Supersolids versus Phase Separation in Two-Dimensional Lattice Bosons

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We study the nature of the ground state of the two-dimensional extended boson Hubbard model on a square lattice by quantum Monte Carlo methods. We demonstrate that strong but finite on-site interaction U along with a comparable nearest-neighbor repulsion V result in a thermodynamically stable supersolid ground state for densities larger than $1/2$, in contrast to fillings less than $1/2$ or for very large U, where the checkerboard supersolid is unstable towards phase separation. We discuss the relevance of our results to realizations of supersolids using cold bosonic atoms in optical lattices.

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The detection of a possible supersolid (SS) state in recent experiments on solid ^{4}He by Kim and Chan [1] has led to renewed interest [2] in a problem that has long [3] intrigued physicists: Can a supersolid phase—with simultaneous diagonal (solid) and off-diagonal (superfluid) long-range order—exist in a bosonic system? While the issue remains controversial [4–6] in a translationally invariant system despite almost 50 years of theoretical research, the situation in lattice models is clearer.

Theoretical studies [7–11] of various *lattice* boson models (which can nowadays be implemented using cold bosonic atoms on optical lattices [12]), appeared to confirm that here SS ground states can indeed exist, particularly when doped away from half filling. Studies of the closely related quantum phase model found SS order in the ground state even at half filling [9]. However, as was pointed out recently, the stability of the SS against phase separation had not been investigated [13]. Indeed, for hard-core bosons on a square lattice, the most widely discussed SS pattern with (π, π) diagonal order is thermodynamically unstable and phase separates into a pure (π, π) solid and a superfluid (SF) for all values of interaction strengths. A striped SS phase with $(0, \pi)$ ordering is stabilized by a finite next-nearest-neighbor interaction.

In this work we analyze stability of crystalline and SS orders of lattice bosons. We present exact strong-coupling arguments showing under which conditions checkerboard supersolids are unstable, and how they can be stabilized with large but finite on-site and nearest-neighbor (nn) energies U and V. We support these arguments by quantum Monte Carlo (QMC) simulations of a two-dimensional (2D) extended Bose-Hubbard model demonstrating that the SS phase is stabilized for densities $\rho > 1/2$ and sufficiently large V (Fig. 1).

Specifically, we study the extended Bose-Hubbard model (EBHM) on a d-dimensional hypercubic lattice with on-site (U) and nn (V) interactions,

$$H = -t\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) - \mu\sum_i n_i + V\sum_{\langle i,j\rangle} n_i n_j + \frac{U}{2}\sum_i n_i(n_i - 1), \quad (1)$$

where $a_i^\dagger$ (a_i) creates (annihilates) a boson at site i with the occupation number $n_i \equiv a_i^\dagger a_i$, t is hopping, μ is the chemical potential, and $\langle i, j\rangle$ runs over all nn pairs.

In the zero-hopping limit $t = 0$, the phase diagram is simple. At low chemical potential $\mu < 0$, no bosons are present. Increasing the chemical potential, the potential energy ($U, V > 0$) is minimized at half-filling $\rho = 1/2$ by the crystal state with one sublattice occupied [checkerboard pattern with (π, π) modulation in 2D]. This state is gapped and remains stable in the presence of a small

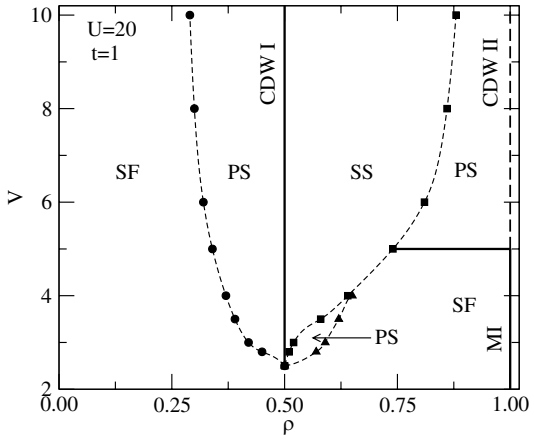

FIG. 1. The ground state phase diagram of the 2D extended Bose-Hubbard model (1) in the $V - \rho$ plane for $U/t = 20$ and densities $\rho \leq 1$, showing superfluid (SF) phases, checkerboard solids formed by single bosons (CDW I) and pairs of bosons (CDW II), a Mott-insulating phase (MI), phase separation (PS), and finally a supersolid phase (SS).

hopping, $t \ll U, V$, with a kinetic energy gain $\Delta E \approx -zt^2/[(z-1)V]$ per boson, where $z = 2d$ is the coordinance. At even larger μ there is another first order phase transition to an insulating state with density $\rho = 1$, which can either be a uniform Mott insulator (MI) with one particle per site for $U > 4V$, or a density wave with two particles per site on one sublattice for $U < 4V$.

Introducing holes into the $\rho = 1/2$ crystal costs chemical potential μ but no potential energy [see Fig. 2(a)]. The kinetic energy gain is slightly increased (compared to $\rho = 1/2$ case) but remains quadratic in t for isolated holes. However, the kinetic energy gain becomes *linear* in t if a number of holes encircle a region of a crystal, forming a domain wall [Fig. 2(b) and 2(c)]. The energy gain is maximized at $\Delta E \approx -ct$, $1 < c < 2$ per hole for a planar [linear in 2D, see Fig. 2(c)] domain wall doped with one hole per two sites. As a result, for a large system with $N = L^d$ sites, the crystalline order is destroyed by introduction of a small density $\rho \sim L^{-1}$ of holes. This instability of the $\rho = 1/2$ crystal to domain wall formation upon hole doping excludes the possibility of a SS phase. On the isotropic square lattice, the instability might develop further, leading to a phase separation between the commensurate crystal at $\rho = 1/2$ and a uniform SF with $\rho < 1/2$ (Fig. 1), as has been discussed previously in Ref. [14].

Doping of the $\rho = 1/2$ crystal with additional bosons works differently depending on the relation between V and U. The energy cost to place a boson at an empty (occupied) site is $E_0 \equiv zV - \mu$ ($E_1 \equiv U - \mu$). For $U > zV$, the additional bosons fill empty sites and mask the checkerboard modulation; for $U - zV \gg t > 0$ the situation is precisely particle-hole conjugate to hole doping. The kinetic energy is again minimized at planar domain walls which destabilize the checkerboard crystal order. In particular, in the hard-core limit $U \to \infty$, the crystalline order is always unstable for $\rho \neq 1/2$.

With $zV \gtrsim U$, however, the bosons can be placed on either an occupied or unoccupied site. The total energy of a single boson delocalized between the two sublattices is $E = E_1 + \Delta - (2z^2t^2 + \Delta^2)^{1/2}$, where $\Delta \equiv (zV - U)/2$. Clearly, for sufficiently small $\Delta \sim t$, the kinetic energy $E - E_1$ is again linear in t and large, which prevents the domain wall formation. As a result, these doped particles will form a SF on top of the density-wave background and hence a SS. Two bosons experience both on-site and nn repulsion ($2U$ and V respectively). Therefore, at sufficiently small densities the condensate should remain stable, which completes the formal argument for the SS existence. We emphasize that this phase requires that putting two bosons onto one site be energetically cheap, which is not the case for hard-core bosons.

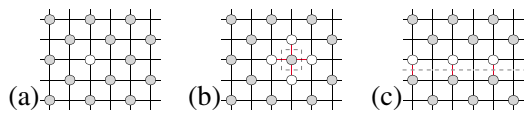

FIG. 2 (color online). The $\rho = 1/2$ checkerboard crystal doped with holes. (a) A single hole. (b) Four holes encircle a boson which can hop between the five degenerate sites. (c) Domain wall doped with holes; bosons can hop freely across the dashed line.

Similarly, at unit filling, $\rho = 1$, the ground state is a MI with one boson per site for $U > zV$, and an ordered solid with two bosons on every other site for $U < zV$. In the former case, additional holes (particles) move along the uniform background with the hopping integral t ($2t$) and experience both nn and on-site repulsion (infinite in the case of holes). They condense on top of the uniform background forming a SF. However, for $zV > U$, the doped particles move on a checkerboard background with the effective hopping, e.g., $t_* = 2t^2/[zV - U + (z-2)V]$ for holes. The resulting kinetic energy gain is only quadratic in t and can be superseded if the holes come together into a SS phase with $\rho \gtrsim 1/2$. Overall, this leads to a thermodynamical instability of the hole-doped checkerboard solid formed by pairs of bosons at $\rho = 1$: the system can minimize its energy by phase separation (PS). Note that here phase separation is not between a SF and a solid but between a SS and a solid. The solid order is not destabilized at this first order phase transition, but just the "Bose-Einstein condensation" transition of holes doped into the solid becomes first order.

We next perform QMC simulations to corroborate these arguments and to show the phase diagram and the existence of a SS phase for the EBHM in the low-density region $\rho \leq 1$. We have used loop-operator updates in a stochastic series expansion QMC method [15] to study the EBHM (1) in the strong-coupling regime $U, V \gg t$. Simulations have been carried out on $N = L \times L$ lattices, with $L = 6, \ldots, 16$. To obtain ground state results we choose an inverse temperature $\beta = 2L$, and find rapid convergence for the system sizes studied (see Fig. 4).

To characterize different phases, we have studied the static staggered [$\mathbf{Q} = (\pi, \pi)$] structure factor,

$$S(\mathbf{Q}) = \frac{1}{N}\sum_{j,k} e^{-i\mathbf{Q}\cdot(\mathbf{r}_j - \mathbf{r}_k)}\langle n_j n_k\rangle - \langle n_j\rangle^2, \qquad (2)$$

which measures the diagonal long-range order (checkerboard solid) in the system, and the SF density ρ_s, measured from the winding numbers of the bosonic world lines (W_x and W_y) in the x and y directions as $\rho_s = \langle W_x^2 + W_y^2\rangle/2\beta m$, where $m = 2/t$ is the effective mass of the bosons. In the thermodynamic limit, a checkerboard solid ground state at $\rho = 0.5$ is marked by (diverging) $S(\pi, \pi) \propto N$ and vanishing ρ_s, whereas a pure SF phase has $S(\pi, \pi)/N \to 0$ and $\rho_s > 0$. A SS phase, on the other hand, is characterized by a finite $S(\pi, \pi)/N$ *and* a nonzero value of ρ_s. For finite systems, both quantities are always finite and estimates for the thermodynamic limit are obtained from finite-size scaling of the observables.

A jump in ρ with varying μ indicates a discontinuous (first order) transition, and has been used to identify re-

gions of PS in the canonical ensemble (fixed ρ). We postpone a more rigorous analysis to accurately identify the nature of transitions and the precise domain boundaries to a later study, and focus on establishing the existence of a SS phase over finite regions of parameter space.

A plot of ρ *vs* μ (Fig. 3) shows clear indications of PS at $\rho < 0.5$ for all values of V—the discontinuity in ρ grows with increasing V. For $\rho > 0.5$, the curves are qualitatively different. For $V < U/4$, there is a small but finite region of positive slope (e.g., $0.5 < \rho < 0.52$ for $V = 3$), followed by PS for $0.52 < \rho < 0.60$, and a region of positive slope for $\rho > 0.6$. At $V = U/4$, there is no evidence of PS for $\rho > 0.5$. With $V > U/4$, the region of PS shifts to large densities, $\rho \lesssim 1$. The location and extent of phase separated regions for small $V(<U/4)$ agrees well with Ref. [13(b)] apart from the extra region of positive slope for $0.5 < \rho < 0.52$ where the ground state has SS order (see Fig. 4). The extent of the SS phase decreases rapidly with decreasing V, becoming vanishingly small in the limit $V \ll U$. We note that for small V the excess density $\rho - 1/2 < 1/L$ and larger L are required to map the SS phase boundary accurately.

Figure 4 displays ground state results for $S(\pi, \pi)/N$ and ρ_s as a function of ρ for three representative values of V. The data are seen to be well converged with system size. For small ρ, the ground state is a SF—the stiffness converges to a finite value while $S(\pi, \pi)/N$ scales to zero. As ρ increases beyond a critical value, there is a discontinuous transition to a (π, π) ordered density-wave (DW) ground state with $\rho = 0.5$. Any intermediate density is inaccessible in the grand canonical ensemble. For$V = 3t(<U/4)$, at $\rho > 0.5$, there are indications of a small region of SS characterized by finite values of *both* $S(\pi, \pi)/N$ and ρ_s, but further finite-size scaling tests are needed to check whether this region remains in the thermodynamic limit. With increasing ρ, there is another discontinuous transition to a SF state with a second region of PS. Finally, at $\rho = 1$, the ground state is a MI with both $S(\pi, \pi)/N = 0$ and $\rho_s = 0$. For $V = 5t(= U/4)$, the extent of the SS region increases substantially and its stability is well established. Additionally, the second phase separated region shrinks to zero and there is a direct SS-SF transition. For $V = 6t(>U/4)$, the SF phase at $\rho \lesssim 1$ is replaced by another region of PS. The ground state at $\rho = 1$ changes from a MI to a (π, π) ordered DW with two particles occupying one sublattice, with a discontinuous transition separating it from the SF phase.

The results are combined to map the schematic ground state phase diagram of the Hamiltonian (1) in the $V - \rho$ (Fig. 1) and $\mu - 1/V$ (Fig. 5) planes. Figure 1 shows the different phases in the (V, ρ) plane at a constant value of on-site interaction, $U = 20$, $t = 1$. For small V, the ground state is a SF for all $\rho < 1$. For $V > 2.5t$, the different

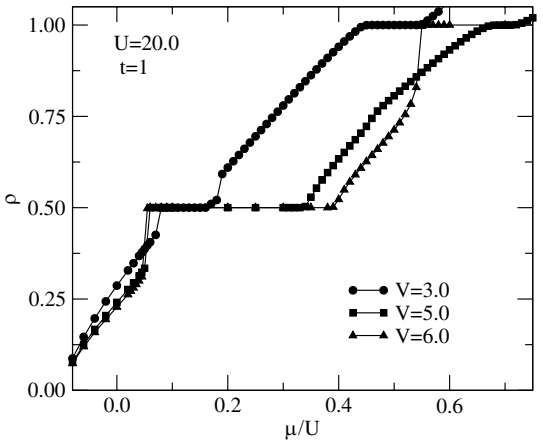

FIG. 3. The average density as a function of the chemical potential for three different values of V ($U = 20$). For clarity of presentation, data for only one system size, $L = 16$, is shown. Error bars are smaller than the symbol sizes. Discontinuous transitions are marked by finite jumps in the particle density.

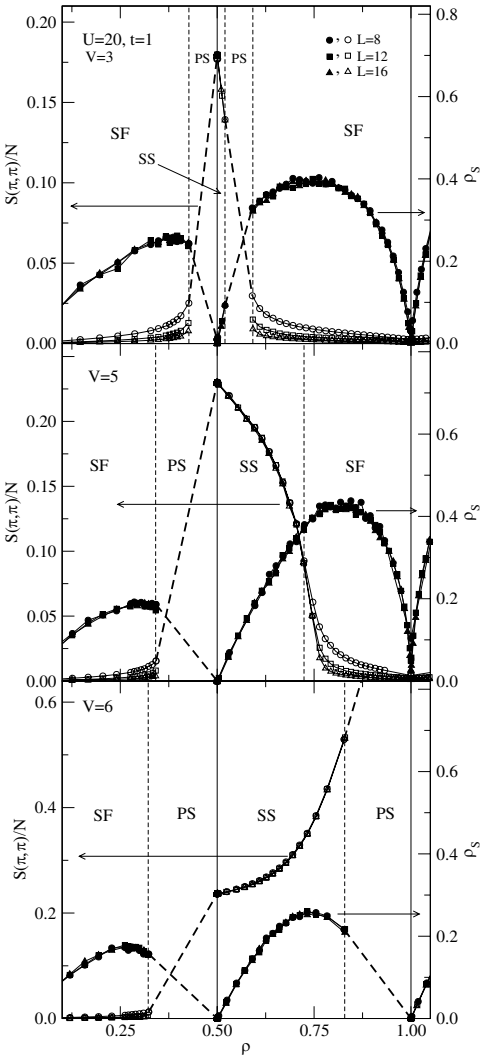

FIG. 4. Staggered structure factor (open symbols) and superfluid stiffness (filled symbols) as a function of particle density ρ for three representative values of V. Dashed lines in the phase separated regions are results obtained by Maxwell construction. See the text for a detailed discussion of the various phases.

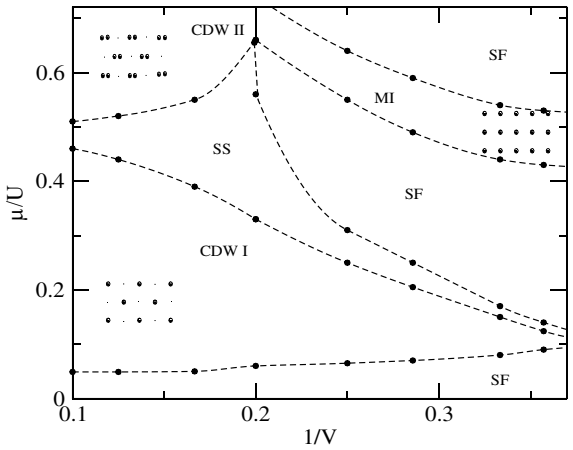

FIG. 5. The ground state phase diagram in the $V - \mu$ plane at $U = 20$, $t = 1$; notations as in Fig. 1. Different solid-ordered phases are shown schematically. The PS regions are manifested as discontinuous transitions across the corresponding phase boundaries (not shown).

phases appear as shown in Fig. 1. The extent of the SS phase and that of the phase separated region at $\rho < 0.5$ increases with increasing V, whereas the phase separated region at $\rho > 0.5$ gets vanishingly small for moderate values of V. It is not clear from the available data whether the PS-SF phase boundary meets the SS boundary at a point, or approaches it asymptotically. At $V > 5.0t$, the SF region at high densities is replaced by a phase separated region, while the ground state at $\rho = 1$ changes from a MI to a (π, π)-ordered DW with two bosons occupying every other lattice site. We note that the phase diagram is qualitative and the phase boundaries approximate.

The features of the phase diagram as a function of $1/V$ (Fig. 5) are markedly different from the "lobe" structure observed in a plot [9] of μ as a function of t/U for the EBHM. The nature of the ground state at $\rho = 1$ changes from a DW to a MI as V is varied across $U/4$. This is accompanied by a change in the curvatures of the phase boundaries. Furthermore, the MI region remains finite even in the limit of $V \to 0$. No evidence of SS phase is found at $\rho = 0.5$, in agreement with the variational studies and previous numerics [7,9].

In conclusion, we have provided strict arguments why a soft-core model with $V > U/z$ and densities $\rho > 1/2$ is sufficient to stabilize a SS phase in a model with nn couplings and substantiated the arguments with QMC calculations of the phase diagram. The existence of a stable SS phase is in contrast to the hard-core case where the system phase separates for all values of nn interaction.

The instability towards PS is also present in higher dimensions and in models with dipolar interactions, although it again does not show up in mean-field calculations [10]. To stabilize a uniform SS phase one needs to reduce the on-site interactions, e.g., with a Feshbach resonance. This will be important for realizations of the SS phases when loading a of chromium atoms [16] into optical lattices.

We finally note that in the studied range of parameters (including very large V up to $12t$), we have not found any nominally gapless phase with both $S(\pi, \pi)/N$ and ρ_s zero which could potentially be identified with a Bose metal [17] (see also Ref. [13(d)]).

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[1] E. Kim and M. H. W. Chan, Nature (London) **427**, 225 (2004); Science **305**, 1941 (2004).
[2] A. Leggett, Science **305**, 1921 (2004); N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **94**, 155302 (2005); A. S. Moskvin, I. G. Bostrem, and A. S. Ovchinnikov, JETP Lett. **78**, 772 (2003).
[3] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).
[4] A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP **29**, 1107 (1969); G. Chester, Phys. Rev. A **2**, 256 (1970); A. J. Leggett, Phys. Rev. Lett. **25**, 1543 (1970).
[5] P. W. Anderson, *Basic notions of Condensed Matter Physics* (Benjamin, New York, 1984).
[6] For review of experimental and theoretical work see M. W. Meisel, Physica B (Amsterdam) **178B**, 121 (1992), and other articles in the same volume.
[7] H. Matsuda and T. Tsuneto, Suppl. Prog. Theor. Phys. **46**, 411 (1970); K. S. Liu, and M. E. Fisher, J. Low Temp. Phys. **10**, 655 (1973); E. Roddick and D. Stroud, Phys. Rev. B **48**, 16600 (1993); **51**, R8672 (1995); G. G. Batrouni *et al.*, Phys. Rev. Lett. **74**, 2527 (1995); R. T. Scalettar *et al.*, Phys. Rev. B **51**, 8467 (1995); R. Micnas, S. Robaszkiewicz, and T. Kostyrko *ibid.* **52**, 6863 (1995); E. S. Sorensen and E. Roddick *ibid.* **53**, R8867 (1996).
[8] E. Frey and L. Balents, Phys. Rev. B **55**, 1050 (1997).
[9] A. van Otterlo and K.-H. Wagenblast, Phys. Rev. Lett. **72**, 3598 (1994); A. van Otterlo *et al.*, Phys. Rev. B **52**, 16176 (1995).
[10] K. Góral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. **88**, 170406 (2002).
[11] H. P. Büchler and G. Blatter, Phys. Rev. Lett. **91**, 130404 (2003).
[12] M. Greiner *et al.*, Nature (London) **415**, 39 (2002).
[13] (a) M. Kohno and M. Takahashi, Phys. Rev. B **56**, 3212 (1997); (b) G. G. Batrouni, and R. T. Scalettar, Phys. Rev. Lett. **84**, 1599 (2000); (c) F. Hébert *et al.*., Phys. Rev. B **65**, 014513 (2002); (d) A. Kuklov, N. Prokof'ev, and B. Svistunov, Phys. Rev. Lett. **93**, 230402 (2004).
[14] N. G. Zhang and C. L. Henley, Phys. Rev. B **68**, 14506 (2003).
[15] A. W. Sandvik, Phys. Rev. B **59**, R14157 (1999).
[16] A. Griesmaier *et al.*, Phys. Rev. Lett. **94**, 160401 (2005).
[17] P. Phillips and D. Dalidovich, Science **302**, 243 (2003); D. Das and S. Doniach, Phys. Rev. B **64**, 134511 (2001).