Quantum melting of a crystal of dipolar bosons

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We investigate the behaviour of dipolar bosons in two dimensions. We describe the large density crystalline limit analytically while we use quantum Monte-Carlo to study the melting toward the Bose-Einstein condensate. We find strong evidence for a first order transition. We characterize the window of experimentally accessible parameters in the context of ultracold bosons and show that observing the quantum melting should be within grasp once one is able to form cold heteronuclear molecules. Close to the melting, we can not conclude on the existence of a supersolid phase due to an insufficient overlap of our variational Bijl-Jastrow Ansatz with the actual ground state.

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I. INTRODUCTION

Quantum melting (the melting of a crystal induced by quantum fluctuations) can be very different from a classical melting (induced by temperature). In two dimensional electronic systems, it was found that near the melting point$, the system is neither in a liquid nor in a solid phase but shares properties with both phases$. In bosonic systems, such an intermediate phase ("supersolid" between the solid and the superfluid phase) was proposed many years ago$. The supersolid phase can be thought as a condensate of either static or dynamical defects$. Some supersolid behaviour (i.e. existence of a non zero superfluid fraction in a solid system) has indeed been recently observed in Helium 4, creating a large renewed of interest on both theoretical and experimental sides. The situation in Helium 4 is however controversial as the predictions of the model studied in this paper are not in agreement with the experimental results, and the experiments seem to be sensitive to the way the solid is prepared (an annealing of the supersolid kills or enhances the superfluid fraction depending on the experiments) indicating that disorder probably plays a key role in this physics and (iii) one gets only access experimentally to macroscopic quantities which make it difficult to infer the physical mechanisms actually involved.

An alternative bosonic system is now promising due to recent progresses in the field of ultracold gases. The production and observation of heteronuclear alkali molecules$ at ultralow temperatures has been reached with various dimers, $e.g.$ KRb, RbCs, or LiCs, yet not in their true molecular ground state. Polar molecules confined in a two-dimensional trap with a perpendicular electric field could be given an important dipole moment (on the order of 1 Debyes$) leading to strong repulsive dipole-dipole interaction on the plane. Although these interactions are not truly long range in 2D, the potential range is larger than for typical van der Waals interaction and smaller densities are necessary to observe crystallization. Moreover the true repulsive character of dipole-dipole interaction should strongly inhibit inelastic three-body recombination. Such systems could be very good candidates for the study of quantum melting as they do not share the usual limitations found in Helium 4: there is a complete control of the external potential seen by molecules (no disorder) and many direct observations can been done (of the spatial distribution of the density for the solid, of the condensate fraction for the superfluid part). It is the purpose of this paper to study this potential use of cold dipolar gases in some detail. We note that two papers with a similar topic and some overlapping results appeared recently$ and hence, whenever appropriate we will compare our findings with these works. Another possible experimental realization of the model studied in this paper are electron-hole heterostructure bilayers where the excitons also interact through dipole-dipole interaction$.

After introducing the model (Bosons in two dimensions with a dipole-dipole repulsion), and briefly the numerical technique (Green Function Monte-Carlo or GFMC) in section$ we proceed with the description of the high density limit where the crystal is expected. In section$ we calculate the phonon spectrum of the crystal, from which we extract the high density expansion of the energy of the system. The nature (first order) of the transition is then discussed in section$ using the GFMC technique.
Particular attention is paid to the sensitivity of the results to the trial wave-function used in the calculation. The quality of the wave-function is usually measured in term of the distance in energy to the true ground state. We find that a better measure can be done by calculating the overlap of the trial wave-function with the true ground-state. In section IV we discuss the possibility of the existence of a supersolid in this system. In the last section we estimate the regime of parameters that should be accessible experimentally. The appendix contains the Ewald summation technique that is applied to the dipole-dipole interaction to reduce finite size effects.

II. THE MODEL: N BOSONS IN 2 DIMENSIONS WITH DIPOLE-DIPOLE INTERACTION

Our system is made of N bosons of mass $M_0$ confined in two dimensions which interact through a dipole-dipole interaction of strength $C_{dd}$, so that the Hamiltonian reads

$$H = -\frac{\hbar^2}{2M_0} \sum_{i=1}^{N} \nabla_i^2 + C_{dd} \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|^3},$$

with dipoles polarized perpendicular to the plane. Measuring lengths in unit of the average distance $\ell$ between bosons (defined as $\pi \ell^2 = 1/n$ where $n$ is the 2D density), and the energies in unit of $E_B \equiv C_{dd} / (2\ell^3)$, the rescaled Hamiltonian depends on a unique dimensionless parameter $r_s$ and reads,

$$H = -\frac{1}{r_s} \sum_{i=1}^{N} \nabla_i^2 + 2 \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|^3}.$$  

The parameter $r_s$ (named in analogy with electronic systems) roughly measures the ratio between interaction energy $\sim C_{dd}/\ell^3$ and kinetic energy $\sim \hbar^2/(M_0\ell^2)$ and reads,

$$r_s = \ell_B^*/\ell,$$

where $\ell_{B}^* = M_0 C_{dd}/\hbar^2$. Contrary to electronic systems, $r_s$ increases with density, so that Bose-Einstein condensation is obtained at low density while at high density the dipole-dipole interaction dominates and the system crystallizes into a triangular lattice (see Sec. III).

A. The Green Function Monte-Carlo technique

The bosonic system is put on a rectangular grid of $L_x \times L_y$ sites with nearest neighbor hopping. Finite size effects are considerably reduced by repeating periodically the simulation box on the two-dimensional plane. This amounts to use periodic boundary conditions for hopping and to replace the dipole interaction by an effective two-body interaction that includes all periodic images. The resulting summation is efficiently performed using a straightforward extension of the Ewald summation technique. This is discussed in more details in appendix A.

The discretized Hamiltonian on the grid reads

$$H = -t \sum_{(\vec{r},\vec{r}')} c_{\vec{r}}^\dagger c_{\vec{r}'} + U \sum_{\vec{r} \neq \vec{r}'} V(\vec{r} - \vec{r}') n_{\vec{r}} n_{\vec{r}'} + (4t + \lambda)N,$$

where the operator $c_{\vec{r}}^\dagger (c_{\vec{r}})$ creates (destroys) a boson on point $\vec{r}$ with the standard commutation relation rules, the sum $\sum_{(\vec{r},\vec{r}')} V(\vec{r} - \vec{r}')$ is done on the nearest neighbor points on the grid. The form of the periodized two-body interaction $V(\vec{r})$ and of the constant $\lambda$ (which accounts for the interaction of a boson with its own images) are given in appendix A. Noting $\nu = N/(L_x L_y)$ the filling factor, the continuous model Eq. (2) is reproduced by choosing the hopping amplitude to be $t = 1 / (r_s \pi \nu)$ and the effective interaction strength $U = 2 / (\nu \pi)^{3/2}$ in the limit $\nu \to 0$. In practice we took $\nu = 1/56$ (some small influence of the presence of the grid) down to $\nu = 1/780$ (no detectable...
influence of the grid). The grid dimensions are also chosen in order not to induce distortion of the triangular lattice of the crystal.

C. The guiding wave-functions

All our Monte Carlo simulations start from a trial wavefunction which is an initial guess for the exact ground state wavefunction. The trial GWF is also used as a guide to converge to the ground state during the GFMC projection. For practical efficiency, i.e. to reduce noise in numerical results, it is important that the GWF is as close as possible from the unknown exact solution. We use here a Bijl-Jastrow form:

$$\Psi_{GWF}(r_1, \ldots, r_N) = \prod_{i=1}^{N} \phi_1(r_i) \prod_{j<k} \phi_2(|r_j - r_k|)$$  \hspace{1cm} (6)

which includes at the variational level one-body and two-body correlations. Two-body correlations are essential in the homogeneous (BEC) limit where it dominates the physics and determines the shape of the wavefunction. On the contrary, one-body terms are sufficient to describe the crystal limit where atoms are almost frozen. It is worth noticing that the two-body scattering problem can be solved exactly at zero energy, leading $\phi_2^{2-b}(r) = AK_0(2\sqrt{r/A})$, where $A$ is an arbitrary constant and $K_0$ the modified Bessel function of the second kind. Its short distance behaviour is $\phi_2^{2-b}(r) \propto (r/r_s)^1/4 e^{-2\sqrt{r/r_s}}$. In practice, we chose

$$\phi_2(r) = \exp\left(-2\sqrt{\frac{r}{r_s}} e^{-r/A}\right),$$  \hspace{1cm} (7)

with a single variational parameter $A$ which sets the length over which two-body correlations are suppressed. In particular, it reproduces the leading short distance behavior for the two-body scattering problem. More complicated variational forms have been tested (with more variational parameters) with the same efficiency. Typical values of $A \simeq 1$ have been found in the vicinity of the quantum melting point $r_s \simeq 27$.

Noting $\Delta y$ ($\Delta x$) the distance between sites along the $y$ ($x$) axis ($\Delta y/\Delta x = \sqrt{3}/2$), we define the vector $q_1 = (0, 2\pi/\Delta y)$ in the reciprocal lattice. Vectors $q_{2/3} = (\pm 2\pi/\Delta x, -\pi/\Delta y)$ are obtained by rotating $q_1$ by an angle of $2\pi/3$ and $-2\pi/3$. We choose for the one-body trial function

$$\phi_1(r) = \prod_{i=1,2,3} \left(1 + \alpha \cos(q_i \cdot r)\right),$$  \hspace{1cm} (8)

where maxima reproduce the triangular lattice expected for the crystal. This function is well-suited to describe quantum melting since it interpolates between a flat liquid (BEC)-type pattern for $\alpha = 0$ and a triangular crystal form for $\alpha \neq 0$. Moreover it conserves the symmetrization property imposed by bosonic statistics in contrast with the Gaussian form often considered in the literature.

III. PROPERTIES OF THE CRYSTAL PHASE

The infinite $r_s$ limit corresponds to a purely classical system of dipoles with interaction energy only. We have compared energies of various lattice configurations and found that the ground state is given by the triangular Bravais lattice of energy per particle $E_0 = 1.59702\ldots$. For comparison, the square lattice energy is $E_0 = 1.62232\ldots$. Ground state properties of the crystal phase can be computed perturbatively for large $r_s$ following Ref.26. For large but finite $r_s$, kinetic energy plays a role as atoms are able to move around the perfect triangular lattice configuration. We treat kinetic terms perturbatively which amounts to an harmonic approximation for the potential felt by the atoms. The emerging collective modes are then a sum of harmonic oscillators over the Brillouin zone. They describe phonons and dominate dynamical properties of the ground state. Moreover first order correction in $1/\sqrt{r_s}$ to the ground state energy derives from zero-point energies of these vibrational modes.

The Hamiltonian Eq. (2) expands around the classical stable position $r_i = R_i + u_i$ where $\{R_i\}$ denotes the triangular lattice configuration. Stopping at second order in atomic displacements, it is straightforward to diagonalize the Hamiltonian in Fourier space. Collective eigenmodes read $u_i(t) = \tilde{u}_q e^{i(q \cdot R_i - \omega t)}$ where the vectors $\tilde{u}_q$ are solutions of the eigenvalue problem

$$\omega^2(q) \tilde{u}_q = \frac{4}{r_s} \Phi(q) \tilde{u}_q.$$  \hspace{1cm} (9)

Here $\Phi(q)$ is a tensor or $2 \times 2$ matrix defined by

$$\Phi_{\alpha,\beta}(q) = \frac{1}{\tilde{u}_{q=0}} \left| \frac{\partial^2}{\partial u_{q\alpha} \partial u_{q\beta}} \sum_{j \neq 0} \frac{1}{|R_j + u_i|^3} (1 - e^{i q \cdot R_j}) \right|_{u_{q=0}}$$ \hspace{1cm} (10)

with Cartesian coordinates $\alpha, \beta = x, y$. For each wavevector $q$ in the first Brillouin zone, Eq. (9) has two solutions which leads to two branches of collective excitations. The symmetry of the triangular lattice under the point group $C_{6v}$ allows to restrict values of $q$ within the irreducible Brillouin zone represented in Fig.1. For illustration we show in Fig.1 the corresponding phonon eigenmodes, solutions of Eq. (9), along the boundary of the irreducible Brillouin zone. We rescale Eq. (9) with the definition

$$\omega_0 = \frac{8}{b^{2}2 \sqrt{r_s}},$$  \hspace{1cm} (11)

where $b = \sqrt{2/\sqrt{3}}$ is the lattice spacing for the triangular lattice with density $1/\pi$. $\bar{\omega}^2 = (\omega/\omega_0)^2$ is now eigenvalue of $\tilde{\Phi} = (b^2/16)\Phi$. For practical purposes, the
The ground state wavefunction is a simple product of all Gaussian ground states of the phonon modes. It can be written as

\[ \Phi_G(\{u_i\}) = N e^{-\frac{1}{2} \sum_{j=1,2} \int_{BZ} \frac{d^2q}{V_{BZ}} \bar{u}_{q,j} \bar{u}_{-q,j} \omega_j(q)/4}, \]

with \( N \) a normalization factor. Vectors \( \bar{u}_q \) are Fourier transforms of the original variables \( \{u_i\} \) and eigenvectors of the system. The reduced onebody wavefunction is obtained by integrating all atomic positions but one. This leads to the following anisotropic Gaussian wavefunction

\[ \Phi_{G,1}(x,y) = N_1 e^{-(x/x_0)^2+(y/y_0)^2}/2, \]

with typical sizes \( x_0 \) and \( y_0 \) respectively in the \( x \) and \( y \) directions. Let \( (\alpha(q),\beta(q)) \) and \( (\gamma(q),\delta(q)) \) be the normalized \( (\alpha(q)^2 + \beta(q)^2) \) eigenstates of Eq. (9), we find

\[ \sqrt{r_s}x_0^2 = \frac{3\sqrt{3} \beta}{2} q^{3/2} \int_{IBZ} \frac{d^2q}{(2\pi)^2} \left( \frac{\alpha(q)^2}{\omega_1(q)} + \frac{\beta(q)^2}{\omega_2(q)} \right), \]

and the same expression holds for \( y_0 \) where \( \alpha(q) \) and \( \beta(q) \) are interchanged. A numerical evaluation yields \( x_0 = 1.3613/r_s^{1/4} \) and \( y_0 = 0.9509/r_s^{1/4} \) in units of \( \ell \).

**IV. FIRST ORDER NATURE OF THE QUANTUM MELTING**

In this section, we use the quantum Monte-Carlo calculations in order to determine the order of the transition. We find strong numerical evidences of a first order transition. Close to a first order transition, the GFMC energies are expected to depend on the GWF \( |\Psi_G\rangle \). To illustrate this point qualitatively, let us expand \( |\Psi_G\rangle \) on the eigenbasis of the Hamiltonian,

\[ |\Psi_G(\alpha)\rangle \propto |\Psi_{BEC}\rangle + c(\alpha)|\Psi_{cry}\rangle + \cdots \quad (14) \]

where \( |\Psi_{BEC}\rangle \) (|\Psi_{cry}\rangle) stands for the BEC (crystal) eigenstate and \( c(\alpha) \) measures the relative projection of the GWF on the two competing eigenstates (a more careful treatment would also include the low lying excitations of the two phases). After projection, one gets a state \( |\Psi\rangle = e^{-\beta H}|\Psi_G(\alpha)\rangle \)

\[ |\Psi\rangle \propto |\Psi_{BEC}\rangle + c(\alpha) e^{-\beta (E_{BEC} - E_{cry})} |\Psi_{cry}\rangle \quad (15) \]

where \( E_{BEC} \) (\( E_{cry} \)) stands for the BEC (crystal) energy. For very large imaginary time \( \beta \), the exponential is very large (or small), and \( |\Psi\rangle \) converges to whichever of the BEC or crystal state is more stable. Real simulations however are done with finite values of \( \beta \) (typically 30t in our case). As one approaches the transition, \( E_{BEC} - E_{cry} \) vanishes, hence the exponential term tends to one, and one is left with a (incoherent) superposition \( |\Psi\rangle \propto \)
smallness of the exponential in Eq. (15) eventually compensates the energy difference $E_{\text{density-density correlation function}}$. As one increases $r_s$ (the last number here, 0.85, is a fitted parameter). Above the critical $r_s \approx 27 \pm 1$, the symmetry breaking state is energetically favored. This plots also demonstrates that the transition is first order. The system contains $N = 72$ bosons in $48 \times 84$ sites.

$|\Psi_{\text{BEC}}\rangle + c(\alpha)|\Psi_{\text{cryst}}\rangle$ whose properties are sensitive to the choice of the variational parameter $\alpha$ of the GWF.

In Fig. 2, we present the GFMC energies as a function of $r_s$ for various choices of the symmetry breaking parameter $\alpha$. Those data support the previous picture: concentrating at first on the $\alpha = 0$ ("BEC" like state, with $c(0) \ll 1$) and $\alpha = 0.75$ ("crystal" like state, with $c(0.75) \gg 1$) curves, we find a crossing around $r_s \approx 27$ above which the crystal becomes more stable than the BEC. When the symmetry is only weakly broken ($\alpha = 0.2$), the GFMC result is close to the BEC state close to the transition. As one increases $r_s$ further, the energy difference $E_{\text{BEC}} - E_{\text{cryst}}$ increases and the exponential in Eq. (15) eventually compensates the smallness of $c(0.2)$ and $|\Psi|$ converges toward the actual ground state $|\Psi_{\text{cryst}}\rangle$.

To further characterize the transition, we now look at the crystalline order parameter. Introducing the static density-density correlation function $g(\vec{r})$ (that roughly measures the probability of finding a particle on point $\vec{r}$ knowing that there is one at point $0$),

$$g(\vec{r}) = \frac{L_x L_y}{N(N + 1)} \sum_{\vec{k}} \left\langle c^\dagger_{\vec{r} + \vec{k}} c_{\vec{k}} c^\dagger_{\vec{r} + \vec{k}} c_{\vec{r}} \right\rangle$$

(16)

the order parameter is usually defined as the Fourier transform of $g(\vec{r})$ taken at a $\vec{k}$ vector belonging to the reciprocal lattice of the expected crystal. A typical example of $g(\vec{r})$ in the BEC (crystal) case can be found in Fig. 3. Here we define the crystalline order parameter $G(r_s)$ (in an equivalent but more convenient way) as the average value of $g(\vec{r})$ at the peaks corresponding to the classical position of the crystal (minus its average value). In Fig. 3, we plot $G(r_s)$ for non broken ($\alpha = 0$), broken ($\alpha = 0.8$) and partially broken ($\alpha = 0.4$) symmetry. The non broken and broken symmetry case have respectively zero and non zero $G$, hence $G$ is discontinuous at the transition which should therefore be first order. The case with partially broken symmetry shows the expected crossover near the transition point.

Far from the transition point, the results are supposed to be independent of the GWF. We checked that this is indeed the case in our calculation: Fig. 4 presents the results before (Variational Monte-Carlo VMC, on the left) and after (RQMC, on the right) projection on the ground state. One can see that although the starting point has no broken symmetry ($\alpha = 0$), the RQMC (or GFMC) algorithm is able to converge to the crystal ground state nevertheless. This result was obtained for a rather small system of $N = 32$ particles however, and for a larger system of $N = 72$ bosons, a small amount of $\alpha$ was needed in order to get the correct ground state.

The above results are consistent with those obtained in Ref. [3, 22]. In Ref. [19], the authors use a finite temperature algorithm and find the transition at $r_s = 32 \pm 7$. Indeed, in our unit, they work at a temperature of the order of $5 \times 10^{-3}$, i.e. several time the difference of energy (per particle) between the BEC and the crystal phase near the transition, see fig. 4. These explain the relatively important error bar on their critical value of $r_s$ and the fact that their superfluid fraction switches back and forth between 0 and 1 close to the transition. In Ref. [20], the authors use the DMC technique, similar to ours. The GWF that they are using to describe the crystal is not symmetric with respect to the interchange of the bosons, and hence describe a crystal of distinguishable particles. However they find a critical $r_s = 30$ which is consistent with ours (we found upon decreasing the filling factor $\nu$
The energy reads, 

\[ E \approx a_0 \bar{n}^{3/2} + a_1/2 \bar{n}^{5/4} + a_1 \bar{n} + \eta \theta(\sqrt{\bar{n}} - r_s^*) \left( \sqrt{\bar{n}} - r_s^* \right) \bar{n}^{3/2} \]  

\[ \text{where } a_0 \approx 1.592, a_1/2 \approx 2.03, a_1 \approx 0.85, \eta \approx 5 \times 10^{-4}, r_s^* \approx 27, \text{ and } \theta(x) \text{ is the Heaviside function discriminating the two phases.} \]

Note that the coefficient \( \eta \) can be directly extracted from Fig. 2. We find that the region where phase separation can occur is very small, given by a width \( \delta r_s = \alpha(r_s^*)^2/(3a_0) \) around the transition point \( r_s^* \). For our parameters, it translates into \( \delta r_s \approx 0.04 \) which is very small.

\[ \rho_S = \frac{1}{2N} \lim_{\beta \to 1} \frac{R^2(\beta)}{\beta} \]  

where \( \beta \) is the imaginary time and \( R^2(\beta) \) is the second moment of the center of mass in one direction (say \( x \)). Such a formula can be easily implemented, but the results should be taken with care. For \( r_s \leq 27 \) (BEC state) we find that \( \rho_S \approx 1 \). For large \( r_s \), we find that \( \rho_S \approx 0 \). However, for \( r_s \geq 27 \) but close to the transition, we could not get a reliable measure of \( \rho_S \) and hence cannot conclude about the presence of a supersolid in this model. This is due to a combination of two difficulties: (i) close to the transition, ”metastable state” can enter into the GWF, hence artificially enhancing \( \rho_S \) (depending on the choice of \( \beta \), see the discussion in section IV), (ii) In the crystal phase, the superfluid fraction is given by rather rare events that contain ”dynamical defects”\(^2\). To illustrate the difficulty of the calculation, let us look at a small system of \( N = 8 \) particles, where using brute force simulations, reliable results could be obtained for any choice of \( \alpha \). Using a very large number of walkers (10^6), and rather long simulations (\( \beta = 80/t \)), we find in Fig. 4 a superfluid fraction \( \rho_S \approx 0.82 \) for all values of \( \alpha \). However, for \( \alpha = 0.5 \) the correct superfluid fraction is only recovered after a (large) simulation time \( \beta \geq 20 \).

A careful analysis shows that for \( \beta < 20 \), the energy is higher than the ground state energy by a very small amount (of the order of \( 10^{-4} \)) usually undetectable in reasonable calculations. In the inset of Fig. 5 (a zoom of the main figure which would correspond to a typical run for a larger system) we find that the datas are perfectly fitted by \( R^2(\beta)/(2N) = 0.41\beta + 1.24(1 - e^{-\beta/3.4}) \) (a usual form) leading to the much smaller (and incorrect) \( \rho_S \approx 0.41 \). Hence, we find that it is very important for practical calculations to check both the convergence of the energy, and the dependence of \( \rho_S \) on the GWF very carefully. A poor choice of the GWF will lead to a slow convergence of the energy (see later in this section) and to incorrect measure of the superfluid density.

V. ON THE PRESENCE OF A SUPERSOLID PHASE

Once the presence of a first order transition has been established, a natural question is whether the superfluid fraction vanishes right at the transition or if there is a region where both the superfluid fraction and the order parameter \( G \) are non zero simultaneously. Such a region would be a supersolid phase and has been searched for for many years. However, to our knowledge, the only model for which it has actually been found are bosons on a lattice\(^{2,27,28,29}\) at large filling factors (i.e. systems similar to our but in the limit \( \nu \approx 1 \) not \( \nu \ll 1 \)) where the crystal is somehow stabilized by the underlying grid. When the crystal is uniquely due to the repulsive interaction (as in Helium 4 or in the system considered here), no convincing evidence could be gathered so far.

There are two alternative way to probe the superfluid character of the system. The direct way consists in calculating directly the superfluid fraction \( \rho_S \) of the system. It is defined as the fraction of the bosons that does not follow when the frame is put (adiabatically) into motion (rotation). It is the bosonic equivalent of the curvature of the energy with respect to an Aharonov flux for electrons. For quantum Monte-Carlo calculations, it is can be conveniently calculated using the diffusive motion of the center of mass of the system (in imaginary time) as

\[ \rho_S = \lim_{\beta \to 1} \frac{R^2(\beta)}{\beta} \]
A second way to find a supersolid is through non diagonal long range order in the one body density matrix

\[ g_1(r', r) = \frac{L_x L_y}{N} \langle c_{r'}^\dagger c_r \rangle. \]

By definition, its largest eigenvalue gives the condensate fraction \( n_0 \). For homogeneous systems it leads to \( n_0 = (1/L_x L_y) \sum_r g_1(r + h, h) \). Alternatively, \( n_0 \) is also given by the long-range asymptotic \( |r - r'| \to +\infty \) of \( g_1(r', r) \) and the two definitions coincide in the thermodynamical limit. In our case, we reduce significantly finite size effects by excluding the short range part of \( g_1 \) with an arbitrary length \( r_0 \),

\[ n_0 = \frac{1}{V_{r_0}} \sum_{|r| > r_0} g_1(h + r, h), \]

where \( V_{r_0} \) is the system volume excluding a disk of radius \( r_0 \). In contrast to density-density correlations, GFMC only provides access to mixed estimators for the condensate fraction since \( g_1(r', r) \) is a non-local quantity. Results then depend on the quality of the guiding wavefunction compared to the exact wavefunction. For small \( r_s \), interactions are weak and our variational Bijl-Jastrow form is quite a good approximation. In that case, the bias due to mixed estimators can be further reduced by computing \( 2n_0^{\text{MX}} - n_0^{\text{VMC}} \) where \( n_0^{\text{VMC}} \) is the variational Monte Carlo result using the same guiding wavefunction. The situation is rather different close to the quantum melting point since the Bijl-Jastrow does not describe the strong correlations between particles. For this case, the mixed estimator for \( g_1 \) leads to results that can not be trusted. To illustrate this point, we plot the condensate fraction for \( r_s = 27 \) and \( N = 50 \) particles and for different values of \( \alpha \) in Fig. 6.

![FIG. 5: (color online). Diffusion of the center of mass \( R^2(\beta) \) for \( N = 8 \) particles in \( 16 \times 28 \) sites at \( r_s = 200 \) using \( 10^6 \) walkers. The various lines correspond to \( \alpha = 0 \) (straight), \( \alpha = 0.2 \) (dotted) and \( \alpha = 0.5 \) (dashed). The thin red (blue dashed) lines are fit \( y = 0.82 \beta \) (\( y = 0.41 \beta + 1.24(1 - e^{-\beta/3.4}) \)) corresponding to a superfluid fraction of 0.82 and 0.41 respectively. Inset: zoom of the main figure.](image)

![FIG. 6: Condensate fraction \( n_0 \) as a function of the variational parameter \( \alpha \), see Eq. \ref{eq:alpha}. The three lines correspond to a VMC calculation with \( n_0^{\text{VMC}} \), a GFMC calculation which gives a mixed estimator \( n_0^{\text{MX}} \) and an extrapolated result \( 2n_0^{\text{MX}} - n_0^{\text{VMC}} \). This last quantity is reduced by a factor 3 between \( \alpha = 0.5 \) and \( \alpha = 0.8 \).](image)
of $\kappa$ shown in Fig. 7 reveals two things: (i) The broken symmetry GWF ($\alpha = 0.5$) actually gets better than the BEC ($\alpha = 0$) around the transition point $r_s = 27$. (ii) However, in the broken symmetry phase, $\kappa$ still increases with $r_s$, indicating that we describe poorly the crystal close to the transition.

VI. DISCUSSION

We conclude this paper by discussing how the above results would apply to actual experiments using ultracold dipolar molecular systems. The system we have in mind could be for instance, RbCs molecules confined by a two-dimensional trap and where electric dipole moments are induced by a perpendicular electric field. Those types of systems typically have three different experimental limitations that constrain the range of parameters ($r_s$) than could actually be observed in practice. (i) First, the dipolar forces that can be induced is limited to $C_{dd} = \gamma (\varepsilon a_0)^2 / (4\pi \varepsilon_0)$ ($\varepsilon$ dielectric constant, $a_0$ Bohr radius) with $\gamma \leq \gamma_{\text{exp}}$ (typically $\gamma_{\text{exp}} \approx 0.25$ for RbCs). (ii) The maximum density is also limited and $\ell \geq \ell_{\text{exp}}$ with a typical value of $\ell_{\text{exp}} \approx 60\mu m$. It means that $r_s$ is limited by $r_s \leq (\ell_{\text{exp}} / \ell_{\text{exp}})$. Noting $\ell_{\text{exp}} = \gamma \ell_0$, we get $r_s \leq \gamma (\ell_0 / \ell_{\text{exp}})$ where $\ell_0 = M_0(a_0)^2 / (\hbar^2 4\pi \varepsilon_0) \approx 20\mu m$ for RbCs. (iii) The temperature is limited to $T_{\text{exp}}$, the order of $T_{\text{exp}} \approx 100 nK$. In order to observe the physics discussed here $T_{\text{exp}}$ should be a fraction $\epsilon$ (say $\epsilon \approx 1\%$) of $T_B$. This imposes, $r_s \geq (T_{\text{exp}} / T_0)^{1/3} \gamma^{2/3}$ with $kT_0 = (\varepsilon a_0)^2 / (8\pi \varepsilon_0 \ell_0^3)$. For RbCs, $T_0 \approx 1.45 nK$. It is an experimental challenge to actually produce ultracold heteronuclear molecules in their vibrational and rotational ground state. However we stress here that, once these molecules are produced, the quantum melting transition itself should be within reach. Putting these three above conditions together, we find the allowed window of parameters shown in Fig. 8.

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APPENDIX A: EWALD SUMMATION

Finite size effects can be reduced by adding periodic images to the original simulation box forming a lattice pattern with rectangular boxes of size $L_x \times L_y$. Each atom in the original box has images in all other boxes. The simple $1/r^3$ dipole interaction between atoms is thus replaced by an effective interaction taking all images into account, or

$$V(r - r') = \sum_{\mathbf{R}_M} \frac{1}{\mathbf{R}_M \cdot (r - r' + \mathbf{R}_M)^3}$$

(A1)

where $\mathbf{R}_M = (nL_x, mL_y)$ denote all vectors of a rectangular lattice. Since the summation has a poor convergence, we extend the well-known Ewald summation trick to this problem. The $y$-integral in the identity

$$\frac{1}{|r|^3} = \frac{4}{\sqrt{\pi}} \int_0^{+\infty} dy y^2 e^{-y^2 |r|^2}$$

(A2)

is splitted in two parts $\int_0^{+\infty} = \int_0^{y_0} + \int_{y_0}^{+\infty}$ and $V(r)$ is splitted correspondingly $V(r) = V^<(r) + V^>(r)$. $y_0$ is...
a parameter that can be chosen arbitrarily. The second part for $y > y_0$ converges exponentially fast when the summation over positions is performed. One finds

$$V^>(\mathbf{r}) = \sum_{\mathbf{R}_M}^{y_0^3} \varphi_{1/2}(y_0 | \mathbf{r} + \mathbf{R}_M|).$$

We have introduced the set of functions

$$\varphi_n(x) = \frac{2}{\sqrt{\pi}} \int_1^{\infty} dt \, t^n e^{-tx^2},$$

which can be expressed as rational functions of Erf($x$), $e^{-x^2}$ and powers of $x$. For the case $y < y_0$, we define the function $F(\mathbf{r}, y) = \sum_{\mathbf{R}_M} e^{-y^2 |\mathbf{r} + \mathbf{R}_M|^2}$ periodic over the rectangular lattice for fixed $x$. Thus we write $F(\mathbf{r}, y)$ as a summation over its Fourier components on the reciprocal lattice

$$F(\mathbf{r}, y) = \sum_{\mathbf{K}_M} e^{i\mathbf{K}_M \cdot \mathbf{r}} \frac{\pi}{L_x L_y} \frac{e^{-K^2 y^2}}{y^2},$$

with reciprocal lattice vectors $\mathbf{K}_M = (2\pi n / L_x, 2\pi m / L_y)$, and the relation

$$V^<(\mathbf{r}) = \frac{4}{\sqrt{\pi}} \int_0^{y_0} dy \, y^2 F(\mathbf{r}, y),$$

yields again an exponentially fast converging expression for $V^<(\mathbf{r})$. After some straightforward calculations and using definition (A3) for functions $\varphi_n(x)$ we finally arrive at

$$V(\mathbf{r}) = \sum_{\mathbf{R}_M}^{y_0^3} \varphi_{1/2}(y_0 | \mathbf{r} + \mathbf{R}_M|)$$

$$+ \frac{\pi y_0}{L_x L_y} \sum_{\mathbf{K}_M} \cos(\mathbf{K}_M \cdot \mathbf{r}) \varphi_{-3/2} \left( \frac{|\mathbf{K}_M|}{2 y_0} \right),$$

(A4)

the effective interaction between atoms in the simulation box. Moreover, subtracting $1/|r|^3$ from the right-hand-side of Eq. (A4) and letting $r \to 0$ leads to the constant $\lambda$ in Eq. (5).

$$\lambda = -\frac{4}{3\sqrt{\pi}} y_0^3 + \frac{\pi y_0}{L_x L_y} \sum_{\mathbf{K}_M \neq 0} \varphi_{1/2}(y_0 | \mathbf{R}_M|)$$

$$+ \frac{\pi y_0}{L_x L_y} \sum_{\mathbf{K}_M} \varphi_{-3/2} \left( \frac{|\mathbf{K}_M|}{2 y_0} \right),$$

which accounts for the self-interaction between each atom and its own images.

The same procedure can be applied to calculate efficiently the kernel (11) describing phonons for the crystal phase. Again we start with Eq. (A2), split the $y$-integral and $\Phi = \Phi^++\Phi^-$ accordingly. The second part converges very rapidly when the summation over the positions $\mathbf{R}_j$ of the triangular lattice is performed, one finds

$$\tilde{\Phi}_{\alpha,\beta}^> = \frac{1}{\delta} \sum_j \frac{2 R_{\alpha,j} R_{\beta,j}}{b^2} \varphi_{3/2} \left( \frac{|R_j|}{b} \right)$$

$$-\delta_{\alpha,\beta} \varphi_{3/2} \left( \frac{|\mathbf{R}_j|}{b} \right) \left(1 - \cos(\mathbf{q} \cdot \mathbf{R}_j)\right),$$

with functions (A3). For convenience, we choose $y_0 = 1/b$ where $b = \sqrt{2/\sqrt{3}}$ is the triangular lattice spacing. The first part is computed more efficiently by going to Fourier space in a similar way as above. The final result reads

$$\tilde{\Phi}_{\alpha,\beta}^< = \frac{\pi^3}{2\sqrt{3}} \sum_j \left( b(G_j + \mathbf{q})_\alpha b(G_j + \mathbf{q})_\beta \times \right.$$

$$\left. \varphi_{-3/2} \left( \frac{|b| G_j + \mathbf{q}_j|}{2} \right) - b G_{\alpha,j} b G_{\beta,j} \varphi_{-3/2} \left( \frac{|b| G_j}{2} \right) \right),$$

where the summation is carried out over all vectors $G_j$ on the hexagonal reciprocal lattice with an exponentially fast convergence.

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