Temperature driven structural phase transition for trapped ions and its experimental detection

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A Wigner crystal formed with trapped ion can undergo structural phase transition, which is determined only by the mechanical conditions on a classical level. Instead of this classical result, we show that through consideration of quantum and thermal fluctuation, a structural phase transition can be solely driven by change of the system's temperature. We determine a finite-temperature phase diagram for trapped ions using the renormalization group method and the path integral formalism, and propose an experimental scheme to observe the predicted temperature-driven structural phase transition, which is well within the reach of the current ion trap technology.

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Ions trapped in a linear Paul trap or a planar Penning trap have become a very useful platform [1], with exciting applications in both quantum information science [2] and precision measurements [3]. Trapped ions also provide a controllable system to simulate and study many-body phase transitions [4]. A well-known phase transition that can be observed in a small ion crystal is the structural phase transition of the Wigner crystal formed with trapped ions, which has raised significant interest and been extensively studied [5–16]. For instance, a linear crystal in a Paul trap can be squeezed to a zigzag shape with change of the aspect ratio between the transverse and the axial trapping frequencies. The structural phase transition for trapped ions so far is formulated on a classical level, determined by the mechanical equilibrium conditions. On a classical level, quantum and thermal fluctuation of the ion positions play no role in the structural phase transition, and this transition is thus independent of the system's temperature.

In this paper, we develop a theoretical formalism to take into account quantum and thermal fluctuation in the structural phase transition, and show for the first time that a structural phase transition can be driven solely by change of the system temperature. The structural phase transition is induced by condensation of phonons into the soft mode (the lowest frequency collective oscillation mode of the ion crystal). Anharmonic coupling between different phonon modes intrinsic in the Coulomb interaction leads to renormalization of the soft mode frequency which affects the phase transition point. We calculate the system's partition function using the path integral approach, and gradually integrate out the high frequency modes with the renormalization group (RG) method to construct the RG flow for the soft mode frequency. With this formalism, we can calculate the finite-temperature phase diagram for the ion crystal. Using the linear ion crystal in a Paul trap as an example, we propose an experimental scheme to detect the predicted temperature-driven linear-to-zigzag structural phase transition and show that the requirements in observing this transition fits well with the current status of the experimental technology.

We consider N ions of mass m subject to external harmonic potentials in both axial (z) and transverse (x, y) directions. To be concrete, we take a linear Paul trap as an example with the trapping frequencies $\omega_y > \omega_x > \omega_z$ (the method can be extended easily to other type of traps). We consider the system near the linear-to-zigzag transition point, with the ions distributed along the z direction with a tendency towards the zigzag transition in the $x - z$ plane. To describe this phase transition, it suffices to consider the ion interaction Hamiltonian in the $x - z$ plane, given by

$$H = \sum_{i=1}^{N} \sum_{\alpha=x,z} [\frac{p_{i\alpha}^2}{2m} + \frac{1}{2} m\omega_\alpha^2 \alpha_i^2] + \sum_{i>j} \frac{\kappa}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (1)$$

where κ is the Coulomb interaction rate. We assume the temperature of the system is significantly below the melting temperature of the ion crystal, which is typically of the order of $0.1 - 1$K [17]. This condition is satisfied straightforwardly in experiments with laser cooling. The ions have well-defined equilibrium positions $\bar{\mathbf{r}}_i$, and we expand $\mathbf{r}_i$ around the equilibrium positions up to the fourth order of the displacement operators $\delta\mathbf{r}_i \equiv \mathbf{r}_i - \bar{\mathbf{r}}_i$. Up to the second order of $\delta\mathbf{r}_i$, the quadratic part of the Hamiltonian can be diagonalized to get the normal phonon modes. For N ions in the $x - z$ plance, there are in total $2N$ normal modes, and we label them from 1 to $2N$ in the ascending order of the mode eigen-frequencies. Expressed with the coordinates of the normal modes, the Hamiltonian has the form

$$\begin{aligned} H &= \sum_{i=1}^{2N} \frac{p_i^2}{2m} + \frac{1}{2} m\omega_z^2 z_0^2 \Big(\sum_{i=1}^{2N} \omega_i^2 q_i^2 \\ &+ \sum_{ijk}^{2N} B_{ijk}\, q_i q_j q_k + \sum_{ijkl}^{2N} C_{ijkl}\, q_i q_j q_k q_l \Big) \end{aligned} \quad (2)$$

where p_i and q_i are the canonical momentum and coordinate for the i^{th} phonon modes and ω_i denotes the corresponding eigen-frequency. We have factorized out

ω_z (axial trap frequency) and $z_0 \equiv (2\kappa/m\omega_z^2)^{1/3}$ (typical distance between the ions) as the frequency and the length units ($\omega_i, q_i, B_{ijk}, C_{ijkl}$ are thus all dimensionless). The terms with B_{ijk} and C_{ijkl} represent the cubic and quartic terms in the expansion of the Coulomb potential, and we need to keep both of them as they lead to the same order of correction to the phase transition point in the following renormalization calculation. The values for ω_i, B_{ijk}, and C_{ijkl} are determined numerically through expansion of the Hamiltonian in Eq. (1) and diagonalization of its quadratic components [18].

The structural phase transition is caused by phonon condensation in the lowest normal mode (soft mode, or mode 1 in our notation, which corresponds to the zigzag mode for an ion chain). This happens when the effective frequency ω_{1eff} of the soft mode crosses zero. In the classical treatment [15], interaction and fluctuation of the phonon modes are neglected and the effective frequency ω_{1eff} is just given by the bare frequency ω_1 in the Hamiltonian (2). As ω_1 is determined simply through expansion and diagonalization of the trapping and the Coulomb potentials, it is apparently determined only by the mechanical conditions and has no dependence on the system's temperature. Here, we take into account the phonon interaction and derive the effective frequency ω_{1eff} through a renormalization group treatment of the partition function corresponding to the Hamiltonian (2) in the path integral formalism. As a qualitatively new result from this treatment, we show that the structural phase transition is not purely mechanical any more and becomes a thermodynamic transition depending on the system temperature.

In the path integral formalism, the partition function of the system $Z = e^{-H/(k_B T)}$ (where T is the system temperature) can be written as [19]

$$Z = \oint \prod_{i=1}^{2N} \mathcal{D} q_i e^{-S}, \tag{3}$$

where the action

$$\begin{aligned} S &= \int_0^{\hbar\omega_z/(k_B T)} \frac{d\tau}{\hbar\omega_z} \frac{1}{2} m\omega_z^2 z_0^2 \left\{ \sum_{i=1}^{2N} \left[(\partial q_i/\partial\tau)^2 + \omega_i^2 q_i^2 \right] \right. \\ &\left. + \sum_{ijk} B_{ijk}\, q_i q_j q_k + \sum_{ijkl} C_{ijkl}\, q_i q_j q_k q_l \right\}. \end{aligned} \tag{4}$$

The RG method provides a way to work out this partition function and to find the effective frequency ω_{1eff} of the lowest mode [20]. The basic idea of the RG method is to integrate out the high frequency modes in the path integral step by step to get a renormalized action for the lower frequency modes. We start from the highest mode $2N$, and the integration over this mode can be done in a perturbative manner with Gaussian integration over the variable $q_{2N}(\tau)$, where τ is the imaginary time in the unit of $1/\omega_z$. We define a small parameter $\epsilon = \delta z/z_0$, where the length scale $\delta z = (\hbar/m\omega_z)^{1/2}$ characterizes the ion oscillation amplitude for a single ion in a trap with frequency ω_z. We consider renormalization correction to the effective parameters up to the order of ϵ^2 (which is the order of C_{ijkl} term in the action). Following the standard procedure to calculate the path integral, we find that after integration of the mode $2N$, the action for the modes 1 to $2N-1$ still takes the form of Eq. (4) up to the order ϵ^2, with the effective parameters renormalized to

$$\begin{aligned} \omega'_{ij} &= \omega_{ij} + \epsilon^2 \left[f_1 \frac{C_{i,j,2N,2N}}{2\omega_{2N}} - f_2 \frac{B_{i,2N,2N} B_{j,2N,2N}}{8\omega_{2N}^3} \right] \\ C'_{ijkl} &= C_{ijkl} + \frac{B_{i,j,2N} B_{k,l,2N}}{4\omega_{2N}^2} + O(\epsilon^2) \\ B'_{ijk} &= B_{ijk} + O(\epsilon^2) \\ f_1 &= \coth\left(\frac{\hbar\omega_z\omega_{2N}}{2k_B T}\right) \\ f_2 &= \coth\left(\frac{\hbar\omega_z\omega_{2N}}{2k_B T}\right) + \frac{\hbar\omega_z\omega_{2N}}{2k_B T} \left[\sinh\left(\frac{\hbar\omega_z\omega_{2N}}{2k_B T}\right) \right]^{-2} \end{aligned} \tag{5}$$

where ω_{ij} and ω'_{ij} denote the coefficients before the quadratic term $q_i q_j$ in the action ($\omega_{ij} = \omega_i^2 \delta_{ij}$ in Eq. (4)), and for the coefficients written as $C_{i,j,2N,2N}$ or $B_{i,2N,2N}$, summation over all possible permutations of the indices are implicitly assumed. After the renormalization, we re-diagonalize the quadratic term from $\sum_{ij} \omega'_{ij} q_i q_j$ to $\sum_i \omega_i'^2 q_i'^2$ and make the corresponding changes to B'_{ijk} and C'_{ijkl} through change of coordinates from q_i to q'_i. With this step, the action then takes the same form as in Eq. (4), with the mode index summarizing from 1 to $2N-1$ and the coefficients renormalized to ω'_i, B'_{ijk}, and C'_{ijkl}. Then we can continue with integration of the next highest mode until we finally integrate out all the modes except for the soft mode 1. The transformation $(\omega_i, B_{ijk}, C_{ijkl}) \to \left(\omega'_i, B'_{ijk}, C'_{ijkl}\right)$ defines the RG flow equations, and after integration of all the modes from mode N to mode 2, the last ω'_1 gives the effective frequency ω_{1eff}. By numerically solving the RG flow equations, the structural phase transition point can be determined by the criterion $\omega_{1eff} = 0$. Since the RG flow equations (see Eq. (5)) depend on the system temperature T, and so does ω_{1eff}, structural phase transition can be possibly driven solely by temperature under a fixed aspect ratio of the trap.

The temperature related functions f_1 and f_2 can be well approximated at temperature $T \gg \hbar\omega_z\omega_{2N}/k_B$ (the latter corresponds to a pretty low temperature compared to Doppler cooling limit) by:

$$f_1 \simeq \frac{2k_B}{\hbar\omega_z\omega_{2N}} T, \qquad f_2 \simeq 2f_1, \tag{6}$$

so the renormalization correction to ω_{1eff} is linear in T for a wide range of temperature. As a result, the critical exponent for temperature induced linear-to-zigzag phase transition should be 1, as long as the critical temperature is above $\hbar\omega_z\omega_{2N}/k_B$. The magnitude of the correction to ω_{ij} at each step is of the order of $k_B T/\left(m\omega_z z_0^2\right)$, which is

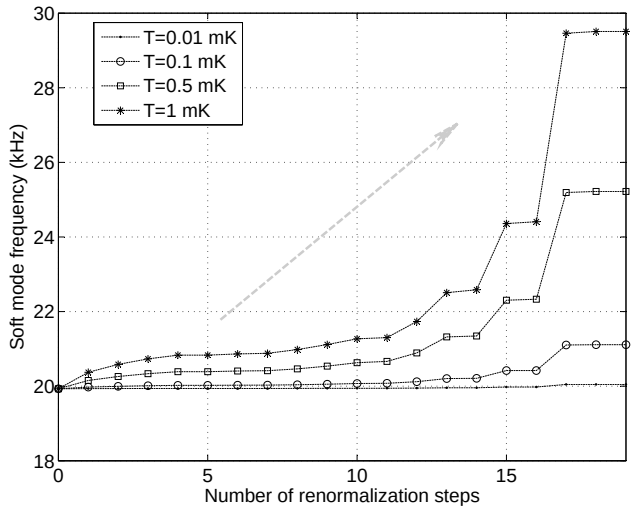

FIG. 1: (a) Change of the soft mode frequency during the renormalization process with the aspect ratio $\alpha \equiv \omega_x/\omega_z = 4.6$. Different curves correspond to different temperature, and the number of the renormalization steps represent the number of high frequency modes that have been integrated out.

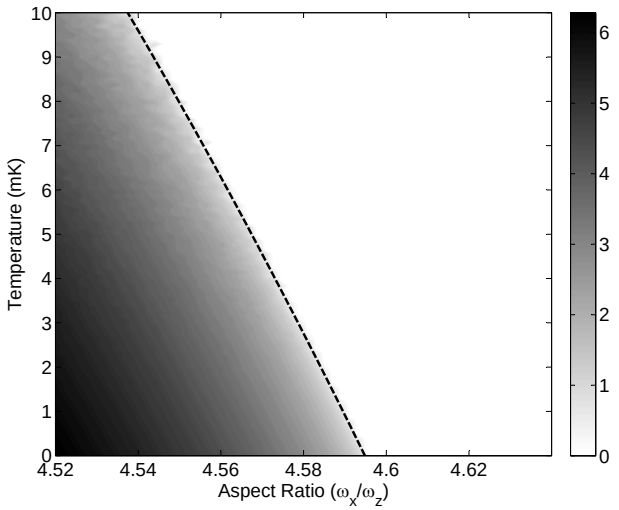

FIG. 2: The map of the order parameter (with value in unit of μm) as a function of temperature and aspect ratio in the linear-to-zigzag phase transition for $N = 10$ ions. The dashed line marks the phase boundary where the order parameter crosses zero.

a small quantity representing the ratio of system temperature to melting temperature. It is also worth mentioning that even for zero temperature, the renormalization correction to ω_{1eff} is nonzero as $f_1 = f_2 = 1$ when $T = 0$, providing correction from quantum fluctuation to this structural phase transition.

In the following, we carry out some explicit numerical calculation to show that it is realistic to observe the predicted temperature driven structural phase transition in the current experimental system. In our calculation, we take 10 ions as an example with the mass of ions set as same as Yb^+ ions. The axial trap frequency is set to 100 kHz and the aspect ratio ω_x/ω_z is chosen around the classical critical value 4.59 [13]. Temperature is varied on the order from μK to mK. Fig. 1 shows the change of soft-mode frequency during the process of renormalization (the RG flow for ω_1) at different temperatures. We find that each renormalization step (integration of one normal mode) increases slightly the soft mode frequency, and the change after $2N-1$ renormalization steps can be quite significant. The change clearly increases with the temperature, as the thermal fluctuation of the ion positions deviate the system from the classical limit where each ion is assumed fixed at its equilibrium position.

To characterize the phase transition, we calculate the order parameter, which is taken as the transverse displacement of the zigzag mode (the mean value of q_1) for the linear-to-zigzag transition. Fig. 2 shows the value of the order parameter and the corresponding phase diagram as a function of both temperature and aspect ratio. The phase boundary has a slope there, which shows that a structure phase transition can be driven vertically at a fixed aspect ratio solely by change of the system temperature. From the figure, we also see that the order parameter is more sensitive to the aspect ratio than to the temperature. Tuning the aspect ratio by about 1% (4.59 to 4.54 for example) at a fixed temperature (around 1 mK) will result in a change of the order parameter by about 5 μm, while the same change with a fixed aspect ratio around 4.54 requires one to cool the temperature from 10 mK to 1 mK.

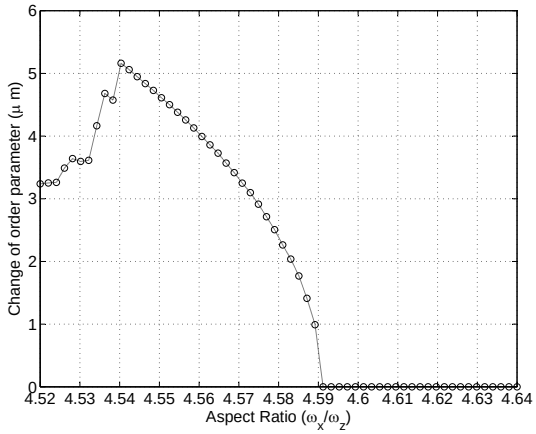

FIG. 3: The change of value of the order parameter as a function of the aspect ratio when temperature is cooled from 10mK to 1mK. By tuning the aspect ratio of the confining trap to an optimum value, cooling the ions can give rise to a change of the order parameter as large as $5\mu m$, resulting in a fairly noticeable transition from linear to zigzag pattern.

Experiment done in Ref. [10] has successfully observed the classcial linear-to-zigzag phase transition in a trapped ion crystal by changing the radial trap frequency with an accuracy of 2 kHz (0.5% for aspect ratio). With such an accuracy (and probably better nowadays), one can pick an optimum value for aspect ratio to maximize the change of order parameter based on the numerical calculation shown in Fig. 3. The CCD camera used in Ref. [10] has a resolution of $0.3 - 1$ μm, which is enough to tell the transition point as the change of order parameter is apparently larger than $1\mu m$ for a relatively wide range of aspect ratios (see Fig. 3).

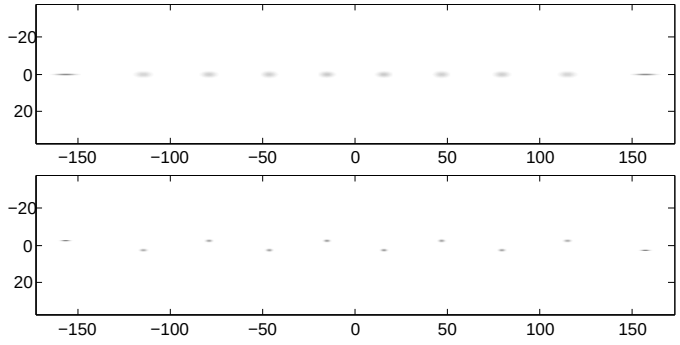

FIG. 4: Plot of ions' probability density in $x - z$ plane (in unit of μm for both axes) due to thermal fluctuation. The upper figure shows the position and the probability density of 10 ions at high temperature (5mK), which characterizes the linear phase. The lower figure is simulating the ion's position after cooling the temperature to 1mK, and the zigzag pattern clearly emerges. The aspect ratio is tuned at about 4.57.

In real experiments carried out at finite temperature, the thermal fluctuation of the ions' positions will blur the image of ions. In this case, we need to calculate whether the image of ions are still sharp enough to show the temperature driven structural phase transition for the ion chain. We calculate the thermal fluctuation of ions' axial and transverse positions, and plot the probability density of the ions' wave-packets above and below the critical temperature (See Fig. 4), with the aspect ratio tuned near classical critical value. Here we only demonstrate the case with a few ions (N=10) where the transverse displacement of all ions can be roughly treated as the same as the order parameter calculated above, but our calculation method works for larger number of ions as well. Our simulation shows that one can clearly observe the structural phase transition from linear to zigzag pattern, as the thermal fluctuation of ions' transverse position in the considered temperature range is much smaller than the change of order parameter across the transition point.

In summary, we have developed a method to characterize the temperature driven structural phase transition in a trapped ion crystal, taking into account contributions from both quantum and thermal flucatuation. We use renormalization group method to calculate the effective soft mode frequency under finite temperature for a given number of ions and show that the system have an interesting phase diagram with respect to the system temperature and aspect ratio. Our predictions can be verified under current experimental conditions, as shown by our explicit calculations taking account of the experiemntal imperfections.

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