The Effect of Different Potentials for Paul Traps and it's Application as a Quantum Simulator

Bachelor Thesis

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March 28, 2018

Under vejledning af
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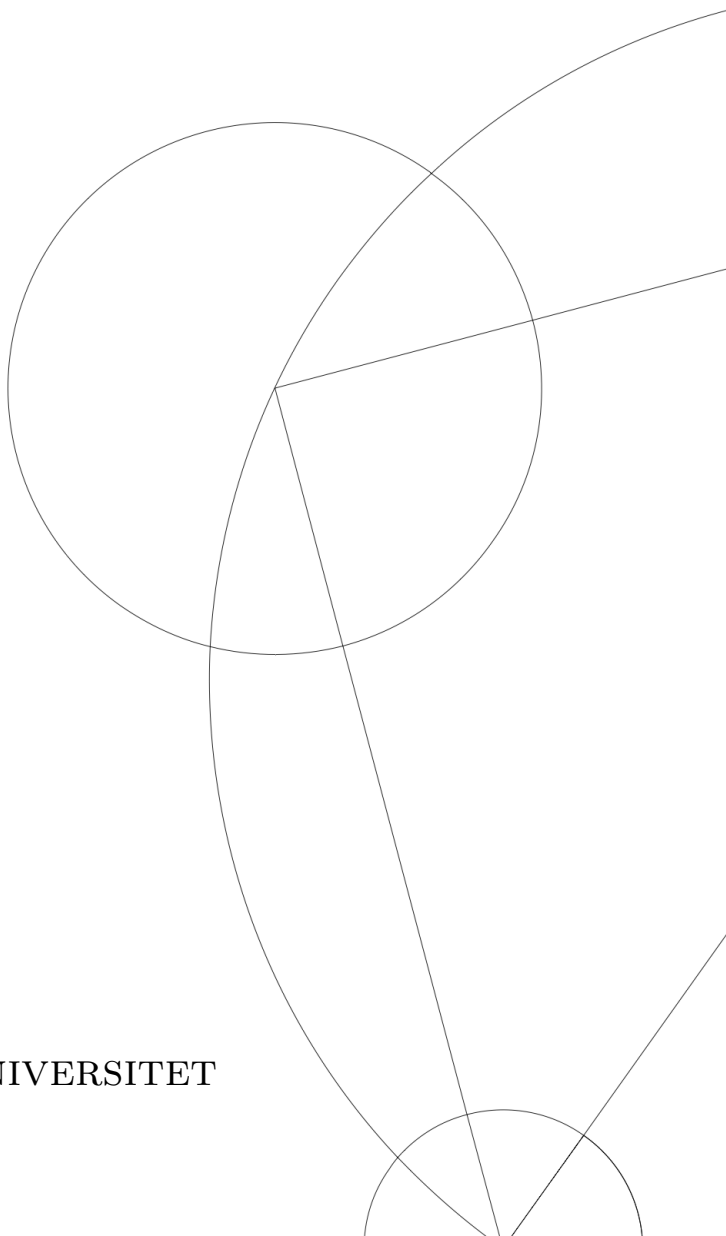

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Hand in date: 28.03.2018

Abstract

In this project we will consider the capabilities of a linear ion trap as a Quantum Simulator. The project considers different choices for potentials along the trap and examines how the different potentials affect the spacing of the ions held in place. Modes of transversal oscillations of the ions are found and used as a basis for the implementation of the *Mølmer–Sørensen gate*. Coupling strength between the ions are found from numerical evaluation.
The proposed changes to the potentials seems to be an improvement over the harmonic potential, especially with detuning of $\delta \sim 1.2\omega_{COM}$ where behaves like a dipole-dipole interaction. For detuning close to the center of mass motion $\delta \sim \omega_{COM}$ the coupling strength will be constant across the ion chain and long range spin-spin interaction can occur.

Contents

1 Introduction

A model of great importance in many areas of physics is the *Ising Model*, which in it's general form is described by the hamiltonian $H = -\sum J_{ij}\sigma_i\sigma_j - \mu\sum h_j\sigma_j$. Models like this forms a basis for our understanding of ferromagnets. To calculate spin coupling for N ions in a lattice one needs to consider 2^N different spin states, which quickly becomes to big of a problem to handle with classical computers. Feynman stipulated the idea of a quantum simulator, which makes use of the quantum mechanical nature of the computer itself to solve problems[1]. One method which has enjoyed succes in recent years is the idea of using a ion trap as a quantum simulator, in which a number of ions are held in place by an electric potential and then controlled by a laser. With this setup it has been possible to confine and control up to $N = 53$ ions in a linear trap paul-trap[2] and $N \sim 300$ ions in a two-dimensional penning trap[3].

2 Linear Ion Trap

Consider a chain of N ions held in place by an electric potential V_{trap} along the direction of the chain. Let $\mathbf{R}_1(t), \mathbf{R}_2(t), \ldots, \mathbf{R}_N(t)$ denote the position of the ions in a coordinate system placed such that the ions are placed along the z-axis. We may number the ions such that $z_m < z_{m+1}$ for $m = 1, \ldots, N-1$. The ions are held in place radially by a rapidly oscillating electrical field, which we'll assume for now is so strong that $x_m = y_m = 0$ for all ions. Along with the potential the ions also interact with each other through coulomb interaction. Therefore the potential energy of the chain is,

$$V = \sum_{m=1}^{N} V_{trap}(z_m) + \sum_{\substack{n,m=1 \\ n\neq m}}^{N} \frac{Z^2e^2}{8\pi\varepsilon_0}\frac{1}{|z_n - z_m|}, \tag{1}$$

where Z is the degree of ionisation of the ions, e is the elementary charge and ε_0 is the vacuum permittivity. The equilibrium positions $z_1^0, z_2^0, \ldots, z_N^0$ are given by the solutions to the N coupled equations

$$\left[\frac{\partial V}{\partial z_m}\right]_0 = 0, \qquad m = 1, \ldots, N, \tag{2}$$

where the notation $[\ \cdot\ ]_0$ means that the term is to be evaluated at $z_m = z_m^0$ for all m. These equations are dependant on the choice of trap potential V_{trap}, and will generally be too complicated to solve analytically. If the trap potential is chosen to

be harmonic $V_{trap}(z) = \frac{1}{2}M\nu^2 z^2$ where M is the mass of the ion, it will be possible to solve the system analytically for $N = 2$ and $N = 3$[4], but generally one have to rely on numerical methods to find the equilibrium positions.

2.1 Choice of Trap Potential

It is generally desirable for the ions in the trap to be equidistance, as it will greatly simplify any models that seek to describe the interaction between the ions. Another wish is for the trap potential to be simple, as that would make it easier to construct and work with experimentally. These two wishes can't be achieved at the same times and thus a compromise between the two is needed.

A harmonic potential is an obvious choice to satisfy these criteria. This is also the potential used in many experiments [2]. This potential has the advantages of being easy to work with both theoretically and experimentally, however it suffers from the fact that the ions are equidistance. To counter this one could change the trap potential used. This thesis examines four different choices of potential,

- $V_{trap}^{(2)}(z) = \frac{1}{2}M\nu^2 z^2$
- $V_{trap}^{(4)}(z) = \frac{\lambda_4}{4l^2}M\nu^2 z^4$
- $V_{trap}^{(6)}(z) = \frac{\lambda_6}{6l^4}M\nu^2 z^6$
- $V_{trap}^{(8)}(z) = \frac{\lambda_8}{8l^6}M\nu^2 z^8$

where the scale length l is defined by,

$$l^3 = \frac{Z^2 e^2}{4\pi\varepsilon_0 M\nu^2}, \tag{3}$$

and λ_4, λ_6 and λ_8 allows us to tune the strength of the potentials such that the length of the ion chain remains the same no matter the choice of potential. The equilibrium positions for these potentials are found by solving (2) numerically. To determine λ_i for the different potentials, a method was used where the equilibrium positions were found with $\lambda_i = 1$. This produced a set of coordinates $z_1', z_2', \ldots, z_N'$ for each potential, these were scaled to be the same length as the chain produced by $V_{trap}^{(2)}$. The scaled coordinates were then plugged back into (2), which this time were solved for λ_i. Then to double check the result (2) were used with the newly found λ_i to ensure that the coordinates matched the scaled coordinates. This was

done for chains consisting from 4 to 100 ions.

We can now compare how the ions are spaced for the different potentials. One way to do this is to find the standard deviation σ for the distance between neighbouring ions

$$\sigma = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N-1}(d_i - \bar{d})} \tag{4}$$

where $d_i = (z^0_{i+1} - z^0_i)/l$ is the spacing between neighbouring ions in units of the scale length l and $\bar{d}$ is the mean spacing. A plot with σ for the different potentials for $4 \leq N \leq 100$ is found in figure 1. From it we can see that the proposed potentials $V^{(4)}_{trap}$,$V^{(6)}_{trap}$ and $V^{(8)}_{trap}$ are significantly better at separating the ions with equal distance than the harmonic potential $V^{(2)}_{trap}$ when theres more than 10 ions in the chain.

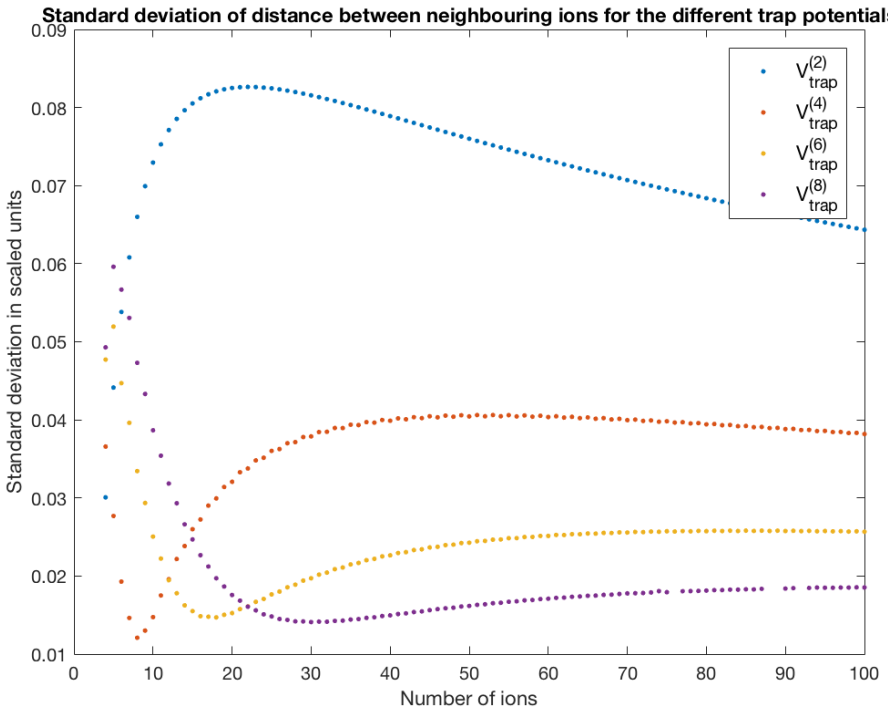

Figure 1: The standard deviation of the distance between neighbouring ions in units of the scale length l as defined in (3). This makes it possible to determine the regime in which the different potentials will the give the most uniform distribution of the ions. For $N = 4$ $V^{(2)}_{trap}$ is the best choice, for $5 \leq N < 12$ it is $V^{(4)}_{trap}$, for $12 \leq N < 22$ it is $V^{(6)}_{trap}$ and for $22 \leq N$ it is $V^{(8)}_{trap}$.

2.2 Longitudinal Oscillations

We now wish to consider the motion of the ions. Let $z_m(t) = z_m^0 + q_m(t)$ such that $q_m(t)$ describes the displacement of the ions compared to the equilibrium as a function of time. The Lagrangian corresponding to this motion is

$$L = \frac{1}{2}\sum_{m=1}^{N} \dot{q}_m^2 M - \frac{1}{2}\sum_{m,n=1}^{N} q_n q_m \left[\frac{\partial^2 V}{\partial q_n \partial q_m}\right]_0 \tag{5}$$

where dot notation is used to denote the time derivative and terms of order q^3 and higher have been omitted. Defining $f_k = \lambda_k(k-1)u_m^{k-2}$ and letting the trap potential be $V_{trap}^{(}k)$, allows the Lagrangian to be rewritten as

$$L = \frac{M}{2}\left[\sum_{m=1}^{N} \dot{q}_m^2 - \nu^2 \sum_{m,n=1}^{N} q_n q_m A_{nm}\right], \tag{6}$$

where

$$A_{nm} = \begin{cases} f_k + 2\sum_{i=1}^{N} \frac{1}{|u_m - u_i|^3}, & \text{if } n = m, \\ -\frac{1}{|u_n - u_m|^3}, & \text{if } n \neq m. \end{cases} \tag{7}$$

The matrix A with as it's entries is real, symmetric and positive semidefinite[4] so its eigenvalues must be non-negative. Number the eigenvalues μ_p and corresponding eigenvectors $\mathbf{b}^{(p)}, p = 1, \ldots, N$, such that μ_1 have the lowest eigenvalue, μ_2 the second lowest and so on. We may assume that the eigenvectors are normalised

$$\sum_{p=1}^{N} b_n^{(p)} b_m^{(p)} = \delta_{nm}, \quad \sum_{m=1}^{N} b_m^{(p)} b_m^{(q)} = \delta_{pq} \tag{8}$$

where $b_m^{(p)}$ is the m^{th} entry of the p^{th} eigenvector. Define the normal modes as

$$Q_p = \sum_m b_m^{(p)} q_m, \tag{9}$$

then

$$q_m = \sum_p b_m^{(p)} Q_p. \tag{10}$$

By defining the angular frequency of the p^{th} mode as $\nu_p = \sqrt{\mu_p}\nu$, allows us to write the Lagrangian as

$$L = \frac{M}{2}\sum_{p=1}^{N}\left[\dot{Q}_p^2 - \nu_p^2 Q_p^2\right] \tag{11}$$

The canonical momentum is $P_p = M\dot{Q}_p$ and thus allows the hamiltonian to be explicitly written

$$H = \sum_p \left[\frac{1}{2M} P_p^2 + \frac{M}{2} \nu_p^2 Q_p^2 \right]. \tag{12}$$

2.3 Transversal Oscillations

Let's now consider transversal ocsillations. The ion trap is set up in the same way as before with the N ions along the z direction. Along the z-direction the ions are still held in place by the four different trap potentials. Along the x- and y-axis the ions are held in place by a rapidly oscillating electrical field which to the second order may be approximated by the effective radial potential,

$$V_{rad} = \frac{1}{2} M \nu_{rad}^2 (x_m^2 + y_m^2). \tag{13}$$

This potential will be added to eq.(1) along with a change from $|z_n - z_m|$ to $|\mathbf{R}_n - \mathbf{R}_m|$ in the coulomb part to reflect that the ions now differ in the radial coordinate as well,

$$V = \sum_{m=1}^{N} \left(V_{trap}(z_m) + \frac{1}{2} M \nu_{rad}^2 (x_m^2 + y_m^2) \right) + \sum_{\substack{n,m=1 \\ n \neq m}}^{N} \frac{Z^2 e^2}{8\pi\varepsilon_0} \frac{1}{|\mathbf{R}_n - \mathbf{R}_m|}. \tag{14}$$

Suppose the ions all oscillate along the x-direction. The Lagrangian that describes this motion is analogue to the longitudinal case

$$L = \frac{1}{2} \left(\sum_{m=1}^{N} \dot{x}_m^2 M - \sum_{m,n=1}^{N} x_n x_m \left[\frac{\partial^2 V}{\partial x_n \partial x_m} \right]_0 \right) \tag{15}$$

Carrying out the differentiation and evaluating at equilibrium position yields

$$\left[\frac{\partial^2 V}{\partial x_n \partial x_m} \right]_0 = \begin{cases} M\nu_{rad}^2 - \frac{Z^2 e^2}{4\pi\varepsilon_0} \sum_{\substack{i=1 \\ i \neq n}}^{N} \frac{1}{|z_i - z_n|^3}, & \text{if } n = m, \\ \frac{Z^2 e^2}{4\pi\varepsilon_0} \frac{1}{|z_n - z_m|^3}, & \text{if } n \neq m. \end{cases} \tag{16}$$

Define the ratio between the radial potential strength and the strength of the harmonic trap potential as $\gamma = \frac{\nu}{\nu_{rad}}$, such that the Lagrangian becomes

$$L = \frac{M}{2} \left[\sum_{m=1}^{N} \dot{x}_m^2 - \nu_{rad}^2 \sum_{m,n=1}^{N} x_n x_m B_{nm} \right] \tag{17}$$

where

$$A_{nm} = \begin{cases} 1 - \gamma^2 \sum_{\substack{i=1 \\ i \neq n}}^{N} \frac{1}{|u_m - u_i|^3}, & \text{if } n = m, \\ \gamma^2 \frac{1}{|u_n - u_m|^3}, & \text{if } n \neq m. \end{cases} \tag{18}$$

Just like before we can find eigenvalues ρ_p and eigenvectors $\boldsymbol{\varphi}_p$ for B, and like before the Lagrangian can be written in terms of the modes defined by $\Phi_p = \sum_m \varphi_{m,p} x_m$ and the angular frequency of the modes $\omega_p = \sqrt{\rho_p}\nu_{rad}$. Thus

$$L = \frac{M}{2} \sum_{p=1}^{N} \left[\dot{\Phi}_p^2 - \omega_p^2 \Phi_p^2 \right]. \tag{19}$$

However this time the eigenvalues could be negative. In the limit $\gamma \to \infty$ the matrix B will be negative definite, which will result in negative eigenvalues and imaginary frequencies. This reflects that the radial potential is not strong enough to keep the lowest energy configuration of the ions to be a linear configuration. The lowest energy configuration will instead be a zigzag or helical configuration.

2.4 Zigzag Configuration of the Ions

In order to avoid a zigzag configuration of the ions in the trap, the strength of the trap potential compared to the radial potential must be weak enough to avoid the lowest energy configuration of the ions to be a zigzag configuration. Start by considering the potential of the ion chain as described in equation (14)

$$V = \frac{1}{2} M \omega_r^2 l^2 \left[\sum_{m=1}^{N} \left(\tilde{V}_z(\tilde{z}_m) + \tilde{r}_m^2 \right) + \sum_{\substack{n,m=1 \\ n \neq m}}^{N} \frac{1}{|\tilde{R}_n - \tilde{R}_m|} \right] \tag{20}$$

where the positions of the ions are described by the scaled cylindrical set of coordinates $\tilde{R}_m(\tilde{r}_m, \theta_m, \tilde{z}_m)$. The lowest energy configuration of this potential is either a linear, a zigzag or a helical configuration [5]. Because of the symmetry of the trap the linear configuration where $\tilde{r}_1 = \cdots = \tilde{r}_N = 0$ will always be at equilibrium. It will however not always be stable, if $\tilde{V}_z$ is too strong a small perturbation such as a laser pulse will cause the ions to decay into a lower zigzag configuration. The linear configuration is stable if $\frac{\partial^2 V}{\partial \tilde{r}_m^2} > 0$, which is equivalent to

$$\frac{\partial^2}{\partial \tilde{r}_m^2} \left[\sum_{m=1}^{N} \left(\tilde{V}_z(\tilde{z}_m) + \tilde{r}_m^2 \right) + \sum_{\substack{n,m=1 \\ n \neq m}}^{N} \frac{1}{|\tilde{R}_n - \tilde{R}_m|} \right] > 0 \tag{21}$$

Carrying out the differentiation and evaluating in the linear configuration yields the rather pleasing

$$2 - \sum_{\substack{n=1 \\ n \neq m}}^{N} \frac{1}{|\zeta_{nm}|^3} > 0 \tag{22}$$

where $\zeta_{nm} = |\tilde{r}_n - \tilde{r}_m|$. In practice it is only necessary to evaluate this expression for $m \approx N/2$ as this is the area with the least seperation between the ions. This equation relates the raidal potential trough the scale length l to the trap potential through the set of z_m. This along with the way of finding z_m as described in a previous section provides a way, although indirectly, to gauge the choices of potential strengths.

For the rest of the thesis we'll treat the transversal case as it produces significantly better results and it is the way the experiments are done today [6][2]. The longitudinal case follows analogously.

3 Quantum Mechanics

Now let's consider the system quantum mechanically. Given the classical hamiltonian of the system

$$H = \frac{1}{2M}\sum_{p=1}^{N} P_p^2 + \frac{M}{2}\sum_{p=1}^{N}\omega_p^2\Phi_p^2 \tag{23}$$

Introduce the ladder-operators $a_p^\dagger$ and a_p which raises and lowers the respective phonon mode and obeys the canonical commutation relations

$$[a_i, a_q] = 0, \quad [a_q^\dagger, a_q^\dagger] = 0, \quad [a_p, a_q^\dagger] = \delta_{qp}. \tag{24}$$

Make the substitution

$$\Phi_p \to \Phi_p = \sqrt{\frac{\hbar}{2M\omega_p}}(a_p^\dagger + a_p) \tag{25}$$

$$P_p \to P_p = i\sqrt{\frac{\hbar M\omega_p}{2}}(a_p^\dagger - a_p) \tag{26}$$

$$\tag{27}$$

which yields

$$H = \frac{1}{2M}\sum_{p=1}^{N}\left(i\sqrt{\frac{\hbar M\omega_p}{2}}(a_p^\dagger - a_p)\right)^2 + \frac{M}{2}\sum_{p=1}^{N}\omega_p^2\left(\sqrt{\frac{\hbar}{2M\omega_p}}(a_p^\dagger + a_p)\right)^2 \tag{28}$$

$$= \sum_p \omega_p\hbar\left(a_p^\dagger a_p + \frac{1}{2}\right) \tag{29}$$

which is the hamiltonian corresponding to the quantum motion of the ions. This is accompanied by an internal hamiltonian

$$H = \hbar\omega_{eg}\sum_{i=1}^{N}\frac{\sigma_{zi}}{2} \tag{30}$$

where $\hbar\omega_{eg}$ is the energy difference between the internal energy levels of a single ion and σ_{zi} is the Pauli matrix corresponding to the i'th ion in the chain. Combined these two yields the complete time independant part of the full hamiltonian

$$H_0 = \sum_p \omega_p\hbar\left(a_p^\dagger a_p + \frac{1}{2}\right) + \hbar\omega_{eg}\sum_{i=1}^{N}\frac{\sigma_{zi}}{2} \tag{31}$$

with the set of eigenstates $\{|f_1, f_2, \ldots, f_N, n_1, \ldots, n_N\rangle\}$ where $f_i = e$ or g and n_p is the excitation of the p^{th} vibrational mode.

3.1 Ion-Laser Interaction

We can now turn our attention to the interaction between the laser and the ions. Consider the system consisting of a single ion which obeys the single ion version of eq. (31),

$$H_0 = \hbar\nu\left(a^\dagger a + \frac{1}{2}\right) + \hbar\omega_{eg}\frac{\sigma_z}{2}. \tag{32}$$

Suppose the system is exposed to a monochromatic electromagnetic plane-wave, described by the E-field,

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + \mathbf{E}_0 e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \tag{33}$$

where $\mathbf{k}$ is the wave vector and is chosen such that the wave propagates in the x-direction. We assume that the internal energy levels couple through the electrical field, so we may write the hamiltonian for this interaction as [7]

$$H_1 = -\boldsymbol{\mu_d}\cdot\boldsymbol{E}(\boldsymbol{r},t), \tag{34}$$

where $\boldsymbol{\mu_d}$ is the electric dipole moment operator. This can be written as

$$H_1 = \frac{\hbar\Omega}{2}(\sigma_+ + \sigma_-)\left(e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\right) \tag{35}$$

where Ω is the Rabi frequency of the transition and is given by $\hbar\Omega = -|\mu_d|E_0/2$ and $\sigma_\pm = \sigma_x \pm i\sigma_y$ are the Pauli matrices relating to the internal energy levels. We'll now transition to the interaction picture by the transformation $U = e^{i\omega_{eg}t|e\rangle\langle e|}$ which we'll expand in a series and utillize that $|e\rangle$ and $|g\rangle$ form an orthonormal basis so a theorem from linear algebra yields $|e\rangle\langle e| + |g\rangle\langle g| = 1$

$$U = 1 + i\omega_{eg}t\,|e\rangle\langle e| + \frac{1}{2}(i\omega_{eg}t)^2\,|e\rangle\langle e| + \cdots \tag{36}$$

$$= |g\rangle\langle g| + |e\rangle\langle e| + i\omega_{eg}t\,|e\rangle\langle e| + \frac{1}{2}(i\omega_{eg}t)^2\,|e\rangle\langle e| + \cdots \tag{37}$$

Collecting the terms with $|e\rangle\langle e|$ and substituting the terms which depends on $|e\rangle\langle e|$ with an exponential yields,

$$U = |g\rangle\langle g| + e^{i\omega_{eg}t}\,|e\rangle\langle e| \tag{38}$$

$$\tag{39}$$

We use this to transform H_1 into the interaction picture,

$$H_{1,I} = UH_1U^\dagger = \hbar\Omega\left[\left(e^{-i(\mathbf{k}\cdot\mathbf{r}-(\omega+\omega_{eg})t)} + e^{i(\mathbf{k}\cdot\mathbf{r}-(\omega-\omega_{eg})t)}\right)|e\rangle\langle g| + h.c.\right] \tag{40}$$

where $h.c.$ is the Hermitian conjugate. We chose a detuning such that the energy of the laser is close to that of the internal energy difference. This means that $\omega - \omega_{eg} \ll \omega + \omega_{eg}$ and we may neglect the terms involving $\omega + \omega_{eg}$ because they are rapidly oscillating and thus will average to 0 on any applicable time scale. Using this approximation which is called a *rotating wave approximation* and transforming back to the Schrödinger picture gives us,

$$H_1 = U^\dagger H_{1,I} U = \frac{\hbar\Omega}{2}\left(\sigma_+ e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + h.c.\right). \tag{41}$$

The generalisation to the chain of N ions is straightforward

$$H_1 = \sum_i \frac{\hbar\Omega_i}{2}\left(\sigma_{+i} e^{i(\mathbf{k_i}\cdot\mathbf{r_i}-\omega_i t)} + h.c.\right) \tag{42}$$

where the sum is over all ions affected by a laser. We have the freedom to let different lasers with different strength and frequency address the different ions. The last thing we'll do is to consider the term $(\boldsymbol{k}\cdot\boldsymbol{r})$ in the exponent. The wave propagates in the x-direction and thus $\boldsymbol{k} = k\hat{x}$. Recall x-coordinate of the ion is described through the transversal modes of oscillation, Φ_p, by $x_m = \sum_p \varphi_{m,p}\Phi_p$ and the modes are given by eq. (25). This allows us to write

$$\boldsymbol{k_m}\cdot\boldsymbol{r_m} = \sum_p k_m \phi_{m,p}\sqrt{\frac{\hbar}{2M\omega_p}}(a_p^\dagger + a_p). \tag{43}$$

Define the *Lamb-Dicke parameter* as,

$$\eta_{m,p} = k_m\phi_{m,p}\sqrt{\frac{\hbar}{2M\omega_p}}, \tag{44}$$

such that we may write the hamiltonian as

$$H_1 = \sum_i \frac{\hbar\Omega_i}{2}\left(\sigma_{+i} e^{i\left[\sum_p \eta_{i,p}(a_p^\dagger + a_p) - \omega_i t\right]} + h.c.\right), \tag{45}$$

which will, along with eq. (31), form the basis of out further analysis.

3.2 Perturbative Treatment of the Transitions

We'll let the laser be bichromatic with the two angular frequencies $\omega_1 = \omega - \delta$ and $\omega_2 = \omega + \delta$. The way the vibrational modes are laid out means that the detuning δ is chosen to over/undershoot the first excitation of the different modes by a small

margin.

Because the lasers are to tuned to be off resonant, the energy dosen't add up for only one ion to be excited. However if two ions are hit by a photon each with different frequencies, they will have enough energy to make the transition $|ggn\rangle \leftrightarrow |een\rangle$ through the intermediate stages $\{|egn_p \pm 1\rangle, |gen_p \pm 1\rangle\}$ which will become virtually excited. This way of controlling the ions is called a *Mølmer–Sørensen gate* and was first proposed in [8].

To find the transition rate we'll use second order perturbation theory, where H_1 will considered a perturbation to H_0. Let the initial state at $t_0 = 0$ be $|\Psi\rangle = \sum_{|i\rangle} c_i |i\rangle$, where the sum is over the eigenstates to H_0 with energy given by $H_0 |i\rangle = E_i |i\rangle$. First order perturbation theory for the transition to the eigenstate $|m\rangle$ yields [9]

$$\dot{c}_m = -\frac{i}{\hbar} \sum_{|i\rangle} c_i \langle m| H_1 |i\rangle e^{i(E_m - E_i)t/\hbar} \tag{46}$$

Integrating to get an approximation for c_m

$$c_m(t') \approx c_m(t = t_0) - \frac{i}{\hbar} \sum_{|i\rangle} c_i \int_{t_0}^{t'} \mathrm{d}t \left[\langle m| H_1 |i\rangle e^{i(E_m - E_i)t/\hbar} \right], \tag{47}$$

To carry out the integration we need to pull out the time dependant part of H_1. Split up H_1 in the following way,

$$H_1 = \sum_j \left(V_{1j} e^{-i\omega_j t} + V_{1j}^\dagger e^{i\omega_j t} \right) \tag{48}$$

Then V_{1j} and $V_{1j}^\dagger$ will be independant of time, so we can carry out the integration,

$$c_m = c_m(t_0) - \frac{i}{\hbar} \sum_{|i\rangle, j} c_i \left[\frac{\langle m| V_{1j} |i\rangle e^{i(E_m - E_i - \omega_j \hbar)t/\hbar}}{(E_m - E_i - \omega_j \hbar)/\hbar} + \frac{\langle m| V_{1j}^\dagger |i\rangle e^{-i(E_m - E_i - \omega_j \hbar)t/\hbar}}{(E_m - E_i + \omega_j \hbar)/\hbar} \right]_{t_0}^{t'} \tag{49}$$

The transitions we are interested in are close to resonant such that $E_i + \hbar\omega_j \approx E_m$, so we may neglect the last term as $E_m - (E_i + \omega_j \hbar) \ll E_m + \omega_j \hbar - E_i$ which corresponds to absorption on a photon. If however that the transition occurred by emission of a photon $E_m + \omega_j \hbar \approx E_i$ and thus the second term would dominate. Throwing away the last term in the bracket and considering a further transition to the final state $|f\rangle$ by plugging c_m back into (46) yields,

$$\dot{c}_f = -\frac{1}{\hbar^2} \sum_{|m\rangle, |i\rangle} c_i \frac{\langle f| H_1 |m\rangle \langle m| H_1 |i\rangle}{(E_m - E_i - \omega_j \hbar)/\hbar} e^{i(E_f - E_m)t/\hbar} (e^{i(E_m - E_i)t_0/\hbar} - 1) \tag{50}$$

where we have assumed that the initial population of the intermediate states $|m\rangle$ and $|f\rangle$ is zero. The probability of finding the system in the state $|f\rangle$ after time $t' - t_0$ is $|P_f| = |c_f|^2$ and so we recognise the Rabi frequency $\tilde{\Omega}$ of the transition as [10],

$$\tilde{\Omega} = -\frac{1}{\hbar^2}\left|\sum_{|m\rangle,|i\rangle}\frac{\langle f|\,H_1\,|m\rangle\,\langle m|\,H_1\,|i\rangle}{(E_m - E_i - \omega_j\hbar)/\hbar}\right| \tag{51}$$

3.3 Evaluating the Rabi frequency

Let's now try to evaluate the Rabi frequency for the transition where the i^{th} and j^{th} ion start out in the ground state and some distribution of vibrational modes are populated, which we will represent with the state $|i\rangle = |g_i g_j n\rangle$. For the intermediate states we'll consider $|m\rangle = \{|e_i g_j n_p \pm 1\rangle, |g_i e_j n_p \pm 1\rangle\}$ where one of the modes is raised or lowered, and as the final state we consider $|f\rangle = |e_i e_j n\rangle$. We'll start by evaluating the terms $\langle f|\,H_1\,|m\rangle$ and $\langle m|\,H_1\,|i\rangle$,

$$\langle e_i g_j n_p + 1|\,H_1\,|g_i g_j n\rangle = \langle e_i g_j n_p + 1|\sum_{m=i,j}\frac{\hbar\Omega_m}{2}\left(\sigma_{+m}e^{i\left[\sum_q \eta_{m,q}(a_q^\dagger + a_q) - \omega_m t\right]} + h.c.\right)|g_i g_j n\rangle \tag{52}$$

The ions are cooled to the Lamb Dicke regime where $|n_p + 1|\eta_{m,q} \ll 1$, such that we may perform the expansion $e^{i\left[\sum_q \eta_{m,q}(a_q^\dagger + a_q)\right]} \approx 1 + i\sum_q \eta_{m,q}(a_q^\dagger + a_q)$. As we are exciting the ions only terms involving σ_{+m} will yield anything when the inner product is taken. So we may throw away the hermitian conjugate.

$$\langle e_i g_j n_p + 1|\,H_1\,|g_i g_j n\rangle = \langle e_i g_j n_p + 1|\sum_{m=i,j}\frac{\hbar\Omega_m e^{-i\omega_m t}}{2}\sigma_{+m}\left[1 + i\sum_q \eta_{m,q}(a_q^\dagger + a_q)\right]|g_i g_j n\rangle \tag{53}$$

Only the first ion is excited so can throw away the sum as only the term involving σ_{+i} will be non-zero.

$$\langle e_i g_j n_p + 1| H_1 |g_i g_j n\rangle = \langle e_i g_j n_p + 1| \frac{\hbar\Omega_i e^{-i\omega_i t}}{2}\sigma_{+i}\left[1 + i\sum_q \eta_{i,q}(a_q^\dagger + a_q)\right]|g_i g_j n\rangle \tag{54}$$

$$= \frac{\hbar\Omega_i e^{-i\omega_i t}}{2}\langle e_i g_j n_p + 1|\left(|e_i g_j n\rangle + \sum_q \eta_{i,q}\left[\sqrt{n_q+1}\,|e_i g_j n_q + 1\rangle + \sqrt{n_q}\,|e_i g_j n_q - 1\rangle\right]\right) \tag{55}$$

$$= \frac{\hbar\Omega_i e^{-i\omega_i t}}{\eta}_{i,p}\sqrt{n_p+1} \tag{56}$$

Similar calculations yields

$$\langle e_i g_j n_p - 1| H_1 |g_i g_j n\rangle = \frac{\hbar\Omega_i e^{-i\omega_i t}}{2}\eta_{i,p}\sqrt{n_p} \tag{57}$$

$$\langle g_i e_j n_p + 1| H_1 |g_i g_j n\rangle = \frac{\hbar\Omega_j e^{-i\omega_j t}}{2}\eta_{j,p}\sqrt{n_p+1} \tag{58}$$

$$\langle g_i e_j n_p - 1| H_1 |g_i g_j n\rangle = \frac{\hbar\Omega_j e^{-i\omega_j t}}{2}\eta_{j,p}\sqrt{n_p} \tag{59}$$

And for $\langle f| H_1 |m\rangle$ we get

$$\langle e_i e_j n| H_1 |e_i g_j n_p + 1\rangle = \frac{\hbar\Omega_j e^{-i\omega_j t}}{2}\eta_{j,p}\sqrt{n_p+1} \tag{60}$$

$$\langle e_i e_j n| H_1 |e_i g_j n_p - 1\rangle = \frac{\hbar\Omega_j e^{-i\omega_j t}}{2}\eta_{j,p}\sqrt{n_p} \tag{61}$$

$$\langle e_i e_j n| H_1 |g_i e_j n_p + 1\rangle = \frac{\hbar\Omega_i e^{-i\omega_i t}}{2}\eta_{i,p}\sqrt{n_p+1} \tag{62}$$

$$\langle e_i e_j n| H_1 |g_i e_j n_p - 1\rangle = \frac{\hbar\Omega_i e^{-i\omega_i t}}{2}\eta_{i,p}\sqrt{n_p} \tag{63}$$

Note that ω_j in the denominator of (51) is the angular frequency of the laser that excites in the $|i\rangle \to |m\rangle$ transition. Plugging in the terms above into (51) yields

$$\tilde{\Omega}_{i,j} = -\frac{1}{\hbar^2}\left|\sum_p \frac{\left(\frac{\hbar i}{2}\right)^2 \Omega_i\Omega_j e^{-i(\omega_i+\omega_j)t}\eta_{i,p}\eta_{j,p}(n_p+1)}{\omega_{eg}+\omega_p-(\omega_{eg}+\delta)} + \cdots\right| \tag{64}$$

$$= \frac{1}{4}\Omega_j\Omega_i\left|\sum_p \eta_{i,p}\eta_{j,p}\left(\frac{n_p+1}{\omega_p-\delta} + \frac{n_p}{-\omega_p-\delta} + \frac{n_p+1}{\omega_p+\delta} + \frac{n_p}{-\omega_p+\delta}\right)\right| \tag{65}$$

$$= \frac{1}{2}\Omega_i\Omega_j\sum_p \frac{\eta_{i,p}\eta_{j,p}\omega_p}{\delta^2-\omega_p^2} \tag{66}$$

Substituting in the expression for η as given by (44) yields

$$\tilde{\Omega}_{i,j} = \omega_i \omega_j \frac{\hbar k_j k_i}{4M} \sum \frac{\phi_{i,p}\phi_{j,p}}{\delta^2 - \omega^2} \tag{67}$$

This gives rise to the effective Hamiltonian $H_{eff} = \hbar \sum_{i,j} \tilde{\Omega}_{i,j}, \sigma_{x,i}\sigma_{x,j}$ which describes the time evolution of the system [11]. In the next section we'll evaluate the sum by using the modes found earlier.

4 Numerical Analysis

We can evaluate (67) by plugging in the values we found for the different transversal modes. The transversal modes are laid out in such a way that the center of mass oscillation has the highest frequency with $\omega_{COM} = \nu_{rad}$. Depending on how γ is chosen all other modes will have an angular frequency in the range $0 < \omega_p < \nu_{rad}$. Therefore we will consider detuning in the range $\delta > \omega_{COM}$. When we have evaluated what is the coupling strength $\tilde{\Omega}_{i,j}$ in the effective Hamiltonian, we'll want to see how it depends on $|i-j|$. Specifically the wish is for $\tilde{\Omega}_{i,j} \propto |i-j|^{-\alpha}$, where $0 < \alpha < 3$ depending on the detuning. The discrepancy ε between the fit $f(|i,j|) = \beta|i-j|^{-\alpha}$ and the values for $\tilde{\Omega}_{i,j}$ is to be measured by

$$\varepsilon = \sqrt{\frac{1}{N_{i,j}} \sum_{i>j} \left(\frac{(f|i,j|) - \tilde{\Omega}_{i,j}}{f(|i,j|)} \right)^2}, \tag{68}$$

where $N_{i,j}$ is the number of term that are summed.

If a detuning is chosen very close to the COM mode the coupling strength between the ions $\tilde{\Omega}_{i,j}$ will be an almost constant function of the distance between the ions, as is seen in figure 2. For detuning in this area alle four potentials perform similarly with roughly the same value for α. The discrepancies ε for this regime of detuning are ordered like $\varepsilon^{(2)} < \varepsilon^{(4)} < \varepsilon^{(6)} < \varepsilon^{(8)}$ (see figure 2 for a specific example), however some of the reason for this is that the α's are in the opposite order, and as we will see later higher α will lead to higher ε.

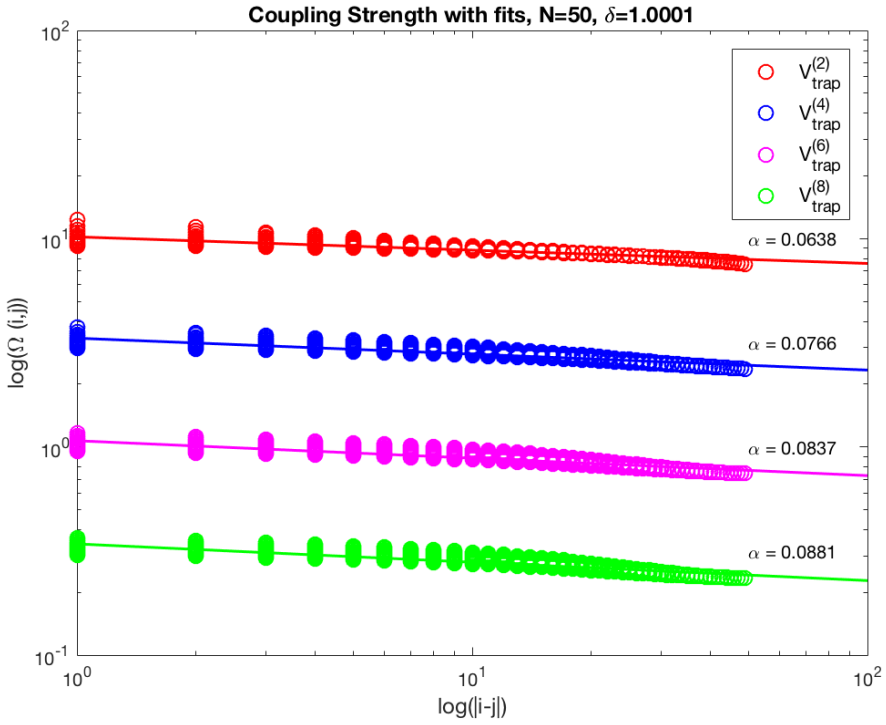

Figure 2: Coupling strength for 50 ions with detuning $\delta = 1.0001\omega_{COM}$ found by evaluating (67) for transversal oscillations. $V^{(2)}_{trap}$,$V^{(4)}_{trap}$ and $V^{(26}_{trap}$ are shifted up by a factor $10^{1.5}, 10$ and $10^{0.5}$ respectively in order to be able to distinguish them. Fits of type $\tilde{\Omega}_{i,j} \propto |i-j|^{-\alpha}$ are indicated by the line, with the value for α above the fit. The discrepancies between fit and $\tilde{\Omega}_{i,j}$ as define by (68) are: $\varepsilon^{(2)} = 0.030, \varepsilon^{(4)} = 0.038, \varepsilon^{(6)} = 0.043$ and $\varepsilon^{(8)} = 0.046$.

If we let the detuning be 1.2 another picture emerges, as seen in figure 3. This time $V^{(2)}$ performs significantly forse than the other three potentials, as is also evident by $\epsilon^{(2)} = 0.481$ compared to the others which are in the range $0.32 < \epsilon < 0.37$.

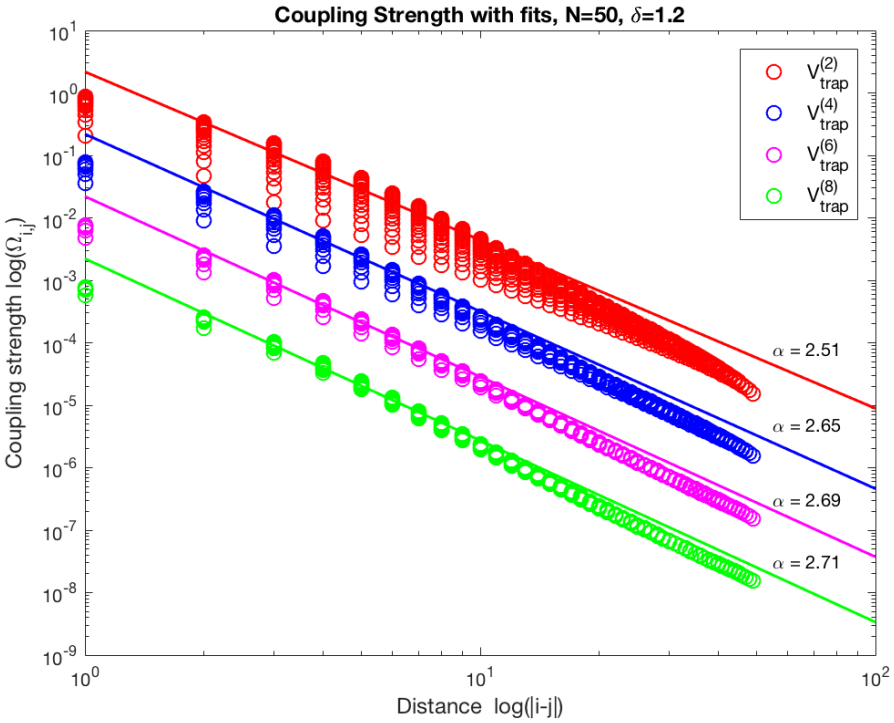

Figure 3: Coupling strength for 50 ions with detuning $\delta = 1.2\omega_{COM}$ found by evaluating (67) for transversal oscillations. $V^{(2)}_{trap}$,$V^{(4)}_{trap}$ and $V^{(6)}_{trap}$ are shifted up by a factor $10^3, 10^2$ and 10^1 respectively in order to be able to distinguish them. Fits of type $\tilde{\Omega}_{i,j} \propto |i-j|^{-\alpha}$ are indicated by the line, with the value for α above the fit. The discrepancies between fit and $\tilde{\Omega}_{i,j}$ as define by (68) are: $\varepsilon^{(2)} = 0.481, \varepsilon^{(4)} = 0.361, \varepsilon^{(6)} = 0.333$ and $\varepsilon^{(8)} = 0.328$.

If we let δ vary between ω_{COM} and $1.2\omega_{COM}$ we see that we can indeed get α in the range $0 < \alpha < 3$ as seen in figure 4. Likewise we see in figure 5 that for detuning bigger than $\sim 1.02\omega_{COM}$ the proposed new trappotential follows the power law closer than the classical harmonic potential.

5 Possible Improvements

One possible further improvement would be to change the profile of the laser, such that it is stronger where the ions are further apart. In the numerical analysis this would correspond to change Ω_i, as the effective Hamiltonian relates to the electrical field through Ω_i. Now we have assumed that the profile is the same across the chain

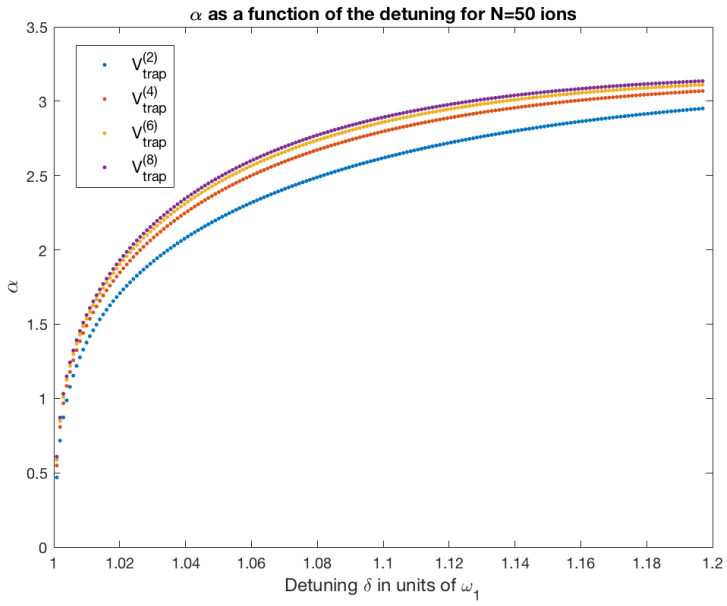

Figure 4: The interaction range (α) as a function of the detuning for N=50. All four potentials have similar performance with $0 < \alpha < 3$. If the detuning is chosen to be close to the center of mass mode ω_{COM} there will be long range interaction. While of the detuning is chosen to be further from the center of mass mode the interaction range will become shorter and the hamiltonian will more or less turn into a nearest neighbour model.

as we chose $\Omega_i = \Omega_j = \Omega$. This can be done independently of proposed improvement of changing the trap potential.
Another possible improvement is to choose another potential than the ones discussed here. The whole method discussed in this thesis might be turned around such that instead of examining the effects of the well known potentials chosen here, one might construct a potential which will result in equal distance between the ions.

6 Conclusion

The proposed changes to the paul trap presentet in this thesis seems to be an improvement. The ability to simulate long-distance spin-spin coupling for detuning close to the center of mass mode seems to be preserved. If detuning are chosen to be further from the center of mass mode the changes proposed will lead to significant improvements, as the coupling strength obeys a power law much more closely.

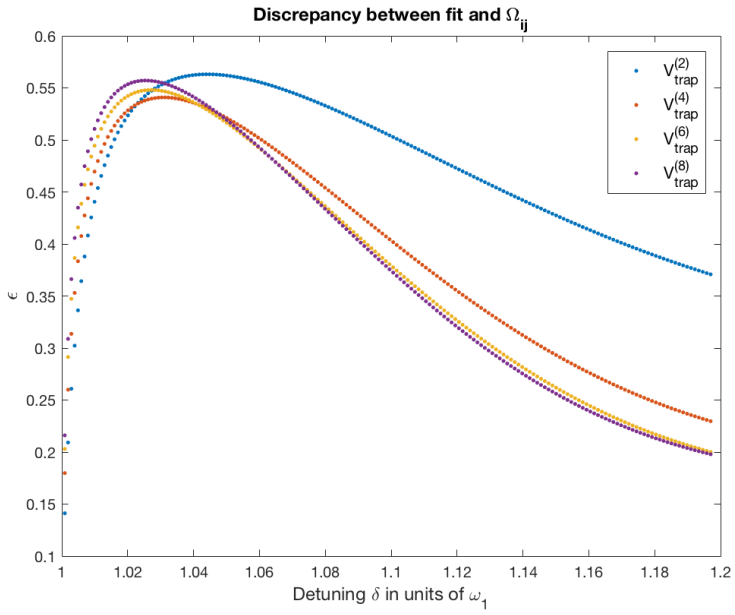

Figure 5: The discrepancy ϵ between the fit and the calculated values for the coupling strength as defined in (68). It is evident that the proposed trap potentials $V^{(4)}_{trap}$, $V^{(6)}_{trap}$ and $V^{(8)}_{trap}$obeys the power law much more strictly for higher detunings, while not performing significantly worse close to resonant.

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