論文の内容の要旨

Planar Coulomb crystals for Quantum Simulation
（量子シミュレーションを目的とした平面クーロン結晶の実現）

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Introduction

Background

Simulating quantum systems is known to be a very difficult computational problem. In the early 1980s Richard Feynman suggested that only a quantum system would be able to efficiently simulate another quantum system. This observation led to the development of quantum information processing. Remarkable progress that has been made in this field, yet the original idea of a quantum simulator has not yet been put into practice although some attempts have been made. However, things are about to change due to the proposal by Porras and Cirac (*Phys. Rev. Lett*. **96**:250501 (2006)) for quantum simulation and computation with planar Coulomb crystals. This scheme is particularly promising because it makes use of the ion trap quantum computation technologies that at the moment are the most successful among the proposed systems for implementing quantum information processing. So far, in ion traps all the required building blocks for quantum computation have been proved. The challenge that is left is scalability. Planar Coulomb crystals also hold the potential for scalable ion trap quantum computation. Moreover, it was estimated that even as few as 30-40 ions would be enough to simulate quantum systems that are beyond the computing power of today's top supercomputers.

Motivation and purpose

Motivated by the prospect of the experimental realization of applications like quantum simulation, scalable quantum computation and even measurement-based quantum computation, we have undertaken the task of investigating in detail the capability of planar Coulomb crystals to implement the above. As the next step, we aim at realizing planar Coulomb crystals in experiment, our long-term goal (beyond the scope of the current work) being the implementation of quantum simulation. For fulfilling our goal, the following steps are required: (i) a detailed investigation of planar Coulomb crystals, (ii) the estimation of the efficiency of Porras-Cirac proposal and the analysis of the implementation issues, (iii) the design and construction of an experimental setup optimized for the realization of planar Coulomb crystals.

Study of planar crystals

Simulation methods

Molecular dynamics simulations have long been used in the study of Coulomb crystals in both Penning and RF traps. Our simulations are designed using the ProtoMol framework, which has been already extensively tested for the simulation of single and multi-component Coulomb crystals in RF traps. We ran the large simulations on a 16 node PC-cluster and the smaller ones on a single machine (Core2Duo 2.4GHz 2GB/RAM). All the nodes of the cluster contain an Intel P4 3.2GHz processor with 2GB of memory and are connected through Gigabit ethernet. At each time step the forces are estimated and the equations of motion are integrated using the Leapfrog algorithm. The Coulomb force between the ions and was usually calculated directly and only when the number of ions exceeds 10,000 the Multi-grid algorithm was used. We also introduced collisions with background gas. Other heating sources like patch fluctuations are insufficiently understood, hence, they were not included.

Planar crystals

Trapped, cooled ions crystallize when the coupling parameter is larger than ~173. In the case of infinite plasmas bcc-crystals are expected. However, in experiments the number of ions is not large enough and the crystal structures are determined by the boundary conditions set by the confining potentials. 1D, 2D and 3D structures varying from strings and zig-zags to spheroidal crystals have been observed in experiments. The shape of Coulomb crystals depends on the confining potentials. In the case of harmonic potentials, the crystal shape depends only on the anisotropy parameter which is the ratio between the axial and radial frequencies. An oblate spheroidal crystal with N ions will turn into a planar one when the anisotropy parameter is larger than a certain threshold. In planar crystals the triangular-lattice ordering occurs near the center while at the edge shell structures appear. We derived the shell structure for planar crystals with 100 to 5,000 ions and we also calculated the radius and average distance between the ions for crystals with different numbers of ions up to 10,000. We simulated 10,000 ions planar crystals in both Penning and RF traps.

Heating

RF-heating results from the chaotic motion of the ions and manifests itself as an increase in the kinetic energy. Several studies have considered the effects of RF-heating and it has been shown that at low temperatures RF-heating is quite small. The dependence of the RF-heating rates on the trapping voltages, temperature and number of ions has never before been studied for planar crystals. We studied these in detail and found that larger crystals heat faster and in general the heating rates are discouragingly large meaning that planar crystal may not be maintained without continuous cooling. However, we also found that the heating rate strongly depends on the trapping conditions and can be significantly decreased by choosing the appropriate trapping parameters. In order to find ways of reducing heating we investigated the RF-heating dependence on the trap parameters. We found that in order to obtain reduced RF-heating rates low voltages are required. Furthermore, we investigated the effect of collisions with background gas in both Penning and RF-traps and we found out that, considering the usual experimental conditions, in Penning traps heating due to background gas collisions is very significant while in RF-traps it is very small.

Multi-component planar crystals

Bicrystals (crystals composed of two ion species or two isotopes of the same species) have been studied theoretically and experimentally before, however, there are no results on planar bicrystals. We studied planar bicrystals in the view of utilizing them for quantum simulation. In bicrystals the heavy ions form an outer shell, while the light ions gather at the center. The separation between the outer and inner shell depends on the ratio of the ions' masses. The advantage of bicrystals is that while continuously cooling the outer shell, the inner shell is also cooled by sympathetic cooling and, therefore, the crystal can be maintained for long times. Moreover, since the inner shell is not cooled directly, it can be used for quantum simulation. We investigated planar bicrystals in RF traps and found that because of the mass dependence of the radial potential interesting features occur. First, the number of ions in the inner shell is limited by the mass difference between the two components. We calculated the maximum number of ions in the inner shell as a function of the ion masses. Second, the spatial separation between the shells depends on the trapping parameters (i.e. the radial frequency shift) as well as the ion masses and charges. We derived the spatial separation between the shells when strong axial confinement both theoretically and numerically. Then we investigated the effect of spatial separation on sympathetic cooling and RF-heating.

Quantum simulation and computation with planar crystals

In planar crystals, in certain conditions, the ions moving in the axial direction can be considered as independent harmonic oscillators weakly coupled by the Coulomb interaction. Therefore, a planar crystal is similar to a microtrap array. Two-qubit interactions necessary for the implementation of quantum simulation and computation are realized by the means of a spin-dependent pushing force. There are several ways in which this pushing force can be induced. We studied the "push-gate" (for quantum computation and simulation) and the effective spin-spin interaction (for quantum simulation) and estimated the error as a function of various trap and laser parameters. When implementing the "push-gate" in the axial direction, the anharmonic terms of the Coulomb force induce a coupling between the axial motion and the hot radial vibrational modes which leads to decoherence. However, it was shown that this is not such a big issue and in principle high fidelity quantum gates could be achieved. In order to be able to realize the "push-gate" in a planar crystal it is necessary that the Coulomb energy is small compared to the potential energy. When studying the effects of heating on the fidelity of the “push-gate” the most important parameters are the temperature and the distance between the ions. The heating of the planar crystal results in the fluctuations of these two parameters so we estimated the error dependence in these cases. Moreover, we estimated the error in the implementation of effective spin-spin interactions.

Design and construction of the ion trap system

The necessity of minimizing the effects of heating and the specific requirements for the realization of planar crystals would make experiments difficult in both Penning and RF traps. However, each type of trap has its own merits and demerits. In RF-traps, while large crystals could not be maintained without continuous cooling, smaller crystals (<100 ions) cooled to very low temperatures and with a careful choice of the operating parameters may be possible to realize in experiment. The suppression of heating from other sources would be also required. The RF-heating is an important issue but low temperatures might be maintained by sympathetic cooling. The high vacuum conditions in RF-trap experiments together with the more flexible architecture of the trap electrodes providing very good optical access and lower voltages, as well as the uncomplicated laser cooling are the advantages of RF-traps. For the "proof-of-principle", small crystals in RF-traps may be easier to realize, therefore, we decided to construct such a trap.

The design of an RF-trap specialized for the realization of planar crystals is not by any means a trivial problem. Three main issues have to be addressed: (a) the operating parameters must have reasonable values (i.e. small voltages), (b) heating must be reduced as much as possible and (c) good optical access is required. After investigating various trap geometries, we found that the linear segmented trap is the most suitable for our purposes. It provides good optical access and has been used by many groups for the realization of Coulomb crystals. We investigated "the best" trap dimensions that would ensure for reasonable operating parameters stable trapping and would fulfill the planar crystal condition. From a parameter survey combined with SIMION simulations we found that the dimensions most suitable for our purposes: r_0 = 3 mm and z_0 = 1.5 mm.

We designed and constructed the trap electrodes and the electrical connections and fixed them inside the vacuum chamber. The chamber has 5 viewports providing optical access from all directions. The trap electrodes are made of stainless-steel rods separated by Macor parts. Each segment is independently connected to a feedthrough using a thin silver-plated copper conductor with Kapton insulation. Ultra-high vacuum conditions are realized using a turbo-molecular vacuum pump together with a rotary vane pump. We use two Littrow type ECDLs for the laser cooling (397 nm and 866 nm for repumping). Ions are loaded by laser ablation with a frequency doubled Nd:YAG pulsed laser on a 99.9% purity Ca disk target. The ions' fluorescence is recorded on a Andor iCCD camera using a custom-made Nikon microscope lens system.

Conclusion

We investigated planar Coulomb crystals for which there are very few theoretical and experimental results. Using large scale Molecular Dynamics simulations we performed an extensive study of planar Coulomb crystals in both Penning and RF traps including the effects of RF heating and collisions with background gas heating. We analyzed planar bicrystals and found out the limit imposed on the number of ions by the mass ratio and derived the dependence of spatial separation on the mass ratios and radial frequency shift

Using the results from the Molecular Dynamics simulations we estimated the error in the "push-gate" in planar Coulomb crystals. We also considered the error in quantum simulation and estimated the fidelity in the simulation of effective spin-spin interactions.

In order to realize planar Coulomb crystals in experiment, we designed and built an RF-trap system optimized for the implementation of planar crystals. The geometry of the designed linear segmented quadrupole trap provides large axial frequencies even for low voltages. Moreover, the RF-heating is drastically reduced.