Two-dimensional Bose-Holstein model for hard-core-bosons – a quantum Monte Carlo study

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We study a two-dimensional system of hard-core-bosons coupled to optical phonons and obtain the ground state phase diagram. The effective Hamiltonian comprises of a nearest-neighbor hopping as well as a next-nearest-neighbor hopping whose relative strengths can be tuned by the electron phonon coupling; additionally, there is also a large nearest-neighbor repulsion which can produce a charge-density-wave. When the transport has a sizeable (negligible) contribution from next-nearest-neighbor hopping, we get a supersolid (phase separated state of a superfluid and a charge-density-wave). We use quantum Monte Carlo simulation with stochastic-series-expansion technique to investigate the nature of coexistence of the charge-density-wave and superfluid. Our calculation reveals appearance of supersolidity in the system at non-half fillings and for intermediate electron-phonon coupling strengths.

I. INTRODUCTION

Competition or coexistence of diagonal long range orders [such as charge-density-wave (CDW), spin-density-wave (SDW), and orbital-density-wave (ODW)] and off-diagonal long range orders [such as superconducting and superfluid (SF) states] in correlated electronic systems is a subject of immense current interest. Coexistence of CDW and superconductivity/superfluidity has been studied in three-dimensional systems [12] (such as helium-4 and BaBiO₃ doped with K or Pb), in quasi-two-dimensional systems [2] (such as the dichalcogenide 2H-TaSe₂ and NbSe₂), and in quasi-one-dimensional systems [4,5] (such as the trichalcogenide NbSe₃ and doped spin ladder Sr₁₄Cu₂₀(O,1)₂).

Hard-core-bosons (HCB) have been studied by the condensed matter community for a number of decades. A lattice model for quantum liquids, such as the interacting bosonic helium-4 at low temperatures, needs a hard-core constraint to account for the exclusion of occupation of more than one atom at each lattice point [6,2]. The behavior of the ground state and low temperature excitations of such systems are largely controlled by the electron-phonon interactions. Furthermore, local Cooper pairs [comprising of two electrons (of opposite spin) at a site] can also be regarded as HCBs. In Bismuthates, such HCB couple to the breathing mode of the oxygen cage surrounding the Bismuth ion [8,2].

Here, in this article, we study a two-dimensional (2D) Bose-Holstein (BH) model for HCBs on a square lattice where they can hop to nearest neighbor (NN) sites and experience the electron-phonon interactions via a Holstein-type term. Previously, exact diagonalization calculations were done on this model [14] for a small system (i.e., 4 × 4 lattice) to study the resulting phase diagrams. Here we use stochastic-series-expansion (SSE) based quantum Monte Carlo (QMC) technique to simulate much larger size lattices so that the behavior of the phases in the thermodynamic limit can be understood more clearly. Unlike the t − V model, a supersolid (i.e., homogeneously coexisting phase involving CDW and SF) is realized in the system at intermediate HCB-phonon interaction strengths.

II. FORMULATION

The BH Hamiltonian is given by

\[ H = -t \sum_{j,\delta} b_j^\dagger b_{j+\delta} + \omega_0 \sum_j a_j^\dagger a_j + g \omega_0 \sum_j n_j (a_j + a_j^\dagger) \]

where \( a_i \) and \( b_i \) denote the annihilation operators for phonons and HCB particles, respectively, and \( n_i = (b_i^\dagger b_i) \) is the number operator for HCBs at site \( i \). Furthermore, \( t \) is the hopping amplitude and \( \omega_0 \) is the frequency of optical phonons [10]. The effective Hamiltonian for the BH model is derived by first transforming to the polaronic frame of reference (by using the Lang-Firsov transformation) and then performing perturbation theory as detailed in Refs. [11] and [12]. Interestingly, second-order perturbation theory yields a next-nearest-neighbor (NNN) hopping term besides the usual NN hopping term; moreover, a NN repulsion also results. Finally, we get a term \( t_1 - t_2 - V \) Hamiltonian on a 2D square lattice [11],

\[ H_e = -g^2 \omega_0 \sum_j n_j - t_1 \sum_{j,\delta} b_j^\dagger b_{j+\delta} \frac{V}{2} \sum_{j,\delta,\delta' \neq \delta} b_{j+\delta}^\dagger b_{j+\delta} - \frac{V}{2} \sum_{j,\delta} n_j (1 - n_{j+\delta}), \]

where \( t_1 = t \exp(\frac{-g^2}{t}) \), \( t_2 = (t_1^2/\omega_0) f_1(g) \) and \( V = (t_1^2/\omega_0)[4 f_1(g) + 2 f_2(g)] \) with \( f_1(g) = \sum_{n=0}^{\infty} g^{2n}/(n!n) \) and \( f_2(g) = \sum_{n,m=1}^{\infty} g^{2(n+m)}/[n!m!(n + m)] \). Thus, we have non-frustrated NN and NNN hoppings. Consequently, our QMC simulation will not suffer from the negative sign problem. We employ SSE technique in our QMC simulation and investigate the co-existence or competition of CDW and superfluidity in various regimes of the parameter space. Here we should mention that our \( t_1 - t_2 - V \) model for HCBs is equivalent to an extended XXZ spin-
TABLE I. $J_{1z}$ and $J_{2xy}$ in terms of $J_{1xy}$ [in Eq. (3)] at various values of the HCB-phonon coupling $g$.

| $g$  | $J_{1z}$ | $J_{2xy}$ |
|------|----------|-----------|
| 0.5  | 0.444    | 0.415     |
| 1.0  | 1.355    | 0.970     |
| 1.5  | 2.725    | 0.960     |
| 1.75 | 4.324    | 0.811     |
| 2.0  | 8.017    | 0.647     |
| 2.25 | 17.601   | 0.505     |
| 2.5  | 45.485   | 0.395     |
| 2.75 | 137.088  | 0.314     |
| 3.0  | 478.571  | 0.255     |

$1/2$ Hamiltonian as shown below:

$$H = \sum_{<i,j>}[J_{1z}S^z_i S^z_j + \frac{J_{1xy}}{2}(S^z_i S^-_j + \text{H.c.})] + \frac{J_{2xy}}{2}\sum_{<<i,j>>}(S^+_i S^-_j + \text{H.c.}) + \frac{J_{3xy}}{2}\sum_{<<<<i,j>>>>}(S^+_i S^-_j + \text{H.c.}) - h_0 \sum_i S^z_i,$$

where $<i,j>,<<i,j>>$, and $<<<<i,j>>>>$ stand for NN pair, NNN pair, and next-next-nearest neighbor (NNNN) pair, respectively. Furthermore, the operators for the HCBs are related to those of spin-1/2 particles as: $S^z_j = n_j - \frac{1}{2}$ and $S^+_j = \vec{b}^\dagger_j$. A comparison of the parameters in Eqs. 2 and 3 yields: $J_{1z} = V$, $J_{1xy} = -2t_1$, $J_{2xy} = -4t_2$, $J_{3xy} = -2t_2$ and $h_0 = g^2 \omega_0$.

Presence of hopping terms for HCBs indicates that superfluidity [i.e., spontaneous breaking of the global U(1) gauge symmetry] can exist. On the other hand, a large interaction strength suggests the possibility of a CDW. Thus, our objective is to study the compatibility of these two long range orders. Now, these two orders can coexist either in a phase separated (PS) form or homogeneously as a supersolid (SS). It should pointed out that, a $t - V$ model on a square lattice does not show a thermodynamically stable SS phase for HCBs. On the other hand, striped SS behavior is found away from half filling when NNN repulsion ($V_2$) is considered in the $t - V_1 - V_2$ model.

III. NUMERICAL COMPUTATION USING SSE-QMC

We will now give details of the SSE-QMC simulation of our $t_1 - t_2 - V$ model, or equivalently, our extended XXZ spin-1/2 model. Finding the phase diagram in the present problem requires exploring various limits (including high anisotropy in our spin model) of the parameters. In our numerical computations we used directed loop update for efficient sampling of the configurations. The ground state properties are captured by simulating at low enough temperature, i.e., $\beta \sim L$ with $L$ being the linear dimension of the square lattice. We employ $\beta = 3L/2$ since our calculations with $\beta = 2L$ yield the same values for the observables (within the error bars of calculations). From calculations involving various large system sizes, we infer the results in the thermodynamic limit.

As can be seen from the expressions of the two-spin matrix elements for Heisenberg spin models used in various SSE-QMC studies, a positive parameter $\epsilon$ is introduced to ensure the positivity of all the matrix elements (see Appendix A for details). This is necessary so that they can be treated as probabilities. The value of $\epsilon$ can also affect the autocorrelation time of the numerical data. We found that, keeping the numerical value of $\epsilon$ equal to at least a quarter of the anisotropy parameter $J_{1z}/J_{1xy}$, particularly near the transition region, helps keep the data in various bins uncorrelated (see Ref. 13 for value of $\epsilon$ used in the XXZ model).

In this work we are concerned with the diagonal order parameter $S(\pi, \pi)$ [i.e., the structure factor at the Neel ordering vector $\vec{Q} = (\pi, \pi)$] and the off-diagonal order parameter of the superfluid density $\rho_S$. A general expression for $S(\vec{Q})$ is given as

$$S(\vec{Q}) = \frac{1}{N} \sum_{i,j} e^{i\vec{Q} \cdot (\vec{R}_i - \vec{R}_j)} (n_i n_j - n_i < n_j),$$

where $<>$ denotes the ensemble average. Since $n_i$ (or $S_z$ in our spin model) are diagonal in the basis, a QMC average can be computed easily.

The SF density is given by $\rho_S = 1/N (\partial^2 F/\partial \theta^2)$, where $F$ is the free energy in the presence of twisted boundary conditions with angle of twist $\theta$. In a QMC calculation, the SF density along $x$-direction is calculated using $\rho_{Sx} = <(N^+_x - N^-_x)^2>/\beta N$ where $N^+_x$ and $N^-_x$ represent the total no. of Hamiltonian operators transporting spin in the positive and negative $x$-directions, respectively.

We first discuss benchmarking of our QMC calculations by comparing our calculated values (using SSE) with those obtained by exact-diagonalization (ED) methods. We consider both the XXZ model and its simple extension, namely, the $J_1 - J_2$ model. We find that the energy, magnetization, structure factor $S(\pi, \pi)$ and SF density $\rho_S$ of our SSE calculations match quite well with those from the ED results. For obtaining the ED data, we use LAPACK and also various results from the literature. The comparisons of the calculated $S(\pi, \pi)$ and $\rho_S$ for the $J_1 - J_2$ model are shown in Fig. 4.

Our SSE results also compare well with various world-line Monte Carlo results as also the SSE QMC results available in the literature.
IV. ANALYSIS OF THE RESULTS AND TECHNICALITIES

Our calculations for the 2D $t_1 - t_2 - V$ model (obtained from the BH Hamiltonian) aim at obtaining the ground state phase diagram of the system and also at extending (to the thermodynamic limit) the findings presented by a Lanczos study on a small cluster in Ref. [11].

To obtain the phase diagram for our system, the interplay between the diagonal and off-diagonal orders and the transition between them needs thorough investigation. As antiferromagnetic order breaks SU(2) symmetry whereas a SF phase breaks U(1) symmetry, a phase transition between them (according to Landau theory) cannot be of second-order type. Furthermore, a transition to a phase separated state occurs when the system undergoes a first-order transition.

We work in the grand canonical ensemble where there is no constraint on the HCB particle number (or the magnetization in the equivalent extended XXZ model). In Fig. 2 we show the variation of $m_z$, $S(\pi, \pi)$, and $\rho_S$ with magnetic field $h$ (expressed in units of $J_{1xy}$) for $g=1.75$ for both our extended model and its XXZ version (i.e., $J_2 = 0$) in $L \times L$ square lattices with $L = 10$, 14 and 16. The comparison shows that the results for different size lattices almost coincide. At small values of the magnetic field, the system manifests half-filling in the case of HCBs (or zero magnetization in the case of the equivalent spin model); the CDW phase is formed with maximum values of $S(\pi, \pi)$ with SF density simultaneously assuming zero value. At large values of the magnetic field, before the system is at complete filling, $S(\pi, \pi)$ decreases to zero while $\rho_S$ becomes finite manifesting the SF phase. In the intermediate magnetic field region, phase transition occurs with both the orders coexisting in our extended XXZ model. The plot of magnetization in Fig. 2(b), indicates a discrete jump during the transition in the case of the XXZ model (i.e., for $J_2 = 0$). This is a typical signature for a first-order transition. Contrastingly, a continuous smooth increase in $m_z$ is observed for the extended XXZ model clearly ruling out the possibility of a phase sepa-
ration. Calculations using a canonical ensemble shows an inhomogeneous phase coexistence due to phase separation (PS)\(^\ddagger\). In the region adjacent to \(m_z = 0\) in Fig. 2(a), where overlap of \(S(\pi, \pi)\) and \(\rho_S\) are observed, the system displays a SS phase. Analysis of various large system sizes confirms the picture in Fig. 2(a) that there is indeed a homogeneous coexistence of CDW and SF long-range orders in the system.

Next, we will do a further detailed case-by-case study for the system with and without the effects of the NNN hoppings.

### A. Only NN hopping present \((t_2 = 0)\)

Here we study the case of \(t_2 = 0\) in Eq. \(2\), i.e., the bare XXZ model. Calculations are done on a \(16 \times 16\) lattice. We find that the system loses its CDW order at half-filling for values of the coupling \(g\) below the critical value of \(g_c = 0.82\) corresponding to the Heisenberg point of the XXZ model. For smaller values of \(g\), superfluidity develops for all values of filling between 0 and 1. The phase diagram for the XXZ model is depicted in Fig. 3. Our calculated phase diagram of the XXZ model is compatible with Fig. 1, Fig. 2a and Fig. 2b of Ref. 27. At half filling (i.e., \(m_z = 0\)), the Heisenberg point denotes the boundary between CDW and SF phases.

Fig. 4(a) shows the jumps in magnetization \(m_z\) as soon as we increase \(g\) beyond \(g_c\). The magnitude of the jump increases as the coupling \(g\) increases. This jump implies a first-order transition and indicates a phase separated coexistence of the CDW and SF phases. A histogram analysis can also capture the jump in \(m_z\) values. In Fig. 4(b), plotted for \(g = 1.50\), the \(m_z\) histograms change when magnetic field values are varied. For instance, when the magnetic field is set at \(h = 4.44\), \(m_z = 0\) even when large number of Monte Carlo sweeps were used in our QMC computation. On increasing the magnetic field to \(h = 4.46\), the \(m_z\) values start showing a double-peaked structure (with one peak at \(m_z = 0\) and another peak at \(m_z \approx 0.18\)) which is indicative of phase separation (see also inset in Fig. 4b). Then, at a slightly higher magnetic field of \(h = 4.48\), all the \(m_z\) values seem to be centered around a mean value close to 0.18. This manifests the first-order transition. All the discontinuous transitions are due to inhomogeneous coexistence of the CDW and SF phases.

### B. Including NNN hopping \((t_2 \neq 0)\)

The phase diagram for our BH model [obtained from Eq. 2] is depicted in Fig. 5. On including the effects of NNN hopping (i.e., \(t_2 \neq 0\)) in the \(t_1 - t_2 - V\) model of Eq. 2, there can be a difference in the densities in the two sublattices owing to NN repulsion and NNN hopping. As shown in Table. 1 at intermediate values of \(g\) (i.e., \(g \sim 1\)), NNN hopping is comparable to NN hopping; consequently, a SS state can occur. Whereas at larger values of \(g\) (i.e., for \(g > 2.5\)), NNN hopping is fairly smaller than NN hopping and we can expect the same behavior as in the \(t - V\) (or the XXZ) model. On account of particle-hole symmetry in our model, the phase diagram is symmetric about half-filling.

We will now examine various features of the phase diagram of Fig. 4. The phase diagram for our model was obtained by identifying the transition regions and the nature of the various phases. The variation of magnetization with magnetic field in a \(16 \times 16\) lattice is shown in Fig. 6 in the transition region. The results for \(g = 1.5, 1.75, \& 2.0\) magnetization increases gradually without any jump as the magnetic field is increased. Hence, in Fig. 6 for \(g = 1.75 \& 2.0\) CDW and SF phases coexist homogeneously resulting in a SS state. Here we must mention that Fig. 2a) (depicting simultaneous coexistence of CDW and SF phases through non-zero values of \(S(\pi, \pi)\) and \(\rho_S\)) corroborates this conclusion.

Large anisotropy [i.e., large values of \(V/t_1\) in Eq. 2]
in the model requires large simulation time. Thus, as we increase the value of $g$ (thereby increasing the value of $V$), the numerical calculation suffers from appreciable slowing down and with our computational constraints we cannot study for large values of $g$ (i.e., $g \gtrsim 2.25$). Here we would like to add that, as $g$ increases, the value of $J_{1z}/J_{1xy}$ increases rapidly (see table I). SSE calculations are presumably good when $J_{1z}/J_{1xy} \sim 12.21$. Given these constraints, we also observe that we can set a cut-off for the anisotropy parameter $\Delta = J_{1z}/J_{1xy}$ above which the essential physics for the system does not change much. More precisely, we find that we can deal with large values of $g$ (i.e., $g \geq 2.1$) by setting $J_{1z}/J_{1xy} = \Delta_0 = 10$ and still get the correct behavior of the observables thereby saving computational time. Fig. 7 shows $S(\pi, \pi)$ against $m_z$ and $m_z$ versus $h$ for $g = 2.15$ where results using actual value of $\Delta = \Delta_0 = 12.595$ are compared with those using the cut-off value $\Delta = \Delta_0$. The good agreement between the two cases justifies our argument for using $\Delta = \Delta_0$ at large values of $g$. Changing $\Delta$ from $\Delta_0$ produces only a shift in the magnetization (or density) curve while retaining the same shape as can be seen from the $m_z$ plots in Fig. 7(b).

With the above simplification, we do the SSE-QMC simulation for larger values of $g$ (such as $g \geq 2.25$) and observe phase separated phases; we explain this based on Fig. 8 plotted at $g = 2.5$. At values of magnetic field $h \leq 18.9$, a single peaked structure occurs. On increasing $h$, at $h = 18.97$, a double-peaked structure results showing simultaneous existence of two phases (with magnetizations centered at $m_z \approx .12$ and $m_z \approx .25$). A further small increase to $h = 19.07$, leads to again a single peak (centered around $m_z \approx 0.26$) signalling that a discontinuous phase transition has occurred. Thus a phase separated state at $g = 2.5$ is clearly captured in

![Image](image1.png)

**FIG. 7.** Results of (a) structure factor vs magnetization and (b) $m_z$ vs $h$ for a $16 \times 16$ lattice and for $g = 2.15$ when the actual $\Delta$ and $\Delta = \Delta_0 = 10$ are considered.

![Image](image2.png)

**FIG. 9.** Magnetization vs magnetic field in a $16 \times 16$ lattice for large values of $g$.

![Image](image3.png)

**FIG. 8.** Magnetization $m_z$ histograms in the transition region showing phase separation through a double-peaked structure at $h = 18.97$ for $g = 2.5$.
with $i$ and $t$ being Monte Carlo times defined in units of Monte Carlo sweeps (MCS). We thus use a large bin size (15,000,000 MCS) in our simulations and also an appropriately large $\epsilon$ to keep the autocorrelation time to stay well within the bin size. The values of the autocorrelation times, for $g = 2.5$ and at various fields $h$ close to the transition, are shown in Table II.

Lastly, we mention that our phase diagrams, both for the XXZ model and our extension of it, are similar (though not identical) to what were obtained earlier using modified Lanczos method in Ref. [11].

V. SUMMARY

We have studied the effective Hamiltonian of a Bose-Holstein model using the SSE-QMC technique and obtained the phase diagram. We find that supersolidity is realized at intermediate couplings; whereas, at large couplings the system phase separates because NNN hopping is not dominant. Our results on a large $16 \times 16$ lattice are similar to those obtained earlier using modified Lanczos technique on a $4 \times 4$ cluster[11]. We overcame computational difficulties for large repulsive interactions by devising a cutoff repulsive strength. Lastly, we say that our work is an exercise in SSE-QMC study on a simple but important model which can be realized in a cold atom system.

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Appendix A

In SSE-QMC study of Heisenberg spin systems, the Hamiltonian is written as a bond Hamiltonian. Particularly, in our case we write $H = -\sum_{i=1}^{N} \sum_{b} h_{b} b_{i} b_{j}$ where $b_{1}, b_{2}, \& b_{3}$ denote the NN, NNN, and NNNN bonds in our spin model, respectively. Each of such $H_{b_{i}}$ consists of the diagonal ($H_{1,b_{i}}$) and the off-diagonal ($H_{2,b_{i}}$) parts and is given as $H_{b_{i}} = H_{1,b_{i}} + H_{2,b_{i}}$ with expressions

$$H_{1,b_{i}} = C - J_{ix} S_{i}^{z} S_{j}^{z} + h_{b_{i}} [S_{i}^{+} S_{j}^{-} + S_{j}^{+} S_{i}^{-}]$$

$$H_{2,b_{i}} = -J_{xy} S_{i}^{+} S_{j}^{-} + H.c.,$$

where $C = J_{ix}/4 + h_{b_{i}} + \epsilon, \epsilon \geq 0$, and $h_{b_{i}} = h/z$ with the coordination number $z = 12$. In our model, a two-spin matrix element of any of these operators can never become negative.

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