\mathbf{q}) = \int \int dx dy e^{-i(q_x x + q_y y)} V(r).$$
(12.55)

d) Generalize (12.52) to two dimensions and show that the dielectric function in the static, long-wavelength limit becomes

$$\epsilon(q) = 1 + \frac{q_s}{q} \tag{12.56}$$

and determine q_s . Calculate the magnitude of q_s for GaAs/AlGaAs heterostructures (cf. Problem 9).

e) Show from these results that the two-dimensional analog of the plasma oscillation has a frequency ω proportional to $q^{1/2}$ in the long-wavelength limit, and determine the constant of proportionality.

PROBLEM 12 A gas of atoms with number density n moves in two dimensions at a temperature T which is sufficiently high that the atoms in equilibrium are described by the Maxwell-Boltzmann distribution. The mass of an atom is denoted by m.

a) Show that the enthalpy per particle, h, is equal to 2kT.

b) Use the relaxation-time approximation to calculate the thermal conductivity of the gas in terms of the relaxation time τ .

c) Calculate the viscosity in the same approximation and determine the Prandtl number.

PROBLEM 13 Consider a gas of electrons of density n moving in two dimensions (the xy-plane) at temperatures much less than the Fermi temperature.

The electrons move under the influence of a constant electric field E along the *x*-axis. The collisions are treated in the relaxation-time approximation with a constant, temperature-independent relaxation time τ .

a) Determine the change $\delta f = f - f^0$ of the distribution function and plot it as a function of the angle ϕ between the electron momentum and the electric field.

b) Calculate the current density j obtained from the distribution function and show explicitly that the associated change in number density is zero. What is the value of the momentum current density Π_{xy} ?

c) Calculate the ratio of the drift velocity u = j/ne and the Fermi velocity for an electric field E = 1 V/m, with $\tau = 10^{-12}$ s and $n = 10^{11}$ cm⁻².

PROBLEM 14 In the present problem we shall consider the thermal conductivity of a two-dimensional gas of electrons, with dispersion relation $\epsilon = p^2/2m$, at a temperature T much less than the Fermi temperature. The number density of the electron gas is denoted by n, and the effect of collisions is treated in the relaxation-time approximation, with a constant, temperature-independent relaxation time τ . The thermal conductivity κ relates the temperature gradient to the heat current \mathbf{j}_{th} according to $\mathbf{j}_{\text{th}} = -\kappa \nabla T$, where

$$\mathbf{j}_{\rm th} = 2 \int \frac{d^2 p}{(2\pi\hbar)^2} \mathbf{v}(\epsilon - \mu) f. \qquad (12.57)$$

Here μ is the chemical potential.

a) Show that the left hand side of the Boltzmann equation becomes

$$-\frac{\partial f^0}{\partial \epsilon} \mathbf{v} \cdot \nabla T \, \frac{\epsilon - \mu}{T},$$

when linearized in the temperature gradient, and use this to obtain an expression for κ .

b) Calculate the ratio $\kappa/\sigma T$, where σ is the electrical conductivity and compare to the three-dimensional case discussed in Section 2.2.4 of *Transport Phenomena*.

PROBLEM 15 Use the model investigated in the previous problem to calculate a) the heat current associated with an electric field in the absence of a temperature gradient and b) the electric current associated with a temperature gradient in the absence of an electric field. Compare the results to the three-dimensional case discussed in Section 2.2.5 of *Transport Phenomena*.

PROBLEM 16 We shall determine the thermodynamic potential Ω of a twodimensional electron gas in a uniform magnetic field of strength *B* in the limit where the temperature is much bigger than the Fermi temperature. 1. Explain, why Ω is given (for arbitrary temperatures) by

$$\Omega = -kT \frac{eBL^2}{h} \sum_{n=0,1,2,\cdots} \ln(1 + e^{(\mu - \epsilon_n)/kT})$$
(12.58)

where $\epsilon_n = (n + 1/2)\hbar\omega_c$. The electron gas is contained within a square of sidelength L (we have neglected the spin of the electron).

2. Determine Ω as a function of the ratio $\hbar \omega_c/kT$, starting from (12.58). Hint: use that $e^{\mu/kT} \ll 1$.

3. Find an approximate expression for Ω in the limit, where $\hbar \omega_c/kT \ll 1$, and use this to determine the diamagnetic susceptibility, which involves the second derivative of Ω with respect to the magnitude of the magnetic field. What is the value of the susceptibility in the classical limit, $\hbar \to 0$?

PROBLEM 17 In this problem we consider the thermodynamic potential of a two-dimensional gas in a magnetic field, in the limit that the temperature is much less than the Fermi temperature $\epsilon_{\rm F}/k$.

1. Use (12.58) to prove that Ω oscillates as a function of 1/B and determine the period.

2. Find how the amplitude of the magnetisation oscillations depends on the ratio $\hbar\omega_c/kT$.

Help: In carrying out a sum of the type $\sum_{n=0,1,2\cdots} F(n)$ one may use the Poisson summation formula

$$\sum_{n=0,1,2\cdots} F(n) = \frac{1}{2}F(0) + \int_0^\infty dx F(x) + 2\operatorname{Re} \sum_{m=1,2\cdots} \int_0^\infty dx F(x) e^{i2\pi mx}$$
(12.59)

where Re denotes the real part. In calculating the last term (which contains the oscillations) one uses partial integration together with the integral

$$\int_{-\infty}^{\infty} dx \frac{1}{4\cosh^2(x/2)} e^{i\alpha x} = \frac{\pi\alpha}{\sinh\pi\alpha}.$$
 (12.60)

PROBLEM 18 We consider a two-dimensional electron gas described by the Hamiltonian

$$H = H_0 + H' \tag{12.61}$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(12.62)

represents the kinetic energy while

$$H' = \frac{1}{2A} \sum_{\mathbf{q}\neq 0, \mathbf{k}, \mathbf{k}', \sigma, \sigma'} \frac{2\pi e_0^2}{q} c^{\dagger}_{\mathbf{k}+\mathbf{q}, \sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}, \sigma'} c_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}.$$
(12.63)

is the electron-electron interaction. The two-dimensional gas is enclosed in a region of area A.

1) Determine the ground-state energy of the system when the interaction between the electrons is ignored. Calculate the corresponding pressure p and the compressibility $-(\partial A/\partial p)/A$.

2) Use first-order perturbation theory to calculate the ground-state energy in the presence of the electron-electron interaction. Compare your result to that obtained for the three-dimensional case in Chapter 3 of Introduction to Many-particle Physics.

3) Use the result obtained in 2) to calculate the compressibility of the electron gas and discuss your result.

4) Compare your calculated compressibility to that measured experimentally by Eisenstein et. al., Phys. Rev. Lett. 68, 674 (1992).

PROBLEM 19 Consider a system given by the Hamiltonian

$$H = E_a a^{\dagger} a + E_b b^{\dagger} b + \Delta (a^{\dagger} b + b^{\dagger} a), \qquad (12.64)$$

where E_a, E_b and Δ are real constants. The field operators satisfy the Fermi commutation rules

$$\{a, a\} = \{a^{\dagger}, a^{\dagger}\} = 0; \ \{a, a^{\dagger}\} = 1,$$
 (12.65)

and

$$\{b, b\} = \{b^{\dagger}, b^{\dagger}\} = 0; \ \{b, b^{\dagger}\} = 1,$$
 (12.66)

while the *a*- and the *b*-operators anticommute with each other,

$$\{a, b\} = \{a^{\dagger}, b^{\dagger}\} = 0; \quad \{a, b^{\dagger}\} = \{a^{\dagger}, b\} = 0.$$
 (12.67)

- a) Write down the Heisenberg equations of motion for a and b.
- b) Show that the equations of motion have solutions of the form

$$a = a(0)e^{-iEt/\hbar}, \quad b = b(0)e^{-iEt/\hbar}$$
 (12.68)

and determine E in terms of E_a, E_b and Δ .

c) Let (12.64) be the Hamiltonian of a single electron. Use the timeindependent Schrödinger equation $H|\psi\rangle = E|\psi\rangle$ to determine the energy eigenvalues (help: Write $|\psi\rangle$ as a linear combination of state vectors $|1_a, 0_b\rangle$ and $|0_a, 1_b\rangle$ with the properties $a^{\dagger}a|1_a, 0_b\rangle = |1_a, 0_b\rangle$ and $b^{\dagger}b|0_a, 1_b\rangle = |0_a, 1_b\rangle$). **PROBLEM 20** In this problem we shall determine the electrical and thermal resistivity of Al with 1 ppm of Na impurities (in its normally conducting state), using the results of the model calculations described in 'Transport Phenomena'.

a) Determine the residual resistivity (in units of ohm cm).

b) Calculate the resistivity due to electron-phonon scattering at T = 10 K (neglecting the contribution of impurity scattering) and compare your answer to that obtained in a).

c) Calculate the thermal resistivity of Al (in units of mK/W) at T = 10 K for each of the scattering mechanisms discussed in a) and b).

PROBLEM 21 The transport properties of layered cuprate materials such as $La_{2-x}Sr_xCuO_4$ have been investigated intensively, due to the occurrence of high-temperature superconductivity (with a transition temperature of 35 K) when x is near 0.15. These materials also exhibit a linear dependence of the resistivity on temperature from the transition temperature up to 1000 K. When x exceeds 0.2 one finds (see H. Takagi et al., Phys. Rev. Lett. **69**, 2975, 1992) a different power law, $\rho = \rho_0 + T^{1.5}$, which also extends up to about 1000 K.

The solution to the present homework problem will not explain these observations but will allow one to compare them to results obtained using conventional models of transport in two-dimensional systems. We shall neglect the periodic potential and assume that the charge carriers of mass m occupy a 'Fermi disk' of radius $k_{\rm F}$. The phonons will be treated in a two-dimensional Debye-model, with linear dispersion $\omega_q = cq$.

a) Show that the in-plane resistivity ρ_{ab} within the relaxation time approximation is given by

$$\rho_{ab} = \frac{h}{e^2} \frac{d}{k_{\rm F} \ell},\tag{12.69}$$

where d is the distance between two parallel neighboring planes, while $\ell = v_F \tau$ is the mean free path, with v_F being the Fermi velocity. For the materials in question d = 6.4 Å. What is the value of $k_F \ell$, when $\rho_{ab} = 10^{-3}$ ohm cm?

b) We shall use a model electron-phonon matrix element given by

$$|g|^2 = \lambda \frac{\hbar \omega_q}{2N(0)A},\tag{12.70}$$

where A is the area and 2N(0) the density of states (per unit area) at the Fermi energy, corresponding to (2.6.21) in *Transport Phenomena*. How does the quantity corresponding to $\alpha^2 F$ in (2.7.2) depend on frequency ω at small frequencies? Determine the energy- and temperature-dependence of the relaxation rate $1/\tau$ and the electrical resistivity, at temperatures much less than the Debye-temperature. How does the resistivity depend on T, when T is comparable to or larger than the Debye-temperature? **PROBLEM 22** We consider the specific heat of a two-dimensional crystal of hexagonal symmetry and treat the phonons in the Debye-approximation. The crystal consists of N identical atoms which form a triangular lattice in such a way that each atom has 6 nearest neighbors. The distance between nearest neighbors is denoted by a, and the transverse and longitudinal sound velocity is called c_t and c_l , respectively.

a) Express the Debye wave vector q_D in terms of a.

b) Determine the specific heat C as a function of temperature.

c) Write down approximate expressions for C at low and high temperatures. Compare your result at high temperatures to the law of Dulong and Petit.

PROBLEM 23 Use the transformation to phonon coordinates given in (2.6.14-15) of *Transport Phenomena* to show that the thermal average $\langle (\delta \mathbf{R}_i)^2 \rangle$ is given by

$$<(\delta \mathbf{R}_i)^2>=\frac{\hbar}{2MN}\sum_{\mathbf{q}}\frac{1}{\omega_{\mathbf{q}}}(2N^0(\omega_{\mathbf{q}})+1), \qquad (12.71)$$

where N^0 is the Planck function (the sum over polarization directions is included in the q-sum). Use this result to prove that one- and two-dimensional crystals are unstable (help: consider the long wavelength limit $q \rightarrow 0$).

PROBLEM 24 The elastic (free) energy F of a two-dimensional cubic crystal may be written in the general form

$$F = F_0 + \frac{1}{2}\lambda_1(\epsilon_{xx}^2 + \epsilon_{yy}^2) + \lambda_2\epsilon_{xx}\epsilon_{yy} + \lambda_3(\epsilon_{xy}^2 + \epsilon_{yx}^2).$$
(12.72)

Here λ_1 , λ_2 , and λ_3 are three independent elastic constants, consistent with cubic symmetry.

The components of the stress tensor σ_{ik} are obtained from this by differentiating,

$$\sigma_{ik} = \frac{\partial F}{\partial \epsilon_{ik}}.$$
(12.73)

The equation of motion is

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ik}}{\partial x_k},\tag{12.74}$$

in the absence of volume forces. The deformation tensor ϵ_{ik} is defined by

$$\epsilon_{ik} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right), \tag{12.75}$$

where u_i with i = x, y are the two components of the displacement vector.

a) Show that the σ_{xy} component of the stress tensor is given by $\sigma_{xy} = 2\lambda_3 \epsilon_{xy}$ and determine similarly σ_{xx} and σ_{yy} .

b) Find the condition that a plane-wave solution of the form

$$\mathbf{u} = \mathbf{u}_0 e^{i\mathbf{q}\cdot\mathbf{r} - i\omega t} \tag{12.76}$$

satisfies the equation of motion (12.74). Determine the sound velocity as a function of the angle θ defined by $\mathbf{q} = q(\cos \theta, \sin \theta)$.

c) Plot the sound velocity as a function of θ for $\lambda_1 = \lambda_2 = \lambda_3 = \lambda$. How do you expect a corresponding plot to look for a two-dimensional crystal with hexagonal symmetry?

PROBLEM 25 In this problem we consider the thermal conductivity of a twodimensional crystal within the relaxation-time approximation, at temperatures much lower than the Debye temperature. The relaxation time τ is assumed to be a constant, independent of energy and temperature.

a) First we consider the situation where the phonon frequencies are proportional to the wave number, with isotropic velocities c_l and c_t for the longitudinal and transverse modes, respectively. Find the thermal conductivity and compare its temperature dependence to the corresponding case in three dimensions.

b) Indicate how the calculation of the thermal conductivity is changed, if the velocities depend on the direction of propagation (compare Problem 24).

PROBLEM 26 In three dimensions isotopic impurity scattering gives rise to an infinite thermal conductivity (cf. *Transport Phenomena*, Section 4.2.2), if no other scattering mechanisms are present. Is this also true in two dimensions?

PROBLEM 27 We consider a two-dimensional Fermi liquid of interacting particles with mass m and number density n = N/A, A being the area within which the particles are confined. For particles moving in two dimensions, we may introduce Fermi-liquid parameters F_{ℓ} by replacing the Legendre-polynomia P_{ℓ} by the functions $\cos \ell \phi$, where ϕ is the angle between \mathbf{p} and \mathbf{p}' .

a) Express the compressibility in terms of F_0^s and F_1^s . Find the hydrodynamic sound velocity c_1 .

b) Write down the Boltzmann equation in analogy with Section 6.3.1 of *Transport Phenomena* with a collision integral corresponding to eq. (6.3.1). Determine the velocity of zero sound in the case where all other Landau parameters than F_0^s are set equal to zero, while $F_0^s \gg 1$. Compare your result to the hydrodynamic sound velocity.

c) Calculate how the sound velocity depends on $\omega \tau$, where ω is the frequency of the sound wave and τ a suitably defined relaxation time. It is assumed that $F_0^s \gg 1$ and that Landau parameters corresponding to ℓ greater than or equal to 3 may be neglected. Find the relative change in sound velocity and the damping coefficient as a function of $\omega \tau$ and the Landau parameters. Discuss the temperature dependence of the attenuation in the hydrodynamic and in the collisionless regime.

Problems

PROBLEM 28 Consider a particle moving in one dimension with the Hamiltonian given by

$$H = \hbar\omega(a^{\dagger}a + \frac{1}{2}) + \hbar\omega_0(a^{\dagger} + a), \qquad (12.77)$$

where the operators a^{\dagger} and a satisfy the commutation rule $[a, a^{\dagger}] = 1$, while the frequencies ω and ω_0 are positive constants.

a) Write down the Heisenberg equations of motion for a^{\dagger} and a.

b) Solve the Heisenberg equations of motion by introducing the operator $\alpha = a + \omega_0/\omega$ and its hermitian conjugate.

c) Express H in terms of α and α^{\dagger} and determine its eigenvalues.

d) What might be the physical origin of the second term in the Hamiltonian (12.77)? Compare your result to that obtained by solving the appropriate Schrödinger equation.

PROBLEM 29 In this problem we shall discuss the *tight-binding* Hamiltonian of an electron which moves in a periodic lattice. For simplicity we start out by treating the motion in one dimension, and subsequently generalize the discussion to two and three dimensions.

Consider the one-dimensional nearest-neighbor hopping Hamiltonian

$$H = -t \sum_{j\delta} c_j^{\dagger} c_{j+\delta} \tag{12.78}$$

where the index j labels the N atomic sites of the one-dimensional chain $(j = 1, 2 \cdots, N)$, while the sum over $\delta = \pm 1$ ensures that only nearest-neighbor sites, separated by the lattice constant a, are coupled. The constant t is assumed to be positive. The operators c^{\dagger} and c obey the anticommutation rules

$$\{c_{j}, c_{j'}^{\dagger}\} = \delta_{jj'}.$$
 (12.79)

a) Use the transformation

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ikj\,a} a_k \tag{12.80}$$

_ _

to diagonalize the Hamiltonian and plot the eigenvalues ϵ_k as a function of k.

b) Generalize your treatment to a two-dimensional square lattice and draw contours of constant energy in the $k_x - k_y$ plane. How does the corresponding dispersion relation look in the three-dimensional case for a simple cubic lattice?

PROBLEM 30 It is often convenient to transform particle operators into spin operators or vice versa. As an example we consider a lattice gas with a fixed

chemical potential μ . The operator $\hat{K} = \hat{H} - \mu \hat{N}$ is given by

$$K = \frac{1}{2}U\sum_{j\delta}n_j n_{j+\delta} - \mu \sum_j n_j$$
(12.81)

where U is a constant, while $n_j = c_j^{\dagger} c_j$ is the number operator belonging to site j. The sum over δ denotes as usual a sum over nearest-neighbor sites.

a) Use the transformation to spin-1/2 operators given by $n_j = S_j^z + 1/2$, $c_j = S_j^-$, $c_j^{\dagger} = S_j^+$ to prove that the lattice gas model is equivalent to an Ising model in an external magnetic field.

b) Show by adding the hopping term from Problem 29 that the resulting quantum lattice-gas Hamiltonian is equivalent to a Heisenberg model with anisotropic interactions in an external magnetic field.

PROBLEM 31 Use (3.13) to determine the zero-temperature pressure $p = -\partial E/\partial V$ and compressibility $\kappa = -(\partial V/\partial p)/V$ of the electron gas. Plot your results as functions of the parameter r_s , and compare them to the case when the electron-electron interaction is neglected. Indicate how your results are modified, when the term given by (3.29) is added to (3.13).

PROBLEM 32 In this problem we consider a spin-polarized electron gas, in which the number of spin-up electrons N_{\uparrow} differs from the number N_{\downarrow} of spin-down electrons.

a) First we consider the non-interacting case, in which the electron-electron interaction is neglected entirely. Determine the ground-state energy per particle, E/N, as a function of the dimensionless ratio $\alpha = (N_{\uparrow} - N_{\downarrow})/N$, where $N = N_{\uparrow} + N_{\downarrow}$, and find the minimum value of E/N as a function of α .

b) Next we include the electron-electron interaction to first order in perturbation theory. Find how (3.13) is modified in the spin-polarized case by determining the energy per particle as a function of α and r_s .

c) Determine the value of r_s for which the ferromagnetic state ($\alpha = 1$) has lower energy than the non-magnetic state ($\alpha = 0$). Sketch the energy per particle as a function of α for this particular value of r_s .

PROBLEM 33 The elementary excitations of an antiferromagnet are spin waves. Here we shall calculate the spin wave dispersion relation for a linear chain, using the method described in Section 5.5.2.

a) Determine the dispersion relation for the linear chain with nearestneighbor coupling and calculate the spin-wave velocity.

c) Generalize your results to a two-dimensional square lattice and draw contours of constant energy.

PROBLEM 34 We consider a one-dimensional chain of atoms, which are

coupled by nearest neighbor antiferromagnetic interactions, corresponding to the Hamiltonian (5.74) with J < 0. The spin-operators associated with the sites of each of the two sublattices a and c are denoted by $\mathbf{S}_n^{(a)}$ and $\mathbf{S}_m^{(c)}$. The z-component of the total sublattice magnetization is given by

$$S_{z}^{(a)} = Ns - \sum_{n} a_{n}^{\dagger} a_{n}$$
(12.82)

and

$$S_{z}^{(c)} = -Ns + \sum_{n} c_{n}^{\dagger} c_{n}, \qquad (12.83)$$

where the a- and c-operators refer to sites in each sublattice. Note that there are N atoms on sublattice a and N atoms on sublattice c.

a) Use the transformation (5.86) to prove that $S_2^{(a)}$ and $S_2^{(c)}$ are given by

$$S_{z}^{(a)} = Ns - \sum_{q} b_{q}^{\dagger} b_{q}$$
(12.84)

and

$$S_{z}^{(c)} = -Ns + \sum_{q} d_{q}^{\dagger} d_{q}.$$
(12.85)

b) Find, using the Bogoliubov transformation employed in Problem 33,

$$b = u\alpha - v\beta^{\dagger}, \quad d = u\beta - v\alpha^{\dagger},$$
 (12.86)

an expression for the zero-temperature sublattice magnetization in terms of the coefficients v_q . Show that the ground state of the antiferromagnet does not correspond to the sublattice magnetization being Ns and -Ns, respectively.

c) Demonstrate that the sublattice magnetization diverges in one dimension. Does the divergence persist in two and three dimensions?

PROBLEM 35 Use the results obtained in Section 5.3 to calculate the expectation value of the particle number operator $a_k^{\dagger}a_k$ in the ground state of the system of interacting bosons. Plot your result as a function of k.

PROBLEM 36 The elementary excitations of a dilute, three-dimensional Bose gas are phonons. Determine the specific heat at low temperatures and compare with the result obtained at low temperatures in the ideal bose gas.

PROBLEM 37 The spin waves for a Heisenberg ferromagnet are gapless, in the sense that their energy $\hbar \omega_q$ vanishes (as q^2) in the limit when q tends to

zero. Show that the spin waves develop a gap, when the interactions become anisotropic, corresponding to the Hamiltonian

$$H = -\sum_{n} J_{\parallel} S_{n,z} S_{n+1,z} + \frac{1}{2} J_{\perp} (S_{n}^{+} S_{n+1}^{-} + S_{n}^{-} S_{n+1}^{+}), \qquad (12.87)$$

where $J_{\parallel} > J_{\perp}$, and find the magnitude of the gap. What happens in the presence of an external magnetic field?

PROBLEM 38 As an example of the use of diagrammatic methods we investigate in this and several subsequent problems a neutral fermion system described by the Hamiltonian

$$H = H_0 + H', (12.88)$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_k c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
(12.89)

represents the kinetic energy, with $\epsilon_k = \hbar^2 k^2/2m$, while the interaction between the fermions is given by the operator

$$H' = \frac{U}{2V} \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}', \sigma, \sigma'} c^{\dagger}_{\mathbf{k}+\mathbf{q}, \sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}, \sigma'} c_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}.$$
 (12.90)

As an example we might think of the quantum liquid ³He, but one should note the basic difference from real ³He: the Fourier-transform of the interaction is taken to be a positive constant, U, corresponding to a repulsive delta-function interaction in real space,

$$V(\mathbf{r} - \mathbf{r}') = U\delta(\mathbf{r} - \mathbf{r}'). \tag{12.91}$$

The number of fermions is denoted by N. In evaluating physical quantities we shall identify m with the mass of a ³He-atom, while the density n = N/Vis given by the molar volume being 36.8 cm³ (corresponding to liquid ³He at saturated vapor pressure). Unless otherwise indicated, U/k is given the (somewhat arbitrary) value of 300 KÅ³, k being the Boltzmann constant.

a) Determine the ground-state energy per particle in the absence of the interaction. Evaluate the corresponding Fermi energy and Fermi temperature.

b) Show that

$$\alpha = N(0)U \tag{12.92}$$

is a dimensionless parameter and express it in terms of the parameters given above. Here N(0) is the density of states at the Fermi energy in the noninteracting system (per spin and per unit volume). Find the value of α in terms of the parameters given above. c) Calculate the magnitude of the compressibility $\kappa = -(\partial V/\partial p)/V$ for the non-interacting system and determine the magnitude of the sound velocity s from the relation $s^2 = 1/mn\kappa$.

PROBLEM 39 We shall now use the model described in Problem 38 to calculate some physical properties within the Hartree-Fock approximation.

a) Determine the single-particle Green function and indicate the position of its poles in the complex-frequency plane. Draw the relevant diagrams that are being summed.

b) Calculate the single particle energies and determine the shift in the chemical potential (at T = 0 K) compared to the noninteracting system. Evaluate the magnitude of the shift for the parameters given above. How does the chemical potential depend on N?

c) Use the result of question b) to determine the total energy of the system (hint: use the thermodynamic definition of the chemical potential).

d) Calculate the inverse compressibility to first order in α . Determine the magnitude of the sound velocity and compare it to the answer obtained in Problem 38 above.

PROBLEM 40 Use the first-order perturbation theory described in Chapter 3 to calculate the ground state energy of the system described in Problem 38, to first order in α . Compare your result to the answer obtained in Problem 39 c).

PROBLEM 41 We shall later make use of the socalled density-fluctuation propagator for spin-1/2 fermions. It is a special case of a two-particle Green function. The density operator in the Heisenberg picture is

$$\rho(\mathbf{x},t) = \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{x},t)\psi_{\sigma}(\mathbf{x},t), \qquad (12.93)$$

where the field operators ψ and ψ^{\dagger} are given by (6.5) and (6.6). In the following we consider only spatially homogeneous systems, where the ground-state expectation value $\langle \rho(\mathbf{x}) \rangle$ of the density is a constant, *n*, equal to the number of particles per unit volume,

$$\langle \rho(\mathbf{x}) \rangle = n. \tag{12.94}$$

The density fluctuation operator $\tilde{\rho}$ is defined as

$$\tilde{\rho}(\mathbf{x},t) = \rho(\mathbf{x},t) - n. \tag{12.95}$$

The density fluctuation propagator $D(\mathbf{x}, t; \mathbf{x}', t')$ is a time-ordered correlation function, which is defined in analogy with the single-particle Green function (6.1),

$$D(\mathbf{x}, t; \mathbf{x}', t') = -i < T\{\tilde{\rho}(\mathbf{x}, t)\tilde{\rho}(\mathbf{x}', t')\} >$$
(12.96)

in terms of a time-ordered product of density-fluctuation operators in the Heisenberg picture.

a) Use (6.62) to prove that the density fluctuation propagator $D^{(0)}$ of the non-interacting system is given by

$$D^{(0)}(\mathbf{x},t;\mathbf{x}',t') = -2iG^{(0)}(\mathbf{x},t;\mathbf{x}',t')G^{(0)}(\mathbf{x}',t';\mathbf{x},t).$$
 (12.97)

b) In a translationally invariant system, the density fluctuation propagator only depends on the differences $\mathbf{x} - \mathbf{x}'$ and t - t'. The Fourier-transform is

$$D(\mathbf{q},\omega) = \int d(\mathbf{x}-\mathbf{x}')d(t-t')e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}e^{i\omega(t-t')}D(\mathbf{x}-\mathbf{x}',t-t').$$
 (12.98)

Show that the Fourier-transform $D^{(0)}(\mathbf{q},\omega)$ is given in terms of the Fourier-transform of the free-particle Green functions by

$$D^{(0)}(\mathbf{q},\omega) = -2i \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{dk_0}{2\pi} G^{(0)}(\mathbf{k}+\mathbf{q},k_0+\omega) G^{(0)}(\mathbf{k},k_0).$$
(12.99)

Use (6.38) to carry out the integration over the internal frequency variable k_0 by means of the residue theorem.

We shall later on carry out the integration over the internal momentum variable k and relate the resulting function of q and ω to the wavevector- and frequency-dependent dielectric function of the electron gas.

PROBLEM 42 Identify all second order diagrams in the expansion of the single-particle Green function, including linked and unlinked diagrams as well as those of the denominator given by (6.89). Verify the Feynman rules up to and including second order and demonstrate explicitly the cancellation of the unlinked diagrams in the numerator against the corresponding terms in the denominator.

PROBLEM 43 Verify the expression (8.29) for the imaginary part of the function F introduced in (8.27). Plot the result as a function of x_0 for fixed values of x, for instance x = 0.2, x = 1 and x = 2.

PROBLEM 44 We consider a noninteracting system of fermions described by the Hamiltonian H_0 given in Problem 38. Use the expressions (7.24) for the particle number N and (7.31) for the internal energy U to determine U at temperatures that are high compared to the Fermi temperature. Calculate the lowest order correction to the classical internal energy and the specific heat per particle and determine the relative size of the correction terms at T = 10K. **PROBLEM 45** Repeat Problem 44 with the interaction term (A.89) included. The Green function appearing in Eq. (7.24) for the particle number N and in Eq. (7.31) for the internal energy U is taken to be the one obtained in the Hartree-Fock approximation. Determine the leading correction to the classical internal energy coming from the interaction and evaluate its relative size at T = 10 K for the parameters given in Problem 38.

PROBLEM 46 Use the expression (8.37), after analytic continuation, for calculating the dispersion of longitudinal plasma waves in the classical limit where the temperature is much larger than the Fermi temperature. Compare your result to (8.33), which is valid at temperatures much less than the Fermi temperature. Indicate how the (Landau) damping of the plasma wave may be determined.

PROBLEM 47 In the present problem we consider a classical plasma in the ultra-relativistic limit, where $kT \gg mc^2$. Use the result (8.37) for determining the dispersion of longitudinal plasma waves in this limit and compare your result to (8.33) (it is permissible to approximate the energy dispersion relation by $\epsilon \simeq cp$, where p is the momentum).

PROBLEM 48 Use (8.45) for determining $\Pi^{(0)}(q,0)$ as a function of the variable $x = q/2k_{\rm F}$ in the cases where the dimension d is 1,2 and 3. Compare your results to the sketch given in Fig. 8.2. For the case d = 3 plot the derivative $d\Pi^{(0)}(q,0)/dq$ as a function of q in the vicinity of $q = 2k_{\rm F}$. Compare the resulting static dielectric function to that obtained within the Thomas-Fermi approximation.

PROBLEM 49 We shall determine the temperature dependence of $\Pi^{(0)}$ in a tight-binding model of a one-dimensional crystal. The length of the crystal is L = Na, where N is the number of atoms. The energy dispersion relation is

$$\epsilon_k = -E_0 \cos ka. \tag{12.100}$$

We assume that the band is half-filled at T = 0 K, implying that $k_{\rm F} = \pi/2a$.

Find $\Pi^{(0)}(2k_{\rm F})$ as a function of E_0/kT for large values of this parameter (hint: introduce the density of states and utilize that

$$\epsilon_{p+\hbar q/2} = -\epsilon_{p-\hbar q/2} \tag{12.101}$$

and

$$f_{p+\hbar q/2}^0 = 1 - f_{p-\hbar q/2}^0 \tag{12.102}$$

for $q = 2k_{\rm F}$. One needs the integral

$$\int_{0}^{\infty} \frac{dx \ln x}{\cosh^{2} x} = -\ln(4e^{\gamma}/\pi), \qquad (12.103)$$

where $\gamma = 0.577\cdots$). There is a close relation between this logarithmic singularity and the so-called Peierls instability in one-dimensional conductors, as we shall see in Problem 51.

PROBLEM 50 We consider a (degenerate) three-dimensional gas of free electrons, coupled to Debye-phonons by the interaction (9.12) with g given by the model form (9.23), for all q less than the Debye cut-off. Use the polarization bubble $\Pi^{(0)}$ and the diagrammatic approximation

$$\approx = \sim + \sim \circ \approx$$

to determine (at zero temperature) the change in the frequency of the phonons as well as their damping, due to the coupling to the electrons. For numerical values, use $\lambda = 0.2$ and an unperturbed sound velocity c equal to 1/100 times the Fermi velocity.

a) Find the relative magnitude $\Delta c/c$ of the change Δc in sound velocity.

b) Find the magnitude of the relative shift $\Delta \omega_q/\omega_q$ of the phonon frequency at $q = 2k_{\rm F}$ (we assume that $2k_{\rm F}$ is less than the Debye cut-off). What is the value of the derivative of the relative shift with respect to q at $q = 2k_{\rm F}$?

c) Calculate the magnitude of the ratio Γ_q/ω_q , where Γ_q is the phonon width (inverse lifetime). Compare your result to (1.14.13) and (2.11.30) in Transport Phenomena.

Help: For the calculation of the shift in phonon frequency one may use the static limit of $\Pi^{(0)}$ (why?). The damping is determined by the imaginary part of $\Pi^{(0)}$.

PROBLEM 51 When $\Pi^{(0)}$ is used for calculating phonon frequencies in a one-dimensional conductor, one finds that the phonon with wavevector $2k_{\rm F}$ "softens" in the sense that its frequency decreases with decreasing temperature and eventually goes to zero at a "transition temperature" T_c . This *Peierls transition* marks the transition from a conducting to an insulating state (note, however, the general arguments against occurrence of phase transitions in one-dimensional systems, cf. Landau and Lifshitz, Statistical Physics, vol. I).

Use the method of Problem 50 to find the transition temperature T_c as well as the temperature dependence of the phonon frequency just above T_c for the system treated in Problem 49. The results should be given in terms of λ and the Fermi temperature $T_F = E_0/k$.

PROBLEM 52 Determine $\text{Im}\Sigma(\mathbf{k}, \xi_k)$ from (9.62) and compare with (2.7.1) in *Transport Phenomena*. Consider the T = 0 limit as well as $\text{Im}\Sigma(\mathbf{k}, 0)$ at low and at high temperatures compared to the Debye temperature. Discuss the relation of these results to the transport times that enter the electrical and thermal conductivity.

PROBLEM 53 The conduction electrons in a spin-1/2 three-dimensional ferromagnet interact with the local spins S_i , where *i* labels the position in the lattice (assumed to be simple cubic). The interaction Hamiltonian is

$$H_{\rm el-spin} = A \sum_{i} \delta(\mathbf{r} - \mathbf{R}_{i}) \mathbf{s} \cdot \mathbf{S}_{i}, \qquad (12.104)$$

where i is the conduction electron spin.

Introduce magnon propagators and write the interaction Hamiltonian in terms of electron (and magnon) creation and annihilation operators. Discuss differences and similarities between the electron-phonon and electron-magnon many-body problem.

PROBLEM 54 The phonon density-of-states in real materials is usually rather different from the quadratic frequency dependence characteristic of the Debye-model, except at low frequencies. In this problem we consider the opposite extreme, an Einstein model with $\alpha^2 F(\omega)$ given by

$$\alpha^2 F(\omega) = C\omega_0 \delta(\omega - \omega_0), \qquad (12.105)$$

where C is a dimensionless constant, which we take to be C = 0.25.

1) Determine the real and the imaginary part of the self-energy at T = 0 K, as well as the spectral density $A(\mathbf{k}, \omega)$.

2) Determine the relaxation rate $1/\tau(\xi, T)$ as a function of $\xi = \epsilon - \mu$ and T, in terms of the characteristic temperature $T_0 = \hbar \omega_0 / k$.

PROBLEM 55 In this problem we consider the interacting Fermi gas introduced in Problem 38 at zero temperature.

1) Determine the dependence of the relaxation rate (the inverse life-time) on $\xi_k = \epsilon_k - \mu$ for states near the Fermi surface, by considering the imaginary part of the self-energy to second order in the parameter α (cf. Problem 38).

2) Calculate (or estimate) the magnitude of the relaxation rate for $\xi/\mu = 0.01$.

Help: Since we only go to second order in α , the chemical potential μ may be set equal to its value in the ground state of the noninteracting system. The calculation of the lifetime may be carried out by use of either the zero-temperature formalism or the Matsubara technique, with $T \rightarrow 0$ at an appropriate stage. The relevant diagrams for the single-particle Green function (from which the self-energy may be extracted) are drawn below. Consider (a) first and convince yourself (without doing a specific calculation) that the contribution from (b) is the same except for a numerical factor.

Appendix A: Fourier-transforms

The Fourier-transform $\tilde{F}(\mathbf{q})$ of a function $F(\mathbf{r})$ is given by the relations

$$F(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{r}} \tilde{F}(\mathbf{q})$$
(A.1)

where

$$\tilde{F}(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} F(\mathbf{r}).$$
(A.2)

One often distinguishes a function and its Fourier-transform by their argument only, thus writing $F(\mathbf{q})$ instead of $\tilde{F}(\mathbf{q})$.

We shall need the Fourier-transform of a Coulomb-potential and its derivative, which enters the electron-phonon interaction. In order to include the case of a screened Coulompotential we first study the Fourier-transform of the function

$$V(r) = \frac{1}{r} e^{-k \cdot r} \tag{A.3}$$

where $1/k_s$ is the screening length. It is convenient to introduce a polar axis along q. From symmetry considerations it is clear that $\tilde{V}(\mathbf{q})$ can only depend on the magnitude of q. Thus

$$\tilde{V}(q) = 2\pi \int_{-1}^{1} d(\cos\theta) \int_{0}^{\infty} r^{2} dr e^{-iqr\cos\theta} \frac{1}{r} e^{-k_{\bullet}r}$$

$$= \frac{2\pi}{iq} \int_{0}^{\infty} dr (e^{iqr} - e^{-iqr}) e^{-k_{\bullet}r}$$

$$= \frac{2\pi}{iq} (-\frac{1}{iq - k_{s}} + \frac{1}{-iq - k_{s}})$$

$$= \frac{4\pi}{q^{2} + k_{s}^{2}}.$$
(A.4)

For $k_s = 0$ we get

$$\tilde{V}(q) = \frac{4\pi}{q^2}.\tag{A.5}$$

We also need the Fourier transform of the gradient of 1/r. Since

$$\frac{1}{r} = \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi}{q^2},\tag{A.6}$$

we obtain, by letting the gradient $\nabla = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$ act on both sides of (A.6), that

$$-\frac{\mathbf{r}}{r^3} = \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi i\mathbf{q}}{q^2}.$$
 (A.7)

Thus the Fourier-transform of \mathbf{r}/r^3 is $-4\pi i \mathbf{q}/q^2$.

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