Simultaneous Diagonal and Off Diagonal Order in the Bose–Hubbard Hamiltonian

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Abstract

The Bose-Hubbard model exhibits a rich phase diagram consisting both of insulating regimes where diagonal long range (solid) order dominates as well as conducting regimes where off diagonal long range order (superfluidity) is present. In this paper we describe the results of Quantum Monte Carlo calculations of the phase diagram, both for the hard and soft core cases, with a particular focus on the possibility of simultaneous superfluid and solid order. We also discuss the appearance of phase separation in the model. The simulations are compared with analytic calculations of the phase diagram and spin wave dispersion.
I. INTRODUCTION

A lot of attention has been focussed on the interacting electron problem in the last several decades, whereas the interacting boson problem has been considered more often in the framework of specific applications only. However, there are a number of important situations where the elementary excitations are either intrinsically bosonic in character or else can usefully be viewed in terms of bosonic models. $^4\text{He}$ is an example of the former situation, [1] while quantum spin systems, [2] granular superconductors, [3] and flux lines in type–II superconductors [4] are examples of the latter. Therefore it is important to understand in detail the features of model boson systems, in much the same way that one studies the Hubbard, Anderson, and t-J Hamiltonians for correlated fermions. In this paper we consider a lattice model of interacting bosons, the Bose Hubbard (BH) Hamiltonian:

$$H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i n_i + V_0 \sum_i n_i^2 + V_1 \sum_{\langle ij \rangle} n_i n_j + V_2 \sum_{\langle \langle ik \rangle \rangle} n_i n_k.$$ (1)

Here $a_i$ is a boson annihilation operator at site $i$, and $n_i = a_i^\dagger a_i$. The transfer integral $t = 1$ sets the scale of the energy, and $\mu$ is the chemical potential. $V_0, V_1$, and $V_2$ are on–site, near–neighbor, and next–near–neighbor boson–boson repulsions.

The interactions $V_0, V_1,$ and $V_2$ promote the formation of “solid” order, where the boson occupations fall into regular patterns, at special densities commensurate with the lattice. The hopping matrix element $t$ favors mobile bosons, and consequently a superfluid phase at $T = 0$. In what follows the nature of the correlation functions will be studied as we change the Hamiltonian parameters and the density $\rho = \frac{1}{N} \sum_i \langle n_i \rangle$.

When $V_0 = \infty$, the BH model maps onto the quantum spin–1/2 Hamiltonian

$$H = -t \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_j^+ S_i^-) + V_1 \sum_{\langle ij \rangle} S_i^z S_j^z + V_2 \sum_{\langle \langle ik \rangle \rangle} S_i^z S_k^z - H_z \sum_i S_i^z.$$ (2)

The field $H_z = \mu - 2V_1 - 2V_2$. Since $n_i \leftrightarrow S_i^z + \frac{1}{2}$, ordering of the density corresponds to finite wave vector Ising type order. Similarly, $a_i \leftrightarrow S_i^-$ so that superfluidity maps to ferromagnetic ordering in the XY plane. One of the things we shall be interested in in this
work is the possibility that density and superfluid order are not mutually exclusive. Indeed, at \( V_2 = H_z = 0 \), the special point \( V_1 = 2t \) corresponds to the Heisenberg Hamiltonian where Ising and XY order coexist. It has been suggested by various authors [5,6] that the addition of further terms like \( V_2 \) or \( H_z \) could stabilize this “supersolid” from a special symmetry point to a broader area of the phase diagram. Precisely at the Heisenberg antiferromagnet (AF), the effect of a field \( H_z \) is known: It breaks the full rotational symmetry and selects ordering in the XY plane since the spins can more easily take advantage of the field energy. This argument has been used to suggest why doping favors the superconducting over the CDW state in the negative–\( U \) Hubbard model [7] where an analogous “supersolid” symmetry exists at half–filling.

While there have been many mean field (MF) studies of the spin Hamiltonian Eq. 2, there have been to date only a few numerical studies [8–10]. Monte Carlo studies of interacting quantum boson and spin models provide a useful, exact method to study the nature of the correlations on finite lattices. Combined with finite size scaling methods, they can be used to extract information concerning the thermodynamic limit. Boson simulations are somewhat easier than related path integral methods for interacting electron systems, since they can utilize algorithms which scale linearly with the lattice size and can reach essentially arbitrarily low temperatures.

This paper is organized as follows: In Section II and III we determine analytically the MF phase diagram, extending past work by considering additional types of order, and describe spin wave calculations of the dispersion relations in the various phases. In Section IV we provide numerical results for the soft core model, extending our earlier studies [10]. In Section V we describe new results for the hard-core phase diagram. Conclusions are presented in Section VI.
II. MEAN FIELD PHASE DIAGRAM

Previous work established the MF phase diagram of the spin Hamiltonian considering only the possibility of superfluidity and Néel–type ordering of the density. At half–filling, or equivalently at zero magnetization $M_z = 0$, for $V_1 > 2$ and $0 < V_2 < V_1 - 2$ the spins form a Néel state, corresponding to a checkerboard Bose solid with an ordering vector $k_s = (\pi, \pi)$. For $V_2 > \max (V_1 - 2; 0)$ a ferromagnetic phase is formed, with a net moment $M_{xy} \neq 0$ and $M_z \neq 0$. This phase corresponds to a superfluid, and is also stable for arbitrary $V_1$ and $V_2$ away from half–filling. A fully polarized magnetic phase in a strong magnetic field $H_z$, where only $M_z \neq 0$, corresponds to a Mott–insulator with precisely one boson per site. As the solid and the superfluid phases possess different broken symmetries, one could expect that the transition between them is first order. However, a rather different scenario has also been put forward, suggesting that the – presumably – first order transition is split up into two distinct second order transitions, where the two order parameters vanish at separate points. In the regime between the two transitions both order parameters are non–zero, hence it has been termed a supersolid. This intriguing possibility is the subject of the investigations reported in this paper.

The mean field analysis indeed finds such a supersolid phase, although in the hard core limit longer range forces ($V_2 > 0$) are needed to stabilize it. However, recently it was claimed that this conclusion changes in the soft core case, and a supersolid phase exists with nearest neighbor interaction alone. Finally, recent studies on the related Heisenberg model with competing first and second neighbor couplings $J_1$ and $J_2$ established the possibility of additional phases: a collinear phase, with alternating lines of up and down spins, at large $J_2/J_1$, and a disordered phase at intermediate values of $J_2/J_1$. These differing results clearly call for a reinvestigation of the problem.

The MF phase diagram of the spin Hamiltonian Eq. 2 worked out by Matsuda and Tsuneto, and described above, allowed only for a two–sublattice magnetic ordering of the spins corresponding to a Néel solid. Representing the spins by classical vectors of length...
we extend earlier MF analyses \cite{6,12} for the case of a square lattice to include also the possibility of a collinear phase which is expected to form for intermediate to large next–near–neighbor repulsion $V_2$ (see Fig. 1). Assuming that the spins are ordered in the XZ plane, the MF energies per spin, $e_N$ and $e_C$, of the Néel and collinear spin configurations are given by

$$e_N = -4S^2 \sin \theta_A \sin \theta_B + 2S^2V_1 \cos \theta_A \cos \theta_B + V_2S^2 \left( \cos^2 \theta_A + \cos^2 \theta_B \right) - \frac{H_z}{2} S \left( \cos \theta_A + \cos \theta_B \right)$$

$$e_C = -S^2 \left( \sin \theta_{R1} + \sin \theta_{R2} \right)^2 + \frac{V_1S^2}{2} \left( \cos \theta_{R1} + \cos \theta_{R2} \right)^2 + 2V_2S^2 \cos \theta_{R1} \cos \theta_{R2} - \frac{H_z}{2} S \left( \cos \theta_{R1} + \cos \theta_{R2} \right).$$

$\theta_A$ and $\theta_B$ are the angles between the spin direction and the z–axis on sublattice $A$ and $B$, respectively. $\theta_{R1}$ and $\theta_{R2}$ are the corresponding angles in the collinear phase on even and odd rows. The different phases are identified as follows:

$$\cos \theta_A = \cos \theta_B < 1 \quad \text{or} \quad \cos \theta_{R1} = \cos \theta_{R2} < 1 \quad \text{Superfluid}$$

$$\cos \theta_A = -\cos \theta_B = 1 \quad \text{Néel Solid}$$

$$\cos \theta_{R1} = -\cos \theta_{R2} = 1 \quad \text{Collinear Solid}$$

$$\sin \theta_A \neq \sin \theta_B \quad \text{and} \quad -1 < \cos \theta_A \neq -\cos \theta_B < 1 \quad \text{Néel Supersolid}$$

$$\sin \theta_{R1} \neq \sin \theta_{R2} \quad \text{and} \quad -1 < \cos \theta_{R1} \neq -\cos \theta_{R2} < 1 \quad \text{Collinear Supersolid}$$

$$\cos \theta_A = \cos \theta_B = 1 \quad \text{or} \quad \cos \theta_{R1} = \cos \theta_{R2} = 1 \quad \text{Mott phase}$$

We performed the MF analysis in the same spirit as in Refs. \cite{5,6,11}. One proceeds by minimizing $e_N$ and $e_C$ separately with respect to the angles $\theta_A, \theta_B$ and $\theta_{R1}, \theta_{R2}$, respectively. Then the results for fixed magnetic field $H_z$ are translated to fixed magnetisation, i.e. boson density. Finally, we compare the energies of the different phases to obtain the complete MF phase diagram of the spin Hamiltonian Eq. 2. Explicitly, for two–sublattice Néel type ordering we find the following phases for $V_1 > 2$ and $0 < V_2 < V_1 - 2$:

$m=0$ \quad \text{Solid}
\[ 0 < m < \frac{1}{2} \sqrt{\frac{V_1 - V_2 - 2}{V_1 - V_2 + 2}} \quad \text{Neel Supersolid} \]

\[ \frac{1}{2} \sqrt{\frac{V_1 - V_2 - 2}{V_1 - V_2 + 2}} < m < \frac{1}{2} \quad \text{Superfluid} \]

\[ m = \frac{1}{2} \quad \text{Mott Insulator} \quad (6) \]

where \( m = |\rho - \frac{1}{2}| \) is the magnetisation of the system. For \( 0 < V_1 < 2 \) there is no Néel order and for \( m \neq 0 \) the MF ground state is always superfluid.

Similarly we analyze the phase diagram following from minimizing \( e_C \) for the ordered collinear spin structures corresponding to an ordering wave vector \( \mathbf{k}_c = (0, \pi) \) or \( (\pi, 0) \). At half–filling the collinear solid (see Fig. 1) is realized for arbitrary values of the near–neighbor repulsion \( V_1 \). The reason is that at half–filling the energy for the collinear solid is \( e_C = -V_2/2 \), i.e. independent of \( V_1 \) due to the cancellation of \( S_i^z S_j^z \) energies for near–neighbor sites on the same and neighboring rows. Away from half–filling only the superfluid minimizes \( e_C \) for \( V_2 < 2 \). For \( V_2 > 2 \) a collinear supersolid appears in the phase diagram and the boundary between the superfluid and the collinear supersolid is determined by

\[ 0 < m < \frac{1}{2} \sqrt{\frac{V_2 - 2}{V_2}} \quad \text{Collinear Supersolid} \]

\[ \frac{1}{2} \sqrt{\frac{V_2 - 2}{V_2}} < m < \frac{1}{2} \quad \text{Superfluid} \quad (7) \]

which is again independent of \( V_1 \). For \( V_2 > 2 \) the collinear supersolid phase occurs in a density strip of width \( \sqrt{(V_2 - 2)/V_2} \) around half–filling.

Given the MF solution for \( e_N \) and \( e_C \) separately, a comparison for the energies of the different phases allows to map out the complete mean–field phase diagram of the spin Hamiltonian Eq. 2. E.g. at half–filling, \( m = 0 \), we have to compare

\[ e_C = -\frac{1}{2} V_2 \quad \text{Collinear Solid} \]

\[ e_N = e_C = -1 \quad \text{Superfluid} \]

\[ e_N = \frac{1}{2} (V_2 - V_1) \quad \text{Neel Solid} \quad (8) \]

The resulting phase diagram is shown in Fig. 2. Interestingly, for \( 2 < V_1 < 4 \) increasing \( V_2 \) drives two transitions: first increasing \( V_2 \) frustrates the Néel solid and leads to a transition
to a superfluid. Increasing $V_2$ further stabilizes collinear order and leads to a transition from a superfluid to a collinear solid. [31]

Away from half–filling, $0 < m < 1/2$, no solids, neither Néel nor collinear are MF solutions. Instead, transitions occur between the superfluid, and the Néel and collinear supersolid phases. The boundaries between the different phases are given by

\[
\begin{align*}
V_2 &= V_1 - 2 \frac{1 + 4m^2}{1 - 4m^2} & \text{Superfluid to Neel Supersolid} \\
V_2 &= \frac{2}{1 - 4m^2} & \text{Superfluid to Collinear Supersolid} \\
V_2 &= \frac{1}{2} V_1 - \frac{4m^2}{1 - 4m^2} & \text{Neel to Collinear Supersolid} 
\end{align*}
\] (9)

Finite doping leads to a rigid shift of the phase boundary lines obtained at half–filling with the solid replaced by supersolid phases. For

\[
2 \frac{1 + 4m^2}{1 - 4m^2} < V_1 < 4 \frac{1 + 2m^2}{1 - 4m^2} 
\] (10)

this still allows for two transitions with increasing $V_2$, from a Néel supersolid to a superfluid to a collinear supersolid. The $V_1$–$V_2$ phase diagram for a fixed magnetisation $m = 0.2$ is shown in Fig. 3. In addition, Figs. 4 and 5 show the phase boundaries in the $V_2$, $m$ plane for a fixed value of $V_1$ and in the $V_1$, $m$ plane for a fixed value of $V_2$, respectively.

Recently it was claimed that a finite core repulsion $V_0 < \infty$ qualitatively changes this picture. [16] Supersolids were found to exist even at half–filling, moreover without the next nearest neighbor repulsion $V_2$. To study these claims we extend the MF analysis by introducing an approximate soft core representation allowing the spin length $S$ to be a variational parameter and adding a term $H_{\text{constraint}} = V_0 \sum_i (S_i^2 - 1)^2$ to the Hamiltonian. The minimization of the ground state energy is now done separately with respect to $S_A^A, S_B^A$ and $S_A^z, S_B^z, S_z$.

We expand the ground state energy around the superfluid phase, and consider the eigenvalues corresponding to small spatial modulations of the density and superfluid order parameter, in effect generating a Ginzburg–Landau type expression. The superfluid–collinear supersolid transition is studied by writing
\[ S^A_z = m - \epsilon \quad S^B_z = m + \epsilon \]
\[ S^A_x = s - \delta \quad S^B_x = s + \delta \]  

(11)

and expanding to second order in the (small) fluctuations \( \epsilon \) and \( \delta \). The expectation value \( \epsilon \) of the ground state energy per site takes the form

\[ \epsilon = \epsilon_{SF} - 4V_2\epsilon^2 + V_0 \left[ (12s^2 + 4m^2 - 1)\delta^2 + (12m^2 + 4s^2 - 1)\epsilon^2 + 16s\epsilon \delta \right], \]
\[ \epsilon_{SF} = -8s^2 + 4(V_1 + V_2)m^2 + \frac{1}{8}V_0(4s^2 + 4m^2 - 1). \]  

(12)

The ground state energy is the sum of eigenvalues of a matrix in the \((\epsilon, \delta)\) space. First we solve for \( s \) at fixed number of particles, i.e. fixed \( m \), in the superconducting state where \( \delta = \epsilon = 0 \), and obtain

\[ s^2 = \frac{1}{4} - m^2 + \frac{2}{V_0}. \]  

(13)

A zero eigenvalue of the energy matrix signals the phase transition. The condition for the vanishing of the determinant can be solved for \( V_2 \) for arbitrary \( m \)

\[ V_2 = 2 + \frac{8m^2}{1 - 4m^2 + 12/V_0}, \]  

(14)

which gives the phase boundary between the superfluid and the collinear supersolid. With the same procedure the phase boundary between the superfluid and the Néel supersolid is at

\[ V_2 = V_1 - 2 - 16m^2/[1 - 4m^2 + 16/V_0]. \]  

As in the hard core case the phase diagram displays Néel– and collinear supersolid, and superfluid phases. At half–filling the supersolid phases vanish, and two insulating solids are direct neighbors to the superfluid, in contrast with the result of Ref. \[9\]. This result is independent of \( V_0 \), i.e. it is true both in the soft and hard core limits, in agreement with the above hard core MF calculation.

III. SPIN WAVE ANALYSIS

The analyses of the spin wave fluctuations which exist in the literature \[5,11,13\] are in disagreement. The spectrum has been found to be either linear \[5\] or quadratic \[11,13\] at
the solid–supersolid phase boundary. This dependence is crucial for numerical studies, as it determines the dynamical critical exponent $z$ and thereby the appropriate finite size scaling of the lattice.

To settle the issue, we redo the linear spin wave theory analysis for the spin model of Eq. 2 and determine the spectrum in the superfluid, the Néel solid and the Néel supersolid. Again we assume that the spins are ordered in the XZ plane with an angle $\theta_{A(B)}$ to the $z$–direction. On each sublattice the spin quantisation axis is rotated to align the spins along the local direction of the magnetisation by

$$
S_{i \in A(j \in B)} = \begin{bmatrix}
\cos \theta_{A(B)} & 0 & -\sin \theta_{A(B)} \\
0 & 1 & 0 \\
\sin \theta_{A(B)} & 0 & \cos \theta_{A(B)}
\end{bmatrix} \hat{S}_{i \in A(j \in B)}.
$$

To diagonalize the spin Hamiltonian Eq. 2 in terms of the rotated spins $\hat{S}$ we introduce spin raising and lowering operators $\hat{a}^+$ and $\hat{a}$ on sublattice $A$ by

$$
\begin{align*}
\hat{S}^+_{i \in A} &= \hat{S}^x_{i \in A} + i \hat{S}^y_{i \in A} = \hat{a}^+ \\
\hat{S}^-_{i \in A} &= \hat{S}^x_{i \in A} - i \hat{S}^y_{i \in A} = \hat{a} \\
\hat{S}^z_{i \in A} &= \frac{1}{2} - \hat{a}^+ \hat{a}
\end{align*}
$$

which obey the usual bosonic commutation relations in the large $S$ limit. Similarly, operators $\hat{b}^+$ and $\hat{b}$ are introduced on sublattice $B$. After Fourier transformation this leads, up to a constant energy shift, to the linear spin wave Hamiltonian

$$
H_{SW} = \sum_k \left[ H_{11} \left( \hat{a}^+_k \hat{a}_k + \hat{a}^+_{-k} \hat{a}_{-k} \right) + H_{33} \left( \hat{b}^+_k \hat{b}_k + \hat{b}^+_{-k} \hat{b}_{-k} \right) + H_{21} \left( \hat{a}^+_k \hat{a}_{-k} + \hat{a}_{k} \hat{a}_{-k} \right) + \\
+ H_{34} \left( \hat{b}^+_k \hat{b}^+_{-k} + \hat{b}_k \hat{b}_{-k} \right) + H_{31} \left( \hat{a}^+_k \hat{b}_k + \hat{a}^+_k \hat{b}_{-k} + \hat{a}_{k} \hat{b}^+_k + \hat{a}_{-k} \hat{b}^+_{-k} \right) + \\
+ H_{41} \left( \hat{a}^+_k \hat{b}_{-k} + \hat{a}^+_{-k} \hat{b}_k + \hat{a}_k \hat{b}_k + \hat{a}_{-k} \hat{b}_{-k} \right) \right]
$$

neglecting higher order terms in $\hat{a}$ and $\hat{b}$. Due to the two–sublattice structure the $k$–sum is restricted to half of the Brillouin zone, i.e. to momenta with $\cos(k_x) + \cos(k_y) \geq 0$. In the superfluid and the supersolid phase the $k$–dependent coefficients in Eq. 17 are given by:
\[ H_{11} = 2 \frac{\sin \theta_B}{\sin \theta_A} + H_{21} \quad , \quad H_{33} = 2 \frac{\sin \theta_A}{\sin \theta_B} + H_{34} \]
\[ H_{21} = \frac{1}{2} V_2 \sin^2 \theta_A \gamma_k^{(2)} \quad , \quad H_{34} = \frac{1}{2} V_2 \sin^2 \theta_B \gamma_k^{(2)} \]
\[ H_{31} = \gamma_k^{(1)} \left[ -1 - \cos \theta_A \cos \theta_B + \frac{1}{2} V_1 \sin \theta_A \sin \theta_B \right] \quad , \quad H_{41} = H_{31} + 2 \gamma_k^{(1)} \]  
(18)

where \( \gamma_k^{(1)} = \frac{1}{2} (\cos(kx) + \cos(ky)) \) and \( \gamma_k^{(2)} = \cos(kx) \cos(ky) \). The coefficients of the first order terms are required to vanish \[22\] which leads to the conditions

\[ \frac{H_z}{2} \sin \theta_A = 2 \cos \theta_A \sin \theta_B + V_1 \cos \theta_B \sin \theta_A + V_2 \cos \theta_A \sin \theta_A \]
\[ \frac{H_z}{2} \sin \theta_B = 2 \cos \theta_B \sin \theta_A + V_1 \cos \theta_A \sin \theta_B + V_2 \cos \theta_B \sin \theta_B . \]
(19)

These two equations determine the angles \( \theta_A \) and \( \theta_B \) for a given value of the magnetic field \( H_z \). The solutions of Eqs. 19 determine the phase diagram of the model. These equations fully coincide with the ones obtained by minimizing the free energy in the previous section.

We have already used Eq. 19 to eliminate the magnetic field in the expressions for the coefficients \( H_{11} \) and \( H_{33} \) in Eq. 18 of the spin wave Hamiltonian. However, for the Néel solid and the Mott insulator phase where both \( \sin \theta_A = 0 \) and \( \sin \theta_B = 0 \) the elimination is not possible and instead \( H_{11} \) and \( H_{33} \) are given by

\[ H_{11} = V_1 - V_2 - \frac{1}{2} H_z \quad , \quad H_{33} = V_1 - V_2 + \frac{1}{2} H_z \quad \text{Neel Solid} \]
\[ H_{11} = H_{33} = -V_1 - V_2 + \frac{1}{2} H_z \quad \text{Mott Insulator} \]  
(20)

Eq. 17 is diagonalized by a generalized Bogoliubov transformation using the equation of motion \( i \partial_t \hat{a}_k = [\hat{a}_k, H_{SW}] \) with \( \hat{a}_k \propto e^{-i\omega_k t} \). In the boson language the Bogoliubov transformation involves coupled density and phase modes. As a result we obtain the spin wave dispersion in the form

\[ \omega_\pm^2 (k) = \frac{1}{2} \left\{ H_{11}^2 - H_{21}^2 + 2 H_{31}^2 - 2 H_{41}^2 + H_{33}^2 - H_{34}^2 \pm \left( \left( H_{11}^2 - H_{21}^2 - H_{33}^2 + H_{34}^2 \right) \right)^2 + 
+ 4 \left[ [H_{11} - H_{21}] [H_{31} + H_{41}] + [H_{33} + H_{34}] [H_{31} - H_{21}] \right] \cdot \left( [H_{33} - H_{34}] [H_{31} + H_{41}] + [H_{11} + H_{21}] [H_{31} - H_{21}] \right) \right\}^{1/2} \]  
(21)
Typical dispersions are shown in Fig. 6 in the different phases and on the phase boundaries. We now overview the dispersion relations in the four phases.

i) In the Néel solid which is realized for $V_2 \leq V_1 - 2$ and $H_z < 2\sqrt{(V_1 - V_2)^2 - 4}$ the spin wave dispersion is given by

$$\omega_{\pm}(k) = \sqrt{(V_1 - V_2)^2 - (2\gamma_k^{(1)})^2} \pm \frac{1}{2} H_z.$$  \hspace{1cm} (22)

Thus, there are two excitation branches in a halved magnetic Brillouin zone. Both branches are gapped.

ii) In the superfluid there is a Goldstone mode of linear $k$ dependence at small $k$, and a well developed minimum around $k_* = (\pi, \pi)$. Taking the continuum limit carefully identifies this with the roton part of the helium dispersion. Explicitly, with $s = \sin \theta_A = \sin \theta_B$, the dispersion in the extended zone is given by

$$\omega^2(k) = 2\left(1 - \gamma_k^{(1)} \right) \left(2(1 - \gamma_k^{(1)}) + s^2 \left[V_2\gamma_k^{(2)} + (2 + V_1)\gamma_k^{(1)} \right] \right).$$  \hspace{1cm} (23)

iii) In the Mott insulator phase for fields $H_z > 2(2 + V_1 + V_2)$ all spins are aligned along the magnetic field direction. There is a single gapped mode in the extended 1st Brillouin zone with the dispersion given by

$$\omega(k) = \frac{H_z}{2} - V_1 - V_2 - 2\gamma_k^{(1)}.$$ \hspace{1cm} (24)

iv) Finally, in the supersolid phase one has a gapless linear mode, and a gapped one, again in the halved magnetic zone.

To clarify the physics of the transitions we concentrate on the dispersion at $k \approx 0$ and $k \approx (\pi, \pi)$ at the phase boundaries. At the supersolid–Néel solid transition the critical mode is the Goldstone mode at small $k$. At the critical magnetic field, $H_z^c = 2\sqrt{(V_1 - V_2)^2 - 4}$, which determines the Néel solid to supersolid boundary by the vanishing of the gap of the lower excitation branch of the solid, we perform the small $k$ expansion for $\omega_{-}(k)$ from Eq. 22. For $V_1 > V_2 + 2$ where the solid exists at half-filling we obtain

$$\omega_{-}(k) \approx \frac{1}{2} \frac{1}{\sqrt{(V_1 - V_2)^2 - 4}} k^2.$$ \hspace{1cm} (25)
This means that the linear mode of the supersolid softens into a quadratic one at the boundary—signalling the destruction of superfluidity—before lifting off into a gapped mode inside the solid phase. This yields a quantum critical exponent $z = 2$. This value of $z$ agrees with that of Chester \[11\] and Cheng \[13\], but differs from that of Liu and Fisher \[5\], who obtain $z = 1$. We feel, however, that the softening of the Goldstone mode is a physically realistic picture, supporting our result.

At the generic superfluid–to–Néel supersolid transition the critical mode is at $k_* = (\pi, \pi)$. Inside the superfluid phase the roton minimum is at this wavevector. However in the solid, because of the zone–halving, this roton minimum is folded back to $k = 0$. In the superfluid where $\sin \theta_A = \sin \theta_B = s$ we study the small $k$ expansion of the single mode in the neighborhood of $k = (0, 0)$ and $k = (\pi, \pi)$. (Note that the Néel supersolid is only realised for $V_2 < V_1 - 2$.)

$$\omega^2(k) \approx \frac{s^2}{2} (2 + V_2 + V_1) k^2$$
$$\omega^2((\pi, \pi) - k) \approx 8\Delta^2 + \left(2 - 3\Delta^2 - V_2s^2\right)$$

where $\Delta^2 = 2 + (s^2/2) [V_2 - 2 - V_1]$. At the boundary to the Néel supersolid which is reached at a magnetic field $H_z = 2\sqrt{(V_1 - V_2)^2 - 4(V_1 + V_2 + 2)/(V_1 - V_2 + 2)}$ the mean field conditions in Eq. 19 tell that exactly at the transition the roton gap $\Delta$ disappears: the solidification is signalled by the softening–out of the roton mode of the superfluid. The dispersion relation of the rotons also changes from a quadratic to a linear minimum, hence $z = 1$.

Two remarks are in order here. First, recalling the original Landau argument about superfluidity it is clear that a vanishing roton energy leads to a vanishing critical velocity. So, while the superfluid order parameter remains finite through the supersolid transition, the critical velocity collapses to zero. Inside the supersolid phase it again assumes a finite value, as the second excitation branch becomes gapped.

Second, one can raise the question of how this picture is going to be modified in the absence of an underlying lattice. In this continuum limit the modes which go soft are located at a finite magnitude of $k$, i.e. on a ring in momentum space. This means that
the phase space for these excitations is much larger than for the usual Goldstone modes, which are centered around \( k \sim 0 \). It then is possible that these excitations may give rise to a fluctuation–induced first order transition instead of the second order one taking place on the lattice \([32]\).

Similar expansions can be used to study the case of half–filling. In this particle–hole symmetric case, not surprisingly both transitions have \( z = 1 \). In a recent Monte Carlo study \([9]\) the same \( z \) value was used in choosing the lattice size to study both the superfluid–supersolid and supersolid–solid transitions, whereas we find \( z = 1 \) and \( z = 2 \), respectively off half–filling. It appears that our results call for the repetition of the numerical simulations with different \( z \) factors when \( \rho \neq 1/2 \).

Finally at high fields, at the superfluid–to–Mott insulator transition the Goldstone mode softens out again, leading to \( z = 2 \), in agreement with earlier field theoretical predictions \([1]\) and numerical simulations \([23]\).

We have repeated the spin wave calculation for the collinear ordering for an ordering wave vector \( \mathbf{k}_c = (0, \pi) \). In this case the coefficients of the Hamiltonian Eq. 17 outside the collinear solid and the Mott insulating phases are given by

\[
H_{11} = \left(1 + \frac{\sin \theta_{R2}}{\sin \theta_{R1}}\right) + \frac{1}{4} \left(V_1 \sin^2 \theta_{R1} - 2 - 2 \cos^2 \theta_{R1}\right) \cos(k_x)
\]
\[
H_{33} = \left(1 + \frac{\sin \theta_{R1}}{\sin \theta_{R2}}\right) + \frac{1}{4} \left(V_1 \sin^2 \theta_{R2} - 2 - 2 \cos^2 \theta_{R2}\right) \cos(k_x)
\]
\[
H_{21} = \frac{1}{4} \sin^2 \theta_{R1} (2 + V_1) \cos(k_x), \quad H_{34} = \frac{1}{4} \sin^2 \theta_{R2} (2 + V_1) \cos(k_x),
\]
\[
H_{31} = \frac{1}{4} \left[-2 - 2 \cos \theta_{R1} \cos \theta_{R2} + V_1 \sin \theta_{R1} \sin \theta_{R2}\right] \cos(k_y) + \frac{V_2}{2} \sin \theta_{R1} \sin \theta_{R2} \gamma^{(2)}_k
\]
\[
H_{41} = H_{31} + \cos(k_y)
\] \quad \text{.} \tag{27}

The MF conditions are read off from the vanishing of the terms linear in the spin wave operators as before

\[
H_z \sin \theta_{R1} = 2 \cos \theta_{R1}(\sin \theta_{R1} + \sin \theta_{R2}) + V_1 \sin \theta_{R1}(\cos \theta_{R1} + \cos \theta_{R2}) + 2V_2 \cos \theta_{R2} \sin \theta_{R1}
\]
\[
H_z \sin \theta_{R2} = 2 \cos \theta_{R2}(\sin \theta_{R1} + \sin \theta_{R2}) + V_1 \sin \theta_{R2}(\cos \theta_{R1} + \cos \theta_{R2}) + 2V_2 \cos \theta_{R1} \sin \theta_{R2} \cdot \tag{28}
\]
For the superfluid and the Mott insulating phase the spin wave dispersions are obtained identical to the ones derived above in Eq. 23 and Eq. 24. In the collinear solid with \( \sin \theta_{R1} = \sin \theta_{R2} = 0 \) the coefficients \( H_{11} \) and \( H_{33} \) are replaced by

\[
H_{11} = V_2 - \frac{1}{2} H_z - \cos(k_x) \quad H_{33} = V_2 + \frac{1}{2} H_z - \cos(k_x). 
\]

The two gapped modes in the collinear solid for magnetic fields \( H_z \leq 2 \sqrt{(V_2 - 1)^2 - 1} \) and \( V_2 \geq 2 \) follow as

\[
\omega_{\pm}(k) = \sqrt{(V_2 - \cos(k_x))^2 - \cos^2(k_y)} \pm \frac{1}{2} H_z. 
\]

As for the Néel supersolid, the collinear supersolid has one gapless linear mode at small \( k \) and a gapped one in the halved magnetic Brillouin zone which in the case of collinear ordering with wave vector \( k_\star = (0, \pi) \) is determined by \( |k_y| \leq \pi/2 \). The transition from the superfluid to the collinear supersolid is now driven by the softening of the roton mode at \( k_\star = (0, \pi) \). The dynamical exponent is again \( z = 1 \). Also the exponents at the superfluid to collinear solid and at the solid to supersolid transition are identical to the exponents found for the Néel ordering transitions.

### IV. Simulations of the Soft Core Model

**Results at half–filling**

In this section we describe the results of numerical simulations, and compare them with the picture gained from the analytical considerations. Our Monte Carlo calculations are performed using a path integral representation on the BH partition function by discretizing the inverse temperature \( \beta \) into \( L_\tau \) intervals, \( \beta = L_\tau \Delta \tau \). A description of the technical details is contained in [24]. In order to characterize the phase diagram, we measure the boson winding number to determine the superfluid density \( \rho_s \). We also measure the density–density correlations \( c(l) \) and their Fourier transform, the structure factor \( S(k) \).

\[
c(l) = \langle n(j, \tau) n(j + l, \tau) \rangle
\]
Our normalization of the structure factor is such that if \( c(l) \) exhibits long range order, \( S(k_\ast) \) will be proportional to the lattice volume \( N = L_x^2 \), where \( L_x \) is the linear extent in the spatial dimension. If \( c(l) \) exhibits only short range order, \( S(k_\ast) \) will be lattice size independent. Here \( k_\ast = (\pi, \pi), (0, \pi), (\pi, 0) \) are the possible ordering wavevectors of the solid phase.

At weak coupling or high temperatures, \( c(l) \) exhibits only short range order. For \( l \) small, \( c(l) \) is enhanced but very rapidly decays to its uncorrelated value \( \rho^2 \). However, at low temperatures for sufficiently large interactions, the density–density correlations show long range oscillations. The associated structure factor \( S(k) \) evolves from being rather featureless to exhibiting a sharp peak at \( k_\ast = (\pi, \pi) \) as \( V_1 \) increases, and a peak at \( k_\ast = (0, \pi) \) or \( (\pi, 0) \) as \( V_2 \) increases. For our 2D system, for sufficiently large \( V_1 \), we expect a transition in the Ising universality class. That is, \( T_c \) is finite. In fact, if \( t = 0 \) we have \( T_c = 0.567 \, V_1 \). But even for a zero temperature phase transition such as would occur at the Heisenberg point of the hard core model, one will still observe “long range order” at finite \( T \) when the diverging correlation length exceeds the spatial lattice size as \( T \) is lowered. In such instances, of course, a careful study of finite size effects is required to draw conclusions concerning the existence of long range order. Here we always report results for temperatures such that \( \xi > L_x \) so that observables have taken on their ground state values. We have checked the scaling behavior to be sure that the ground state is genuinely ordered, when so claimed.

Fig. 7 shows the superfluid density \( \rho_s \) and structure factor \( S(\pi, \pi) \) as a function of \( V_1 \) for \( V_0 = 7 \) and \( V_2 = 0 \). We see that at \( V_1 \approx 2.5 \) there is a phase transition from a superfluid to a solid phase. The transition on the \( 8 \times 8 \) lattice shown is already rather sharp; finite size rounding in the raw data for the structure factor and superfluid density near the transition point is further reduced as one goes to \( 10 \times 10 \) lattices. That one has true diagonal long range order in the solid phase is confirmed by the fact that the structure factor scales linearly with the lattice volume. Indeed, at \( V_1 = 8 \), \( S(\pi, \pi) \) is almost precisely \( 100/64 \) times as large on the \( 10 \times 10 \) lattice than the \( 8 \times 8 \). There does not appear to be any window of coexistence.
between the superfluid and solid phases at half-filling. To within limits set by rounding, the transition points for $S$ and $\rho_s$ coincide almost precisely. We can make this statement more quantitative by performing the appropriate scaling analysis on the data. For example, we have plotted $L^a_x S(\pi, \pi)$ and $L^b_x \rho_s$ versus $V_1$ for different values of the exponent ratios $a, b$. Curves for different lattice sizes should cross at the same critical value of $V_1$ for the appropriate choices of $a, b$. A complication is that the imaginary time lattice size must be scaled as the appropriate power of the spatial extent, and the dynamic exponent $z$ could be different for the two transitions. Making the simplest assumption that $z$ is the same, however, as was already suggested by the raw data, this scaling procedure shows that the transition points for the two observables are within 0.5% of each other. While the structure factors do indeed cross nicely, the superfluid density curves come together rather than pass through each other. This seems to be a rather generic feature of simulations of the Bose Hubbard model \cite{25} as opposed to related conserved current models \cite{24,9}.

As $V_2$ is increased, $c(l)$ shows a similar transition from featureless uncorrelated behavior to long range order, although in this case $V_2$ favors the formation of a “striped” collinear phase with alternating lines of occupied and empty sites. The structure factor $S(k)$ develops a peak at $k_\ast = (\pi, 0)$ or $(0, \pi)$.

In order to determine whether $V_2$ can drive a supersolid phase at half-filling, we turn on $V_2$ close to the point where the transition between superfluid and solid occurs in Fig. 7. The density $\rho = 0.5$. We show in Fig. 8 a plot of $\rho_s$ and $S(k)$ for $k = (0, \pi), (\pi, 0)$ and $(\pi, \pi)$. We see that $V_2$ drives the Néel solid into a superfluid, and then at yet larger values causes the formation of a striped solid phase. Again, the plots suggest that there is no supersolid phase at $\rho = 0.5$. Scaling plots similar to those constructed at $V_2 = 0$ do not reveal any evidence for distinct critical points for superfluid and solid transitions to within our numerical accuracy.

We can put data from Figs. 7 and 8 together with similar runs for different sweeps of $V_1$ and $V_2$ to obtain the ground state phase diagram of the soft core BH model at $V_0 = 7$ and $\rho = 0.5$. This is shown in Fig. 9. At weak couplings we have a superfluid phase, while at
strong couplings there are two possible solids: checkerboard and striped. A strong coupling analysis predicts a phase boundary between the solid phases at $V_2 = \frac{1}{2}V_1$. The superfluid phase extends out along this line in a very robust manner, as opposed to the situation in 1D, where the superfluid window was rather narrow. This is a consequence of the highly degenerate nature of the strong coupling ($t = 0$) ground state along the line $V_1 = 2V_2$. As can easily be seen, not only do the Néel and checkerboard solids have the same energy, but an infinite number of defect states are degenerate as well for $V_1 = V_2$. For example in a horizontally aligned collinear solid a whole column can be shifted up and down without energy cost. This large degeneracy stabilizes superfluidity, even at large coupling. We will comment further on this point when discussing the hard-core phase diagram.

Results off half–filling

Although it does not appear that the BH model exhibits a supersolid phase at $\rho = 0.5$, we can see the coexistence of diagonal and off–diagonal long range order when the filling is shifted away from $\rho = 0.5$. In Fig. 10 we show $\rho_s$ and $S(\pi, \pi)$ for the same parameters as Fig. 7 except now $\rho = 0.53$. We see that although $\rho_s$ declines significantly when the solid forms, the excess boson density $\delta = \rho - 0.5$ (the magnetization $m$ is spin language) remains mobile in the solid background. Indeed, simulations at different densities (we found supersolids out to dopings of 0.675) show that the tail in $\rho_s$ is precisely proportional to $\delta$. Fig. 11 shows the analogous plot for a striped supersolid. Note that we have here separately displayed $\rho_{sx}$ and $\rho_{sy}$. As expected, the superfluid density in the $x$ and $y$ direction is correlated with the direction in which the striped solid channels run, as determined by the ordering wavevector $k_* = (\pi, 0)$ or $(0, \pi)$. If we had separately measured $\rho_{sa}$ and $\rho_{sb}$ on the two sublattices of the checkerboard solid, we would have found an analogous symmetry breaking. The nonzero value of $\rho_{sa} - \rho_{sb}$ is closely related to the appearance of a nonzero order parameter $m_{xa} - m_{xb}$ in the language of the spin Hamiltonian Eq. 2.

If we were to use finite size scaling techniques to locate the precise phase boundaries, it would be necessary to scale the imaginary time length $L$ as a power of the spatial length $L^2$, where $z$ is the dynamic critical exponent. As we have earlier described, it may be that
different values of $z$ are associated with the two transitions off half–filling, in which case the finite size scaling analysis is much more delicate. [9,10] We do not see the necessity of such a study here, since the supersolid phase occupies an extended portion of the phase diagram, and its existence is not predicated on proving the distinctness of two transition points.

Figures 10 and 11 provide compelling evidence for the existence of a supersolid phase. Our physical picture of this supersolid is one in which $\rho = 0.5$ of the bosons freeze into a rigid solid structure, while the remaining $\delta$ remain mobile. As we have seen, a signal of long range order then is present in both the diagonal $\langle n_in_j \rangle$ and off–diagonal $\langle a_i a_j^\dagger \rangle$ channels.

We have conducted our simulations of the BH Hamiltonian in the canonical ensemble, and have presented our results by specifying the density $\rho$ rather than the chemical potential $\mu$. In describing the nature of the phase diagram it is important to note that due to the existence of a gap in the solid phases, the $\mu–\rho$ relation is non–trivial. If the gap is nonzero, when we dope our system even slightly away from half–filling, the chemical potential is shifted by a considerable amount. In the language of the spin Hamiltonian, Eq. 2, a sizeable field $H_z$ is required to change the magnetization of the gapped Ising phase. In Fig. 12 we illustrate this point by drawing the $\mu/V_1–1/V_1$ phase diagram. A sweep at constant chemical potential reveals a supersolid window. A sweep at fixed density skirts the pure solid and remains in the supersolid phase. This is why we see in Figs. 10 and 11 a supersolid for an extended region $V > V_{\text{crit}}$ rather than in some narrow region between phases exhibiting a single type of order.

If we now examine densities $\rho < 0.5$, we find qualitatively similar results: a superfluid phase gives way to a striped supersolid phase as $V_1$ increases. By these measures, hole or particle doping appears qualitatively similar. The same is true of the checkerboard supersolid, where results for hole doping are entirely reminiscent of the analogous particle doped case.

In fact, however, something rather different does go on with particle and hole doping. In Fig. 13 we show the ground state energy as a function of doping for $V_0 = 7$, $V_1 = 3$, and $V_2 = 3$. For these parameters, as we have seen, we have a striped supersolid off half–filling
and a striped solid at $\rho = 1/2$. The change in slope of $E_0$ at $\rho = 1/2$ reflects a jump in the chemical potential which is, in fact, just the gap in the solid phase. [24]. There is nothing particularly unusual here. The strange feature occurs for the checkerboard case. In Fig. 14 we show the ground state energy as a function of doping for $V_0 = 7$, $V_1 = 3$, and $V_2 = 0$. The fact that $E_0(\rho)$ is concave down for $\rho < 0.5$ indicates an instability to phase separation. Previous studies [29] have suggested the possibility of phase separation in systems with attractive boson interactions. However, we do not have these Lennard–Jones type potentials here, only purely repulsive ones. It is not immediately apparent why mobile holes (or particles) in a rigid solid background should segregate themselves.

A possible explanation, however, is as follows: Consider an isolated doped hole in a checkerboard solid. In order to move to another site of the same sublattice, it must pass through an intermediate site on the opposite sublattice, a state of energy $2V_1$. Thus the hole’s effective hybridization is $t_{\text{eff}} = t^2/2V_1$. (This sort of argument has previously been used to predict the shape of the phase boundary in the one dimensional extended BH Hamiltonian, in good agreement with simulations. [31]) If two holes are near each other, the intermediate state is lower in energy, so the effective hybridization is increased. This suggests a possible mechanism for phase separation: increased mobility of holes which propagate coherently. Of course, the increase in $t_{\text{eff}}$ is partially offset by the entropy cost of confining one hole near the other. Unfortunately, there appears to be an analogous increase in $t_{\text{eff}}$ for doped particles which are proximate, so this reasoning does not explain the fact that $E(\rho)$ is concave down for $\rho < 0.5$ only. Nevertheless, the simulations provide compelling evidence for a lack of particle-hole symmetry.

In principle, one can also examine the issue of phase separation through anomalies in $S(k)$ for small $k$. However, our use of the canonical ensemble makes this approach non-trivial. Further work on the question of phase separation is needed.
V. SIMULATIONS OF THE HARD CORE MODEL

We now examine the phase diagram in the hard core case. This is important to do for a number of reasons. First, it allows us to make a connection to the spin model limit, Eq. 2. Second, as we have seen at $V_0 = 7$, some of the interesting transitions occur at $V_1$ and $V_2$ values which are getting rather large, while we expect in most physical situations that the on–site $V_0$ should be substantially greater than the near neighbor interactions. One consequence of this, is that the doped bosons in the supersolid phase for our soft–core model could move on the occupied sublattice, since the cost of $V_0$ was less than the coordination number $z$ times the near neighbor interaction strengths. In the hard core model such multiple occupancies are forbidden, and we want to make sure that our conclusions are not affected by this change.

Fig. 15 shows results for the superfluid density and structure factors for the half–filled case. We sweep $V_2$ at fixed $V_1 = 3$. A Néel phase appears at small $V_2$. For larger $V_2$ the superfluid phase appears before making a transition into a collinear solid for yet larger $V_2$. If $V_1$ is sufficiently small, the Néel phase at weak $V_2$ is eliminated, and the system remains superfluid down to $V_2 = 0$. Data for this and other sweeps is summarized in Fig. 16 where the resulting ground state phase diagram is shown. Note that we find the superfluid–Néel solid transition at $V_2 = 0$ occurs at a value $V_1$ close to $2t$, which is the result expected based on the mapping to the spin model, Eq. 2.

As in the soft core case the weak coupling superfluid extends out along the $V_2 = V_1/2$ strong coupling boundary between the two solid phases. Unlike analogous studies [31] in 1D, this superfluid wedge is difficult to close, a phenomenon which we earlier explained by the large degeneracy of competing solid phases along the strong coupling line. We have conducted simulations along the line $V_2 = V_1/2$ and find that the superfluid density vanishes at $V_1 \approx 7$. Interestingly, there is no inset of solid order at this point. This needs further study, for example to understand if some disordered dimer phase might exist in this regime, in analogy with related spin systems.
Fig. 17 is a plot for a doped lattice with $\delta = \rho - 1/2 = 0.0625$. The main difference is that, as in the soft-core case, there is a superfluid tail after the structure factor exhibits the transition into the solid phase. That is, there is a supersolid in the hard-core case as well. As expected, doping inhibits somewhat the formation of crystalline order, so that stronger couplings are required to induce the crystalline order as is seen by comparing the doped phase diagram, Fig. 18, with Fig. 16, the phase diagram at half-filling. Despite considerable rounding of the transitions, scaling analyses conclude that the regions where $S$ is large are indeed ordered.

Finally, Figs. 19a,b show the ground state energy as a function of filling for the hard-core model at $V_1 = 8, V_2 = 0$ (Néel solid), and $V_1 = 8, V_2 = 4$ (collinear solid), respectively. The data are qualitatively similar to the soft-core model. In the collinear solid $E_0$ is concave up, with a change in slope at $\rho = 1/2$ which is the gap. In the Néel solid $E_0$ shows a tendency for phase separation.

**VI. RELATED ISSUES**

Up to now we have focussed on the ground state phase diagram of the BH Hamiltonian. It is interesting to consider also the behavior of the system at finite temperatures. Here the motion of doped bosons in the BH model which we have studied with our simulations has a close connection with the idea of “defectons” in a solid [14] where quantum tunneling caused by the finiteness of the de Boer parameter delocalizes lattice defects at low temperature. It is also of interest to study the behavior of the diffusion constant $D$ for the full range of temperature. Here we expect that defects are localized at high $T$, and $D$ first decreases exponentially as $T$ is lowered in this classical regime. $D$ should then exhibit a plateau as quantum diffusion takes over, and ultimately increase again as delocalization occurs. While they focus largely on the behavior of single defectons, Andreev and Lifshitz also consider the possibility of long range Coulomb interactions causing localization into a “defecton superlattice”. Our insulating checkerboard solid is in fact an illustration of this. The Bose-
Hubbard model with only on–site $V_0$, has no solid phase at $\rho = 0.5$, but when $V_1$ is turned on, an ordered lattice does form.

We have focussed here on zero temperature, the finite temperature phase diagram of the 2D BH model would be interesting to study as well. The solid transitions are in the Ising universality class, and hence have a finite $T_c$. Similarly one expects a Kosterlitz–Thouless type finite critical temperature for the superfluid transition. As for the topology of the phase diagram, several possibilities have been explored by Liu and Fisher [5]. One intriguing case is the appearance of a tetracritical point; where the three ordered phases (superfluid, supersolid and solid) come together, giving way to the disordered phase with further increase of the temperature. This happens within a limited, but finite range of parameters on the mean field level. The corresponding scaling theory was developed by Nelson and Fisher [33]. Other alternatives include a supersolid phase which exists only at finite temperatures, and that the tetracritical point is split into bicritical points. [5] We hope to take up some of the issues in a further publication.

In the path integral representation of the BH partition function used in our simulations, the particle number conservation leads to boson “world lines” propagating in the original 2 spatial dimensions plus an additional imaginary time direction which runs from 0 to $\beta$. This picture has been used to suggest close analogies between the physics of vortices in Type II superconductors [34] and the phase diagram of the 2D Bose–Hubbard Hamiltonian. Frey, Nelson, and Fisher, [35] have recently discussed both thermally driven and quantum phase transitions, for example as caused by the introduction of defects or interstitials into the Abrikosov lattice, in these vortex systems. This also has close connections with the results we have discussed here.

VII. CONCLUSIONS

In this paper we have considered quantum phase transitions in the Bose–Hubbard hamiltonian. We identified several phases: solid and supersolid phases with Néel and collinear
patterns, furthermore a superfluid and a Mott type insulating phase. The phase diagram has been determined analytically and the spin–wave spectrum has been calculated. The dynamical critical exponents at each transitions were calculated and preexisting controversies were settled. Our numerical work – utilizing Quantum Monte Carlo methods – provided a detailed study of the different phases. Concerning the phase diagram the existence of supersolid phases has been forcefully confirmed. These phases exist only off half–filling, in accordance with the mean field results, but in disagreement with some recent claims. The possibility of phase separation in the model has been investigated as well, and provides evidence for a violation of the previously assumed particle–hole symmetry of the model.

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Figure Captions

Fig. 1: Mean field phases MF of the XXZ spin Hamiltonian Eq. 2 on a 2D square lattice.

Fig. 2: Hard core mean field phase diagram at half–filling $\rho = \frac{1}{2}$ from comparing the energies of superfluid, Néel and collinear solid.

Fig. 3: Hard core mean field phase diagram (bold lines) away from half–filling for $m = |\rho - \frac{1}{2}| = 0.2$ from comparing the energies of superfluid, Néel and collinear supersolid. Thin lines indicate the phase boundaries at half–filling $m = 0$ (see Fig. 2).

Fig. 4: Hard core mean field phase diagram, magnetisation $m$ versus $V_2$, for fixed $V_1 = 3$. SS denotes the supersolid phases.

Fig. 5: Hard core mean field phase diagram, magnetisation $m$ versus $V_1$, for fixed $V_2 = 1$.

Fig. 6: Spin wave dispersions in the (a) Néel solid, (b) at the Néel solid–Néel supersolid boundary, (c) in the Néel supersolid, (d) at the Néel supersolid–superfluid boundary, and (e) in the superfluid. In all plots $V_2$ and $V_1$ are fixed to $V_2 = 1.5$, $V_1 = 4.5$, and the magnetic field $h$ ($H_z$ in the text) is varied.

Fig. 7: The superfluid density $\rho_s$ and $S(\pi, \pi)$ as a function of $V_1$ for $V_0 = 7$ and $V_2 = 0$. The density $\rho = 0.5$ and $\beta = 4$. The transitions in $\rho_s$ and $S(\pi, \pi)$ appear to occur at roughly the same value of $V_1$.

Fig. 8: The superfluid density and structure factor as a function of $V_2$ at $V_0 = 7$, $V_1 = 2.75$, and $\rho = 0.5$.

Fig. 9: The ground state phase diagram of the BH model at $\rho = 0.5$ and with a soft core on–site repulsion $V_0 = 7$.

Fig. 10: The superfluid density and structure factor for the same parameters as in Fig. 7, except now the system is doped to $\rho = 0.53$. A superfluid tail remains in the (checkerboard) solid phase.

Fig. 11: The superfluid density and structure factor for the same parameters as in Fig. 8, except now the system is doped to $\rho = 0.56$. A superfluid tail remains in the (striped) solid phase.
**Fig. 12:** The qualitative $T = 0$ phase diagram of the Bose–Hubbard model is illustrated. A sweep at constant $\mu$ (full arrow) could cut across the phase boundaries as shown, revealing a supersolid window, while a sweep of constant density (dashed arrow) remains in the supersolid phase at strong coupling. The Mott insulating phase at large $\mu$ has density one boson per site.

**Fig. 13:** The ground state energy as a function of density for $V_0 = 7$, $V_1 = 3$, $V_2 = 3$.

**Fig. 14:** The ground state energy as a function of density for $V_0 = 7$, $V_1 = 3$, $V_2 = 0$.

**Fig. 15:** Superfluid density and structure factors versus $V_2$ for $V_1 = 3$. The density $\rho = 0.500$.

**Fig. 16:** The phase diagram of the half-filled hard-core model. The dashed lines are the results of the Mean Field analysis presented earlier in the paper.

**Fig. 17:** Superfluid density and structure factors versus $V_2$ for $V_1 = 3$. The density $\rho = 0.563$.

**Fig. 18:** The phase diagram of the doped hard-core model.

**Fig. 19:** Ground state energy versus density for the hardcore model. (a) $V_1 = 4, V_2 = 0$ and (b) $V_1 = 4, V_2 = 4$. 
Collinear Solid

SF

Neel Solid

\[ V_2 \]

\[ V_1 \]
\[ V_1 = 3 \]
$V_2 = 1$

- Superfluid
- Neel
- SS

Variables:
- $m$ vs. $V_1$
$V_2 = 1.5$, $h = 2.6$, $V_1 = 4$

Diagram showing $\varphi$ vs $q_x = q_y$.
$V_2=1.5$, $h=3.0$, $V_1=4$
$V_2=1.5$, $h=3.8$, $V_1=4$
\( V_2 = 1.5, \ h = 5.0, \ V_1 = 4 \)
$V_2 = 1.5$, $h = 5.6$, $V_1 = 4$
$\rho = 0.5, V_0 = 7, V_1 = 2.75$
$V_0 = 7, V_1 = 3, V_2 = 3$
$g = 8 	imes 8 	imes 32, \tau = 0.125$
$V_0 = 7$, $V_1 = 3$, $V_2 = 0$

$8 \times 8 \times 32$, $\tau = 0.125$
HARDCORE, $\rho = 0.5$

$S(\pi,0)$

Superfluid

$S(\pi,\pi)$
