Determining the sound wave spectrum of a trapped ion crystal manipulated by optical tweezers

AMEP Lab Project Report

Zeger E.D. Ackerman
Student nr. 11061138

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Examiner:
Dr. Rene Gerritsma

Daily Supervisor:
Dr. Rima X. Schüssler

1 Introduction

Many phenomena in nature cannot be understood by simulating them using a classical computer. In particular, for quantum effects in which frustration plays a role, these systems can only be simulated by quantum simulators, which, in theory, are able to reduce calculation times to achievable orders of magnitude.[Ber+11]

In this research, we use trapped $^{171}Yb^{+}$ ion crystals as quantum simulators.[Olm+07] In these trapped ion quantum simulators, the interactions between ion qubits are mediated by sound waves, whose quanta are phonons.[Jam97] We aim to control the sound wave spectrum of the trapped ion crystal using optical tweezers.[Esp+21; Teo+21] Here, we investigate theoretically how the sound wave spectrum looks along one axis, given a specific tweezer pattern.

For this, we calculate the ion state populations in a trapped ion crystal when it is irradiated by a laser that couples the ground states of the ions to a metastable excited state.[Lei+03] The level diagram including the relevant transitions is shown in figure 1. The 411 nm transition is from the ground state $^2S_{1/2}$ to the excited state $^2D_{5/2}$. The 369 nm transition is from the ground state to the state $^2P_{1/2}$, allowing for fluorescence detection when the ion relaxes from $^2P_{1/2}$ to $^2S_{1/2}$. The 935 nm and 760 nm transitions are used to return the ion from the unwanted states $^2D_{3/2}$ and $^2F_{7/2}$, respectively.

By state-dependent fluoresence detection, it is possible to measure the excitation probability. We calculate the probability for each ion to be in the excited state as a function of the frequency of the applied laser pulse. The obtained probability spectrum of each ion depends on both the mode amplitudes for each ion and the respective mode frequencies.[Kim+09] Together, the mode amplitudes and frequencies constitute the whole sound wave spectrum. As an example, we used a 12-ion crystal and calculated a clear dependence on the optical tweezers. Further experiments will implement the spectroscopic fluoresence technique in experiment on trapped $^{171}Yb^{+}$ ion crystals. Likely experimental limitations include finite laser linewidth, the AC Stark shifts and the Fourier limit as discussed in the outlook.

A quantum simulator has qubits, particles with a spin-up and a spin-down state, which interact with each other. In $^{171}Yb^{+}$, the $^2S_{1/2}$ ground state and the $^2D_{5/2}$ metastable excited state are pseudospin states of the ions. The ions can engage in spin-spin interactions, which are generated by sound waves

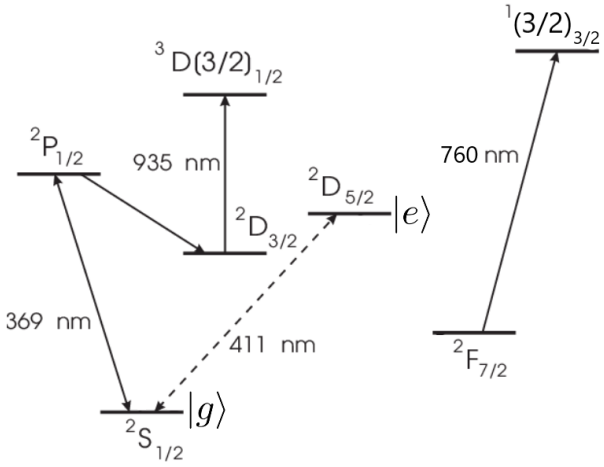


Figure 1: A level diagram of $^{171}Yb^+$ with the relevant states and laser transitions. The ground and excited states are marked with $|g\rangle$ and $|e\rangle$, respectively. Adapted from Madej *et al.* (2001).[MB01]

in the crystal. A sound wave has modes m in which each ion j is displaced with a specific amplitude $b_{m,j}$ at frequency ω_m. Here, we calculated the effect of the sound waves in a 1D ion chain, an example of which is shown in figure 2.

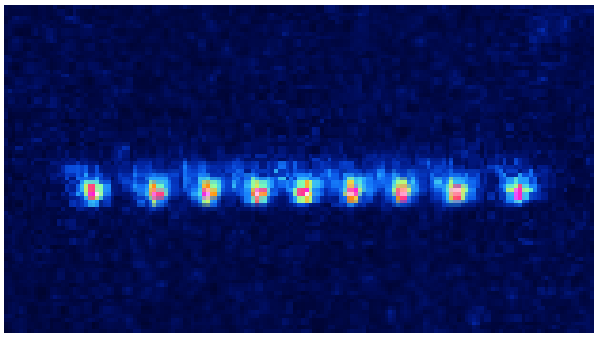


Figure 2: A chain of 9 ions in a Paul trap.

1.1 Single ion case

The interaction of single two-level ions with a laser field closely resembles the (anti)-Jaynes-Cummings Model. The two electronic states are the ground state $|g\rangle$ and the excited state $|e\rangle$. These are the pseudospin-down and pseudospin-up state. The internal state of the ion is represented by the Hamiltonian

$$H_e = \frac{1}{2}\hbar\nu_0\sigma_z, \tag{1}$$

where ν_0 is the frequency of the transition between the two states and σ_z is the Pauli-spin operator.[Kir10] The motion of an ion in a harmonic potential is described by

$$H_m = \hbar\omega(a^\dagger a + \frac{1}{2}), \tag{2}$$

where ω is the oscillation frequency of the ion in a harmonic potential and $a^\dagger$ and a are the creation and annihilation operators of phonons, respectively.

The laser-ion interaction, after applying the rotating-wave approximation, is given by

$$H_l = \hbar\Omega e^{i\eta(a^\dagger + a)} e^{-i(\nu_l t - \phi)}\sigma_+ + \hbar\Omega e^{-i\eta(a^\dagger + a)} e^{i(\nu_l t - \phi)}\sigma_-, \tag{3}$$

where Ω is the Rabi frequency, a parameter describing the coupling, ν_l is the laser frequency, ϕ is the phase of the laser, $\eta = \frac{2\pi}{\lambda_l}\sqrt{\frac{\hbar}{2M\omega}}$ is the Lamb-Dicke parameter, λ_l is the wavelength of the laser and M is the mass of an ion. Due to the interaction with the laser, the ion can change its internal state from $|g\rangle$ to $|e\rangle$ and vice versa, described by the Pauli-spin operators σ_+ and σ_-.

The Hamiltonian describing the whole system is

$$\begin{aligned} H &= H_m + H_e + H_l \\ &= \hbar\omega(a^\dagger a + \frac{1}{2}) + \frac{\nu_0}{2}\hbar\sigma_z + \hbar\Omega e^{i\eta(a^\dagger + a)} e^{-i(\nu_l t - \phi)}\sigma_+ + \hbar\Omega e^{-i\eta(a^\dagger + a)} e^{i(\nu_l t - \phi)}\sigma_-. \end{aligned} \tag{4}$$

Therefore, a system of a single two-level ion interacting with a laser field is described by

$$H = \omega a^\dagger a + \frac{\nu_0}{2}\sigma_z + \Omega\big(e^{i\eta(a^\dagger + a)} e^{-i\nu_l t}\sigma_+ + h.c.\big), \tag{5}$$

where in the last step the zero-point energy is removed and Planck's constant is set to $\hbar \equiv 1$. This Hamiltonian has a time-dependence, which is removed by applying the unitary time-evolution operator

$$U = e^{i\frac{\nu_l}{2}\sigma_z t} \tag{6}$$

to the transformation rule

$$\widetilde{H} = UHU^\dagger - i\hbar U\dot{U}^\dagger. \tag{7}$$

The first part on the right-hand side is

$$UHU^\dagger = \omega a^\dagger a + \frac{\nu_0}{2}\sigma_z + \Omega\big(e^{i\eta(a^\dagger + a)}\sigma_+ + h.c.\big) \tag{8}$$

and the second part is rewritten as

$$-iU\dot{U}^\dagger = i\Big(-i\frac{\nu_l}{2}\sigma_z\Big)UU^\dagger = -i\Big(-i\frac{\nu_l}{2}\sigma_z\Big) = -\frac{\nu_l}{2}\sigma_z, \tag{9}$$

which results in the transformed Hamiltonian

$$\begin{aligned} \widetilde{H} &= \omega a^\dagger a + \frac{\nu_0 - \nu_l}{2}\sigma_z + \Omega\big(e^{i\eta(a^\dagger + a)}\sigma_+ + h.c.\big) \\ &= \omega a^\dagger a - \frac{\Delta}{2}\sigma_z + \Omega\big((1 + i\eta(a^\dagger + a))\sigma_+ + h.c.\big), \end{aligned} \tag{10}$$

where $\Delta = \nu_l - \nu_0$ is the detuning of the laser. The Hamiltonian is Taylor expanded to the second term in the Lamb-Dicke regime, $\eta \ll 1$.

1.2 Multiple ion case

The vibrations along a chain of two ions can be described by two eigenmodes m. One is the centre-of-mass (COM) mode, where both ions move in the same direction. The other is the stretch mode, where both ions move in opposite directions. Each eigenmode has its own frequency given by the corresponding eigenvalue ω_m. For multiple ions in a chain, there is one COM mode of the chain as a whole, and several stretch modes, together describing the vector space of all possible chain vibrations.

In the case of multiple ions forming a crystal, the system has different operators for each ion, as well as for each mode. This system of N_{ions} ions and $N_{\text{modes}} = N_{\text{ions}}$ modes is described by

$$\widetilde{H} = \sum_{m}^{N_{\text{modes}}} \omega_m a_m^\dagger a_m - \frac{\Delta}{2} \sum_{j}^{N_{\text{ions}}} \sigma_z^{(j)} + \Omega\Big(\sum_{j}^{N_{\text{ions}}} \big(1 + i \sum_{m}^{N_{\text{modes}}} \eta_{m,j}(a_m^\dagger + a_m)\big)\sigma_+^{(j)} + \big(1 - i \sum_{m}^{N_{\text{modes}}} \eta_{m,j}(a_m^\dagger + a_m)\big)\sigma_-^{(j)}\Big), \tag{11}$$

where $\eta_{m,j} = \frac{2\pi}{\lambda_l}\sqrt{\frac{\hbar}{2M\omega_m}} b_{m,j}$ is the Lambe-Dick parameter for an ion chain. λ_l and $b_{m,j}$ are scalars, since we only measure along one axis.

In the calculation, the system starts in the ground state $|g\rangle$. We assume that when the laser power as well as the time period of laser exposure t is small enough, the probability of one ion or mode excitation is also small, especially ruling out states with several ions or mode excitations. Typically, we assume $\Omega t \lesssim 1$, since the Rabi frequency is proportional to the square root of the laser power. We also neglect ion and mode relaxation. Due to these approximations, the Hilbert space of a 12-ion crystal contains 157 states ($(1 + N_{\text{ions}})N_{\text{modes}} + 1$), whereas it would contain $2^{12} \cdot 12^{12} \approx 3.65 \cdot 10^{16}$ states ($N_{\text{ions}}^2 \cdot N_{\text{modes}}^{N_{\text{ions}}}$) if multiple ion and mode excitations were allowed. Since we assume the system starts in the ground state and there are only single excitations, $a\sigma_+$ and $a^\dagger\sigma_-$ terms are not included. This results in a simplified Hamiltonian

$$\widetilde{H} = \sum_m \omega_m a_m^\dagger a_m - \frac{\Delta}{2}\sum_j \sigma_z^{(j)} + \Omega \sum_j \Big(\big(1 + i\sum_m \eta_{m,j} a_m^\dagger\big)\sigma_+^{(j)} + \big(1 - i\sum_m \eta_{m,j} a_m\big)\sigma_-^{(j)} \Big) \tag{12}$$

which can be described in matrixform. For example for a two ion system:

$$\widetilde{H} = \begin{pmatrix} 0 & \Omega & \Omega & -i\Omega\eta_{1,1} & -i\Omega\eta_{1,2} & -i\Omega\eta_{2,1} & -i\Omega\eta_{2,2} \\ \Omega & -\Delta & 0 & 0 & 0 & 0 & 0 \\ \Omega & 0 & -\Delta & 0 & 0 & 0 & 0 \\ i\Omega\eta_{1,1} & 0 & 0 & \omega_1 - \Delta & 0 & 0 & 0 \\ i\Omega\eta_{1,2} & 0 & 0 & 0 & \omega_1 - \Delta & 0 & 0 \\ i\Omega\eta_{2,1} & 0 & 0 & 0 & 0 & \omega_2 - \Delta & 0 \\ i\Omega\eta_{2,2} & 0 & 0 & 0 & 0 & 0 & \omega_2 - \Delta \end{pmatrix}. \tag{13}$$

The first row and column correspond to coupling between the ground state $|g\rangle = \begin{pmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}$ and the excited states. In the first excited state the first ion is excited, in the third excited state the first ion and the first mode are excited, and so on. The $-\Delta$ term on the diagonal corresponds to the carrier part of the Hamiltonian, with an ion excitation but no mode excitation. The $\omega_m - \Delta$ term corresponds to the creation and annihilation of a mode in combination with an ion excitation. This matrix can be generalised for any number of ions.

1.3 Probability spectrum

The state of the system after some time t is

$$|\Psi(t)\rangle = U(t)\,|\Psi(0)\rangle = e^{-iHt/\hbar}\,|\Psi(0)\rangle\,. \tag{14}$$

The probabilities to find the system in any state $|m, j\rangle$ after time t is

$$P_{g\to m,j}(t) = |\,\langle m, j|\,U(t)\,|g\rangle\,|^2 \tag{15}$$

Since individual ions are not coupled to individual modes, the probability that an ion is in the excited state $P_j(t)$ is calculated by summing over all modes:

$$P_j(t) = \sum_m^{N_{\text{modes}}} P_{g\to m,j}(t) \tag{16}$$

For example, the probability that a system of two ions is in the state with the first ion and the first mode excited after time t is

$$P_1(t) = P_{g\to 0,1}(t) + P_{g\to 1,1}(t) + P_{g\to 2,1}(t). \tag{17}$$

The probability to find ion j in mode m can be measured by exciting the system with different frequencies and recording the fluorescence. When the frequency is on resonance, the peak amplitude corresponds to the mode amplitude $b_{m,j}$ and the peak position to the mode frequency ω_m. In this research, we focus on the effect of the optical tweezers on the sound wave spetrum. Therefore, we aim to find the relation between the calculated mode frequencies $\widetilde{\omega}_m$ and mode amplitudes $\widetilde{b}_{m,j}$, manipulated by optical tweezers, and the mode frequencies $\widetilde{\omega}_m$ and mode amplitudes $\widetilde{b}_{m,j}$ observed from the measured probability spectrum of each ion.

1.4 Simulation with an ion crystal and optical tweezers

The spin-spin interactions in a trapped ion crystal can be manipulated by changing the sound wave spectrum. This is done with optical tweezers, which make it possible to use controlled mode amplitudes $\widetilde{b}_{m,j}$ and mode frequencies $\widetilde{\omega}_m$. The potential energy of the optical tweezers is

$$V_{\text{tweezer}}(\vec{\rho}_j) = \sum_{j=1}^{N_{\text{ions}}} \sum_{\alpha\alpha'} \frac{M}{2} \Omega^2_{j,\alpha,\alpha'} (\alpha_j - \alpha_j^{(0)})(\alpha'_j - \alpha_j^{\prime(0)}), \tag{18}$$

where $\vec{\rho}_j$ is the position of ion j, $\Omega^2_{j,\alpha,\alpha'}$ is the local optical pinning curvature, α_j is the ion position and $\alpha_j^{(0)}$ is the equilibrium position, both in the α direction.[Esp+21] Taking the effect of the optical tweezers into account, the total potential energy of ion j in a 1D ion chain changes to

$$\begin{aligned} V(\vec{\rho}_j) =& V_{\text{trap}}(\vec{\rho}_j) + V_{\text{tweezer}}(\vec{\rho}_j) + V_{\text{Coulomb}}(\vec{\rho}_j) \\ =& \frac{1}{2} \sum_{\alpha,j} M\omega_\alpha^2 \rho_{j,\alpha}^2 + \sum_{j=1}^{N_{\text{ions}}} \sum_{\alpha\alpha'} \frac{M}{2} \Omega^2_{j,\alpha,\alpha'} (\alpha_j - \alpha_j^{(0)})(\alpha'_j - \alpha_j^{\prime(0)}) \\ &+ \frac{1}{2} \sum_{j\neq i} \frac{e^2}{4\pi\epsilon_0 |\vec{\rho}_j - \vec{\rho}_i|}, \end{aligned} \tag{19}$$

where ω is the trap frequency, e is the Coulomb constant, ϵ_0 is the vacuum permittivity.

The solutions of $\nabla V = 0$ are the equilibrium positions. To find the mode frequencies the Hessian matrix $\mathbf{A}$ is constructed, where

$$A^{(i,j)}_{\alpha,\alpha'} = \left(\frac{d^2 V}{d\alpha_j d\alpha'_i} \right)_{\alpha_j, \alpha'_i \to 0} \tag{20}$$

is the Hessian matrix element on position (i, j). The eigenvalues of the Hessian matrix are the squares of the mode frequencies $\widetilde{\omega}$ in direction α. We only use the motion along one axis.

The probability spectrum of a 1D system of anti-ferromagnetic spin-spin interactions between the 12 particles is determined by first simulating a 12-particle chain of $^{171}\text{Yb}^+$ ions manipulated by optical tweezers, which resulted in new eigenvectors and eigenvalues of the Hessian. The strength of the optical tweezers for each ion is shown in table 1. We substitute these controlled mode frequencies $\widetilde{\omega}_m$ and mode amplitudes $\widetilde{b}_{m,j}$ into the Hamiltonian of equation 12 and used equation 16 to calculated the probability spectra of the ions.

Table 1: Local optical pinning frequencies Ω_j, in terms of the trap frequency ω and with an error of 0.03 ω, for simulating anti-ferromagnetic spin-spin interactions between 12 particles in a chain.

Ion number	Ω_j (ω)
1	0.51
2	1.71
3	2.27
4	2.57
5	2.80
6	2.93
7	2.93
8	2.80
9	2.57
10	2.27
11	1.71
12	0.51

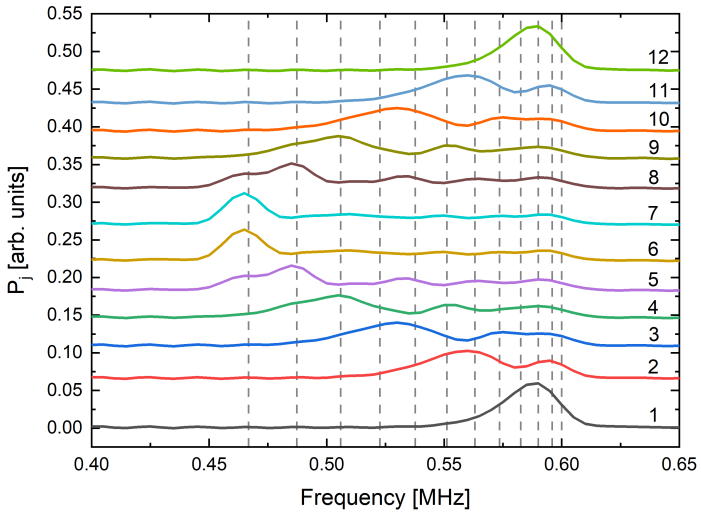
2 Results

For a 12-particle chain of $^{171}Yb^+$ ions, the excitation probability as a function of the laser frequency of the 369 nm laser was calculated for each ion.

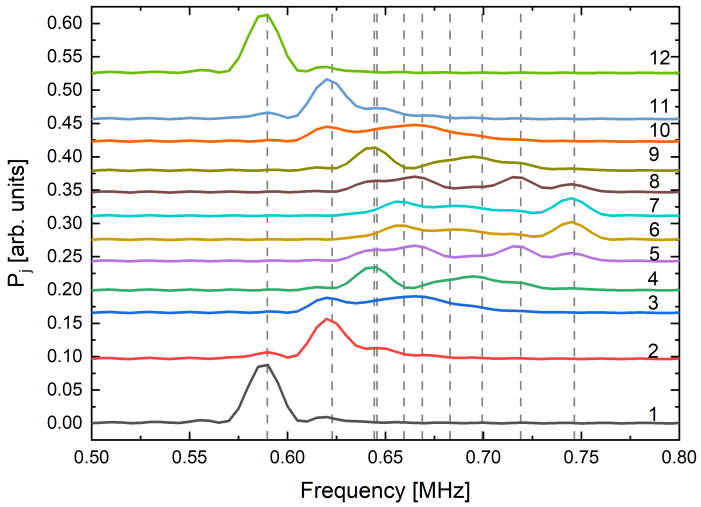
2.1 Probability spectra

The probability spectra of a 12-particle chain of $^{171}Yb^+$ ions without the influence of optical tweezers, where $\Omega t = 3$ is shown in figure 3a. Along the ion chain the spectra are symmetric, suggesting that the modes are also symmetric. The dominant modes of the middle ions have a lower mode frequency than the dominant modes of the outer ions. Ions in the middle are closer together, and since they move symmetrically, those ions resemble more one single, larger mass moving than the outer ions. A larger mass in a harmonic potential corresponds to a lower frequency, which explains the lower mode frequencies for the middle ions. The dashed lines are the calculated mode frequencies. They are shifted from the center of the peak to lower frequencies, resulting from the AC Stark shift.

The probability spectra of a 12-particle chain of $^{171}Yb^+$ ions manipulated by optical tweezers, with local optical pinning frequencies as given in table 1, to simulate a 1D system of anti-ferromagnetic spin-spin interactions between the 12-particles is, with an offset, shown in figure 3b. Along the ion chain, the spectra are symmetric for this system as well, suggesting the modes remain symmetric. The dashed lines are the calculated mode frequencies. Ten are distinguishable, while there are two degenerate modes, at $\omega_m = 0.589$ MHz and at $\omega_m = 0.623$ MHz. Contrary to the case without optical tweezers, the dominant modes of the middle ions now have a higher mode frequency than the dominant modes of the outer ions. This clearly shows that there is an effect of the optical tweezers on the sound wave spectra in the calculation.



(a)



(b)

Figure 3: Probabilities of excitation P_j, with an offset of each ion for clarity, as a function of frequency for different ions j in a 12-ion chain (a) without optical tweezers and (b) manipulated by optical tweezers. The dashed lines represent the calculated mode frequencies ω_m.

2.2 Mode amplitudes and mode frequencies

The mode amplitudes $b_{m,j}$ calculated from the probability spectra that is shown in figure 3b, as well as the expected mode amplitudes of the anti-ferromagnetic tweezer pattern, are shown as a function of ion number for all different modes in figure 4. The calculated and expected values show strong resemblance, suggesting that it is possible to derive mode amplitudes from a measured probability spectrum. Limitations are the spectral resolution and the width of the peaks in the probability spectra.

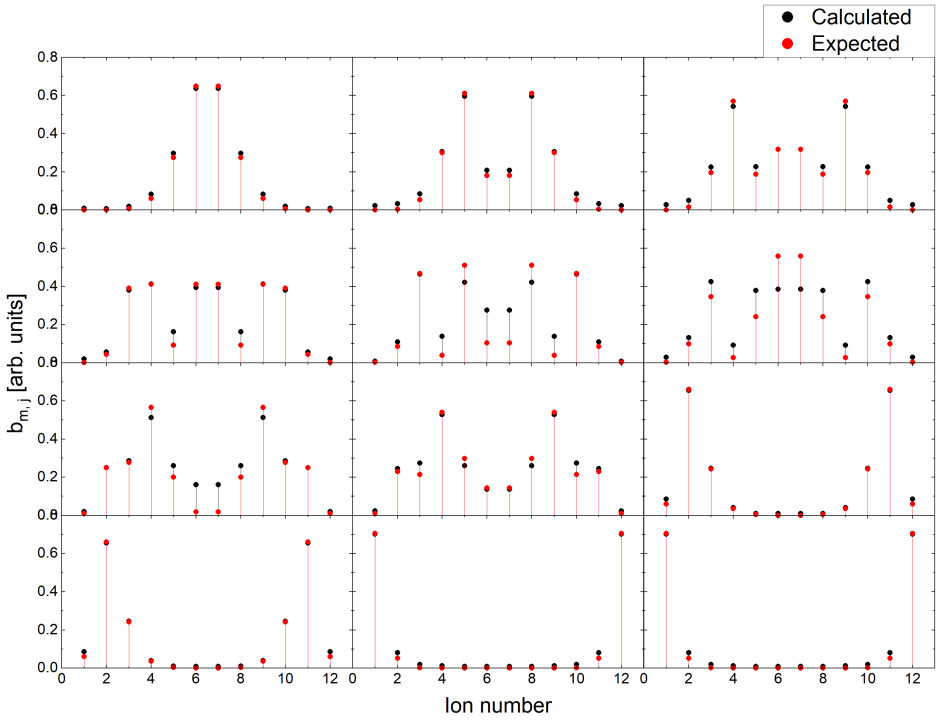


Figure 4: In the case of 12 ions and an anti-ferromagnetic tweezer pattern: Calculated (black) and expected mode amplitudes $b_{m,j}$ as a function of ions j for different modes m. There is strong agreement between them for most of the modes.

3 Outlook

The goal of our research is to be able to simulate a system by recreating the wanted Hamiltonian using a 2D ion crystal, whose sound wave spectrum is manipulated by optical tweezers, and reading out the result of the spin-spin interactions after some time t. To achieve this, $^{171}Yb^{+}$ ions will be cooled by a Doppler laser, formed into a crystal in a Paul trap, and excited using a 411 nm laser.[Fel+20] Ions in the $D_{5/2}$ state cannot be excited by the 411 nm laser and thus cannot fluoresce. Thus, the electronic state can be determined from the fluorescence, since bright ions correspond to the $S_{1/2}$ ground state and dark ions correspond to the $D_{5/2}$ metastable excited state. Repeating this experiment many times will result in a similar probability spectrum to figure 3a when there are no optical tweezers.

When the crystal is manipulated by optical tweezers in the way described in subsection 1.4, a probability spectrum similar to figure 3b is expected. The locations of local maxima of the probability spectrum are the ω_m, the heights of the maxima are proportional to the squared of the $b_{m,j}$. In this way, spectroscopy can be performed on ion systems to study the effect of optical tweezers on the sound wave spectrum.

During simulation of the probability spectrum, multiple ion or mode excitations were not taken into account. These can occur during experiments, but the approximation on the size of the Hilbert state remains valid if those events are discarded during measurements.

Some effects that do need to be taken into account are the AC Stark shift, which is the shift of spectral lines due to the oscillating electric field, the effect of the Fourier limit, where the short laser time results in a minimum possible spectral width of the laser. Another limitation is a finite laser linewidth. These limit the spectral resolution of the probability spectrum.

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