Double peaks in the momentum distribution of cold polar molecules in the supersolid state

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Abstract. We study the checkerboard supersolid of hard-core bosonic polar molecules in a 2D square lattice. This supersolid shows a novel double-peak structure in the momentum distribution of bosons. The double peaks indicate coexistence of superfluidity and solidity. The corresponding peaks can be measured by the time-of-flight experiment and will become a clear evidence for the supersolid state. By exact quantum Monte Carlo calculations, we reveal temperature dependence of the momentum distribution in the supersolid phase. As a result, we observe successive developments of the two peaks.

1. Introduction
A quantum gas of ultracold polar molecules has possibilities of realizing new physics due to the dipole-dipole interaction and attracts great interest motivated by recent experimental advance\cite{1, 2, 3}. One of such fascinating physics is supersolid, which is characterized by the coexistence of superfluidity and solidity. Numerically, it has been confirmed by quantum Monte Carlo simulations that supersolid phases exist in a 2D square lattice system of hard-core dipolar bosons\cite{4}. More specifically, checkerboard-type supersolid phases are found for $\rho < 1/2$ and $\rho > 1/2$, and star-type supersolid phases are also found for $\rho < 1/4$ and $\rho > 1/4$, where $\rho$ is the particle filling factor.

In our recent work\cite{5}, we discussed the mechanism for the checkerboard supersolid mentioned above. This supersolid is realized by the second-order hopping process of defects (interstitials or vacancies) in the crystal. In other words, condensed defects are delocalizing on a strongly non-flat potential of the checkerboard-type background. Owing to the mechanism, the supersolid has a characteristic feature; by our quantum Monte Carlo simulations, we observed a novel double-peak structure of the momentum distribution $n(k)$ in the supersolid state. One of the peaks is a conventional peak at $k = (0,0)$ that indicates superfluidity. The other is a new one at $k = (\pi, \pi)$, which is attributed to the checkerboard order. The corresponding momentum distribution can be measured by the time-of-flight experiment and will become a clear evidence for supersolid. Therefore, it is important to investigate this double-peak structure in the momentum distribution.

In this paper, we study temperature dependence of the momentum distribution of dipolar bosons and reveal how the peaks appear when the system is cooled. In our choice of system...
parameters, the system shows the phase transition from the normal disordered phase to the superfluid phase at a higher critical temperature. Then, the crystalization of bosons realizes at a lower temperature. By our simulations, we show a crucial difference between the supersolid state and the superfluid state in the momentum distribution, which is distinguished by the presence of the peak at \( k = (\pi, \pi) \).

2. Model and Method

We consider a system of hardcore dipolar bosons in a 2D optical square lattice, where dipole moments are induced perpendicularly to the 2D plane by an electric field. In this situation, the dipole-dipole interaction becomes an isotropic repulsive long-range interaction of \( 1/r^3 \). The effective Hamiltonian is given by

\[
H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + V \sum_{i<j} \frac{n_i n_j}{r_{ij}^3} - \mu \sum_i n_i.
\]

Here, \( b_i(b_i^\dagger) \) is the annihilation(creation) operator of hard-core bosons on the site \( i \), \( n_i = b_i^\dagger b_i \) is a particle number operator. \( t, V, \) and \( \mu \) indicate the hopping parameter, the strength of the dipole-dipole interaction, and the chemical potential respectively. \( r_{ij} \) is the distance between the site \( i \) and \( j \). \( \langle i,j \rangle \) means nearest-neighbor pairs. In what follows, we take the lattice spacing as the unit of distance. Through this paper, we consider the square lattice and the system size is defined by \( N = L \times L \). The periodic boundary condition is imposed.

To perform exact computations for Eq. (1), we use a world-line quantum Monte Carlo method based on the worm algorithm[6, 7]. To treat long-range interactions exactly without any cutoff, we apply the Ewald summation method[8]. In long-range interacting systems, there is a notorious difficulty in performing the numerical studies, because it requires the high computational cost of \( O(N^2) \). To overcome this difficulty, we applied the \( O(N) \) Monte Carlo method[9] which realizes Monte Carlo simulations with \( O(N) \) time even in the presence of long-range interactions.

3. Results

Before we study the double-peak structure of the momentum distribution in the supersolid, we show the finite-temperature transitions in this state. For this purpose, we calculate the superfluid stiffness \( \rho_s = \langle W^2 \rangle / (\beta t) \) and the structure factor \( S(k) = 1/N \sum_{i,j} e^{i\mathbf{k} \cdot \mathbf{r}_{ij}} (\langle n_i n_j \rangle - \langle n_i \rangle^2) \). Here, \( \mathbf{W} = (W_x, W_y) \) denotes the winding number vector in the world-line configurations[11] and \( \beta \) is the inverse temperature. The superfluidity and the checkerboard order are characterized as finite values of \( \rho_s \) and \( S(\pi, \pi)/N \) in the thermodynamic limit respectively. The results are shown in Figure 1.

Figure 1. Temperature dependence of the superfluid stiffness \( \rho_s \) (full points) and the structure factor \( S(\pi, \pi)/N \) (empty points) for different system sizes. At first, the superfluid transition occurs at \( T/t = 0.255(5) \), which is obtained by the finite-size scaling of \( \rho_s \) for the Kosterlitz-Thouless transition[10]. When the temperature is lowered, the checkerboard order also develops successively.
in Fig. 1. In these simulations, we chose the parameters as $t/V = 0.15, \mu/V = 3.24$. At this parameter set, the superfluidity in the supersolid phase is caused by condensed vacancies, i.e. $\rho < 1/2$. As we can see in the figure, we observe the two successive finite-temperature transitions, where the checkerboard-order transition follows the superfluid transition when the system is cooled. In Ref. [4], the other type of successive finite-temperature transitions has already been shown; the superfluid transition follows the checkerboard-order transition. These two types of successive transitions occur depending on the model parameters. Let us consider first a supersolid region close to the checkerboard insulating phase at $\rho = 1/2$. In that region, since the number of condensed vacancies is small, the superfluidity is suppressed and the checkerboard-order develops. As a result, the latter type of successive transitions is realized. On the other hand, in a supersolid region close to the superfluid phase, the former one occurs, because the number of condensed vacancies is increased and the checkerboard order is nearly destroyed. In the following, we focus on the former-type successive finite-temperature transitions, because it results in novel successive changes of the momentum distribution.

We next reveal temperature dependence of the momentum distribution in the supersolid phase considered above. In Fig. 2, we show the momentum distribution $n(k) = 1/N \sum_{i,j} \langle b_i b_j^{\dagger} \rangle e^{i k \cdot r_{ij}}$, the superfluid correlation function $C_{\text{SF}}(r_{ij}) = \langle b_i b_j^{\dagger} \rangle$, the density-density correlation function $C_{\text{CDW}}(r_{ij}) = (n_i n_j) - (n_i) (n_j)$ along the $x$-axis. At a high temperature $T/t = 1.0$, the correlation functions show neither long-range order nor quasi-long-range order. As for $C_{\text{SF}}(r_{ij})$, this is
also confirmed from absence of sharp peaks in the momentum distribution of bosons in the
normal state[Fig. 2(a)]. When the temperature is lowered, the system turns into the superfluid
phase[Fig. 2(b)]. In this phase, the power-law decay of $C_{\text{SF}}(r_{ij})$ is observed. The appearance
of the quasi-long-range order implies that the Kosterlitz-Thouless-type superfluid occurs[12]. On
the other hand, $C_{\text{CDW}}(r_{ij})$ still shows no long-range order. Resulting momentum distribution
has a conventional sharp peak at $k = (0, 0)$ associated with superfluidity. When the system
is cooled further, it finally becomes the supersolid state[Fig. 2(c)]. In this phase, $C_{\text{CDW}}(r_{ij})$
has a long-range order. Since the checkerboard-order develops, it shows a zig-zag pattern. At
the same time, $C_{\text{SF}}(r_{ij})$ still has a power-law decay. However, its behavior is different form
the one in the superfluid state; $C_{\text{SF}}(r_{ij})$ also shows the zig-zag pattern. This is due to the
fact that condensed doped defects delocalize on a strongly zig-zag potential of the checkerboard
background. Consequently, the second smaller peaks at $k = (\pi, \pi)$ and its equivalent points
appear in the momentum distribution. In the experiment, we can observe the signals of
superfluidity and solidity simultaneously by the time-of-flight method. Therefore, observation
of these peaks will become a clear evidence for supersolid of ultracold polar molecules in optical
lattices.

4. Summary and Discussion
To summarize, we have studied the double-peak structure of the momentum distribution in the
checkerboard supersolid state. In our simulations, we observed the successive developments of
the two-types of peaks. This is because we have considered the case where the checkerboard-
order transition follows the superfluid transition when the system is cooled. On the other hand,
in the opposite case where the superfluid transition follows the checkerboard-order transition,
we can expect that the double peaks appear simultaneously when the system turns into the
supersolid phase. The presence of the two types of successive finite-temperature transitions will
be more obvious if a finite-temperature phase diagram is obtained.

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