Simulating dynamics of 2D trapped ion crystals

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Abstract
Increasing the number of ions in ion crystals can be used to make more powerful quantum computers. In order to do this, there must be a thorough understanding of the dynamics of ion crystals. In this research, I have improved upon the 2D trapped ion crystal simulation used by our team by implementing a cooling laser which cools the crystals to the doppler limit. This laser works by a random and discrete process which causes the velocities of the ions to change as ions transition between the ground states and excited states. To show possible future uses for the simulation, I have compared the phase behavior between an unstable 8 ion crystal and a stable 4 ion crystal as well as investigated a 4 ion crystal during the melting process.

INTRODUCTION

Quantum computing is an exciting field of physics today. The fundamental principle behind quantum computing is the qubit, a quantum particle which is used as the basic unit of information. Because of the quantum behavior of these qubits, quantum computers will be able to do certain operations much faster than conventional computers. This technology will soon find many uses in commercial and research applications.

There are many kinds of particles which can be used as qubits such as neutral atoms, monatomic ions, or molecular ions. Our group is interested in using trapped barium ions. In order to make effective quantum computers from trapped ions, there needs to be in the order of hundreds of ions. Understanding the dynamics of these trapped ion systems is necessary in order to increase the number of ions that we can crystalize.

The ions are trapped using electric fields oscillating at a radio frequency (RF). As a result of the oscillating RF electric field, there are two oscillations in the ions motion: an overall motion around the ions' equilibrium positions and also a micro-motion oscillation at the RF due to the electric field. One challenge of ion trapping is to limit the effect of the micro-motion.

Trapped ions are cooled using the doppler cooling technique. A laser detuned below the atomic resonant frequency of the ions is shot at the ion crystal. When ions absorb photons, they will gain momentum $\mathbf{p} = \hbar k$ in the direction of the laser. Absorption happens preferentially when the ions are moving opposite to the direction of the laser propagation which causes the temperature of the ions to lower. When ions return to the ground state, they gain momentum $\mathbf{p} = \hbar k$ in a random direction. The emission process can be thought as a random 'walk' in momentum space, with each step equal to $\mathbf{p} = \hbar k$. Because of these random emissions, there is a limit to how low the temperature can be with the doppler cooling technique called the doppler temperature. Foot [1] describes the Optical Molasses Technique which involves three pairs of counter propagating lasers each detuned to $\delta = -\Gamma/2$, where the doppler

TABLE I: Average temperature of various sized ion crystals cooled with 2 step and 1 step laser functions

Crystal Size	2 Step Laser	1 Step Laser
1	1.605 mK	1.810 mK
2	1.439 mK	1.593 mK
4	1.328 mK	1.789 mK
8	1.515 mK	1.789 mK

temperature is $T_D = \hbar\Gamma/2k_B$.

These simulations of trapped ion systems run parallel to experiments happening in the University of Washington, Seattle lab, and they help validate things we see in the lab. Additionally, simulations which record the exact positions of ions can help us understand what is happening in the crystals even when fluorescence is limited due to the effects of micro-motion or when the laser is turned off. The overall goal of this research is to improve the trapped ion simulations. One improvement made was the implementation of a cooling laser function which would cool the ions to the doppler temperature.

METHODOLOGY

The simulation was made using the Python programming language. The equations of motion for the ions are solved using the velocity-verlet algorithm:

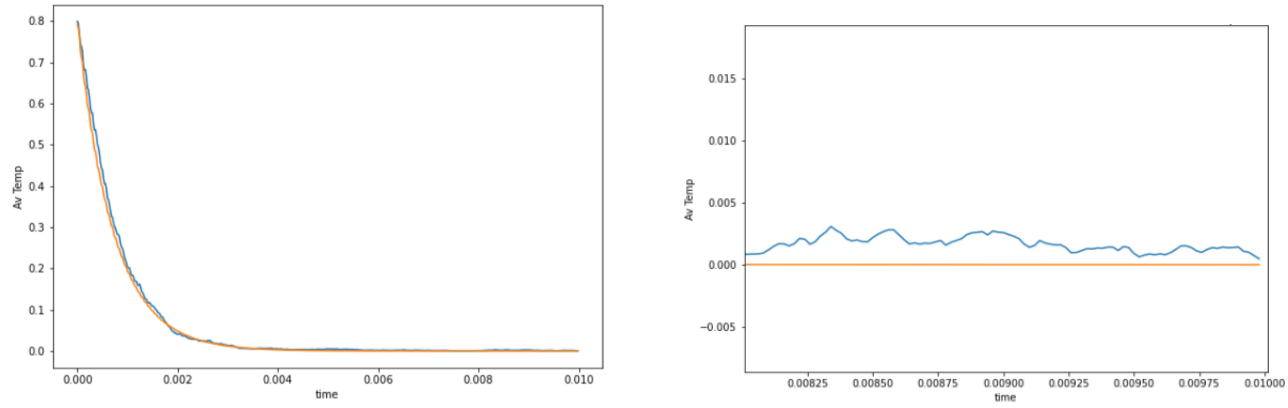
$$\mathbf{x}(t+\Delta t) = \mathbf{v}(t)\Delta t + \frac{1}{2}\mathbf{a}(t)\Delta t^2\,, \tag{1}$$

$$\mathbf{a}(t+\Delta t) = \frac{1}{m}\mathbf{F}_{net}(t+\Delta t)\,, \tag{2}$$

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) + \frac{1}{2}\left[\mathbf{a}(t) + \mathbf{a}(t+\Delta t)\right]\Delta t\,, \tag{3}$$

During each time step, the simulation records the positions and velocities of each ion. Forces on the ions include the laser force, the force from the electric field from the Paul trap, and the ion-ion Coulomb force. Aspects of the Paul trap field were explored in a previous REU project by Martinez [3]. The trap field can either be the actual RF field or a parabolic pseudo field which has the same magnitude as the RF field over one RF period. The Coulomb force on one ion due to all other ions is given by.

$$\mathbf{F}_j = \sum_{j\neq i} \frac{q}{4\pi\epsilon_o}\frac{(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}\,, \tag{4}$$



(a) **(b)**

FIG. 1: Comparison of two laser functions, time averaged laser in orange and two step discrete laser in blue. (a) shows the entire simulations. (b) shows the last 2ms of the simulations.

An early version of the laser force used a time averaged approach:

$$F = \hbar q_i \frac{s\Gamma/2}{1+s}\left(1 + \frac{2\delta v_i}{(1+s)(\delta^2 + \Gamma^4/4)}\right) \equiv F_0 - v\,, \tag{5}$$

A derivation of this can be found in Metcalf (2003) [4]. Because this laser force did not include random emissions of the scattering process, the ions would cool past the doppler limit. A more realistic laser function was made capturing the random and discrete process of laser cooling. An early stage of this discrete laser function assumed that absorption and emission happened simultaneously in the scattering process. The probability that a photon would get absorbed and emitted was given by

$$R_{scatt} = s_0 \frac{\Gamma/2}{1 + s_0 + [2(\delta - \mathbf{k}.\mathbf{v})/\Gamma]^2}\,, \tag{6}$$

and the ion would gain momentum $\mathbf{p} = \hbar k$ in the direction of the laser for absorption and $\mathbf{p} = \hbar k$ in a random direction for emission. A later version of this discrete laser function separated the scattering into two steps: absorption and emission. This function would keep track of the state of the ions. If an ion was in the ground state, the probability of absorption would be:

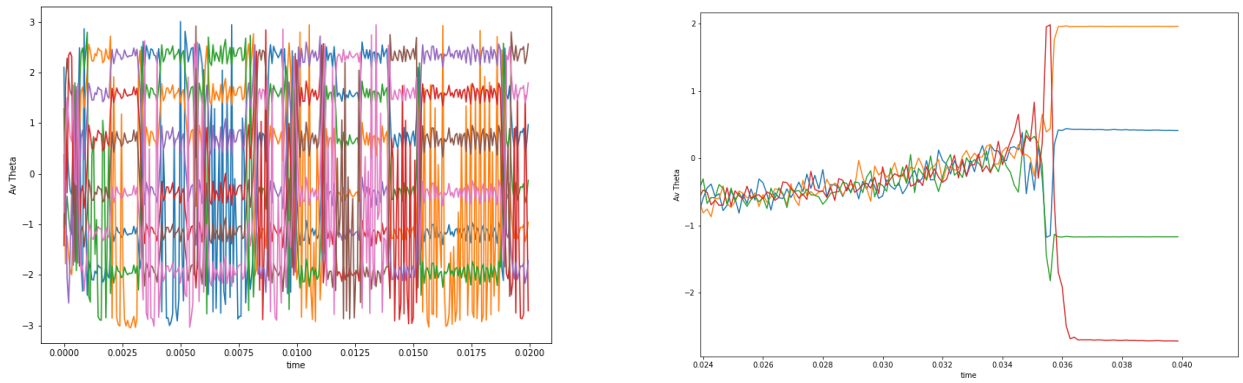
$$P_{abs} = \frac{R_{scatt}}{1 - R_{scatt}/\Gamma}\Delta t\,, \tag{7}$$

and if the ion was excited, the probability of emission would be:

$$P_{em} = \Gamma \Delta t\,, \tag{8}$$

A comparison of the average steady-state temperature of ion crystals with 1, 2, 4, and 8 ions in the parabolic pseudo field cooled by the 1 step discrete laser and the 2 step discrete laser is shown in figure **table 1**.

A comparison of the temperature of one ion cooled by the two step discrete laser and one ion cooled by time average laser is shown in **figure 1**. Temperature is calculated using the equipartition theorem $T = |v|m/3k_b$. This definition of temperature is acceptable in simulations where the pseudopotential is



(a) **(b)**

FIG. 2: (a) Angular positions (colors) of ions in the outer ring of an unstable 8 ion configuration. (b) Angular position of 4 ion system during crystallization phase transition.

used. When using simulations with the RF potential, velocity should be averaged over the RF period before calculating temperature in order to filter out the micro-motion.

RESULTS

Table 1 shows that the two step laser cools ions to lower temperature than the 1 step laser. All simulations were run in a reasonable time, none longer than ten minutes. Because there is a noticeable difference between the 1 step and 2 step laser simulations, the 2 step laser should be used because it simulates the cooling process more realistically and without a major time loss.

Figure 1 shows that both the time averaged laser function and the two step laser function cool a single ion at the same overall rate because their curves are overlapping for most of the simulation time. This is expected because the time averaged laser force is an approximation of the cooling process happening in the 2 step laser function. We can see the difference in these two functions in **(b)** as the temperature of both simulations gets closer to 0 K. The time average laser temperature continues to decay past the doppler temperature while the two step laser function oscillates about T= 1.605 mK. This result is promising because this laser function is better at capturing the asymptotic behavior of the doppler cooling process. Additionally, the value of T= 1.605 mK is in the order of magnitude of the doppler temperature expected in the optical molasses technique with 3 pairs of counter propagating lasers. However, this does not prove that this is the doppler temperature for this one-ion-one-laser system, so theoretical justification for this number should be found.

Preliminary Research

Some preliminary figures were made as a way to explore phase transitions in trapped ion systems. These preliminary figures show in what direction future research could be headed in the future. **Figure 2 (a)** shows the angular position of ions in an 8 ion crystal. We can see that this number of ions makes the crystal unstable. Once the ions have crystalized, the ions do not stay locked into their angular equilibria. Instead, the crystal remelts and recrystallizes, exchanging the ions from their previous equilibria. In comparison, **(b)** shows the crystallization process for 4 ions. Once the 4 ions crystallize, they do not

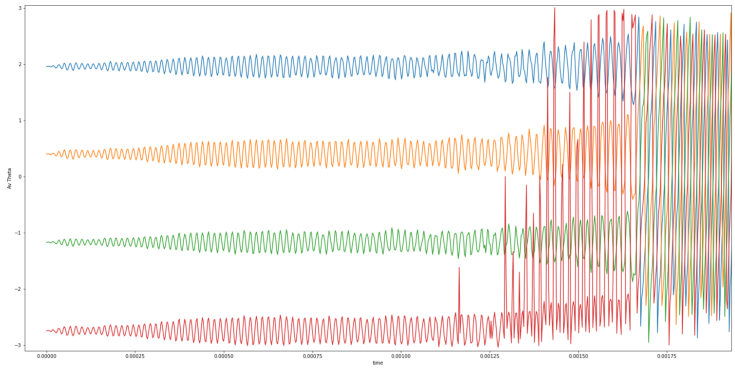


FIG. 3: Angular position (colors) of ions in a 4 ion crystal while subject to a heating laser and cooling laser such that the heating laser is more efficient than the cooling laser.

remelt.
I also explored adding an additional heating laser. **Figure 3** shows a 4 ion crystal in a system with a laser tuned to $\delta_1 = \Gamma/2$ and another laser tuned t0 $\delta_2 = -\Gamma$ so the heating laser was more efficiently tuned. We can see that the ions oscillate farther away from their equilibria as time goes on until finally the crystal melts.

CONCLUSION

In this research, improvements were made in the simulations of trapped ions in a modified paul trap. In particular, a laser function which realistically cools ions to their doppler temperature was added into the simulation. Preliminary research shows where this research could go in the future. One goal of ours is to make larger ion crystals by using two cooling lasers that are detuned separately to accommodate for the different magnitudes of micromotion in a large ion crystal. Currently, in the lab we have made crystals as large as 40 ions. These simulations will help us make even larger crystals.

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