Supersolid in a one-dimensional model of hard-core bosons

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We study a system of hard-core boson on a one-dimensional lattice with frustrated next-nearest-neighbor hopping and nearest-neighbor interaction. At half filling, for equal magnitude of nearest- and next-nearest-neighbor hopping, the ground state of this system exhibits a first-order phase transition from a bond-ordered solid to a charge-density-wave solid as a function of the nearest-neighbor interaction. Moving away from half filling we investigate the system at incommensurate densities, where we find a supersolid phase which has concurrent off-diagonal long-range order and density-wave order which is unusual in a system of hard-core bosons in one dimension. Using the finite-size density-matrix renormalization group method, we obtain the complete phase diagram for this model.

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I. INTRODUCTION

Supersolid phases of matter which feature both off-diagonal superfluid order and long-range crystalline order have been a subject of intense research in the last decade. While there is still no clear evidence for the occurrence of this phase in solid helium [1], there are proposals for creating such a state in optical lattices of cold atoms [2]. Model Hamiltonians which describe supersolid phases exist, of which one of the most rigorously studied is that of hard-core bosons on a lattice with further neighbor interactions [3–8]. Supersolid phases have also been predicted in models of soft-core bosons and binary mixtures [9–12] and quantum spin systems [13,14]. It has been proposed that a system of polar gases in optical lattices is a suitable test bed to observe this exotic phase of matter. Pioneering experiments on chromium Bose-Einstein condensates (BECs) [15] have been recently followed by the realization of quantum gases in other highly magnetic species, including dysprosium Bose and Fermi gases [16] and erbium condensates [17]. Significantly more dipolar gases may be realized by means of polar molecules, which have large electric dipole moments of the order of a debye or larger. Seminal experiments on KRb molecules at the Joint Institute for Laboratory Astrophysics [18] have opened the door towards achieving a quantum degenerate gas of polar molecules, and various experimental groups worldwide are currently involved in this enterprise [19,20]. Rydberg gases constitute yet another possible realization of highly dipolar gases [21]. The successful manipulation of polar lattice gases in optical lattice experiments could lead to the observation of supersolid phases.

On the other hand, the ability to produce frustration in optical lattices of cold atoms has opened up possibilities to realize interesting superfluid and Mott states which have additional kinds of order arising from the kinetic frustration [22–24]. Kinetic frustration in these systems is produced by the competition of two different hopping processes from a site to different sites with different signs of the hopping amplitude. The two different hopping processes could be to a nearest-neighbor site and a next-nearest-neighbor site. It is thus interesting to study the interplay between nearest-neighbor interaction and kinetic frustration away from commensurate densities, which can potentially stabilize a supersolid phase.

In this paper, we study such a model of hard-core bosons hopping on a one-dimensional lattice with nearest-neighbor hopping and interaction and next-nearest-neighbor hopping that induces kinetic frustration as shown in Fig. 1(a). This model is equivalent to a system of a triangular ladder as shown in Fig. 1(b). The model describing such a system can be described by the Hamiltonian

$$H = -t\sum_i (a_i^\dagger a_{i+1} + \text{H.c.}) - t'\sum_i (a_i^\dagger a_{i+2} + \text{H.c.}) + \sum_i V\left(n_i - \frac{1}{2}\right)\left(n_{i+1} - \frac{1}{2}\right), \quad (1)$$

where $a_i^\dagger$ and a_i are creation and annihilation operators for hard-core bosons at site i, and $n_i = a_i^\dagger a_i$ is the boson number operator at site i; t and t' are the nearest- and next-nearest-neighbor hopping amplitudes; and V represents the nearest-neighbor repulsion. Frustration in this model is introduced by choosing $t > 0$ and $t' < 0$. The model described by Eq. (1) can also be thought of as a triangular ladder where the nearest-neighbor hopping and interaction are along the rungs and the next-nearest-neighbor hopping is along the legs. In this work we scale the energies with respect to t by considering $t = 1$; therefore, all the parameters considered are dimensionless. As discussed in Ref. [25], this model does not have a simple representation in terms of spinless fermions due to the presence of the next-nearest-neighbor hopping term. At half filling and for $V = 0$, apart from the trivial point $t' = 0$, there exists one more point corresponding to $t' = -t/2$, where the exact ground state can be obtained [25].

The model of Eq. (1) has been studied recently by us at half filling [25]. The ground-state phase diagram has three different phases, a uniform superfluid (SF), an insulating charge-density-wave (CDW) crystal, and a bond-ordered (BO) insulator. When $t = |t'|$, only the insulating (gapped) phases occur and there is a first-order transition between them as a

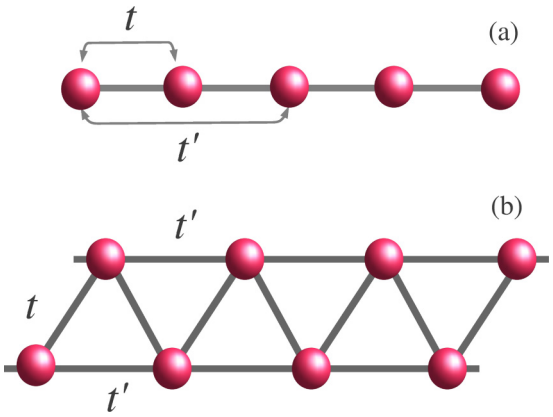

FIG. 1. (Color online) (a) One-dimensional lattice with nearest- and next-nearest-neighbor hopping. (b) Equivalent triangular ladder geometry. The arrows indicate the hopping directions.

function of V. In this paper we study the system by doping it away from half filling to see what types of gapless phases might arise. By performing a detailed analysis using the finite-size density-matrix renormalization group (DMRG) method, we obtain a complete ground-state phase diagram for this model. Our main result is that in addition to the gapped CDW and BO phases, the phase diagram contains a gapless supersolid (SS) phase, which is a phase with concurrent superfluid and charge-density-wave order. This is summarized in the phase diagram of Fig. 2, which is plotted as a function of the chemical potential μ and interaction V. In the following sections, we present details of our calculations.

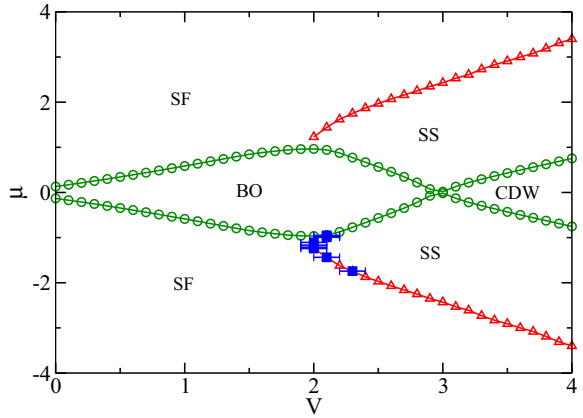

FIG. 2. (Color online) Phase diagram of the t-t'-V model commensurate and incommensurate with $t' = -t$ in the chemical potential and interaction (μ, V) plane. Both μ and V are in units of t and $\mu = 0$ corresponds to the case of half filling where only the CDW and BO phases occur. For other values of μ, we obtain the additional supersolid phase (SS). The phase boundaries marked with (green) circles are those between gapped and gapless phases and are obtained by calculating the charge gap. The phase boundaries marked with (red) triangles and (blue) squares with error bars for some values of V are between the gapless superfluid and the supersolid phases and are determined by looking at the diverging compressibility and the structure factor, respectively, as explained in the text.

II. DETAILS OF THE DMRG METHOD

We study the model described by Eq. (1) using the finite-size DMRG method with open boundary conditions [26,27]. This method is best suited for (quasi-)one-dimensional problems [27]. For most of our calculations we study system sizes of up to 200 sites and retain up to 256 density matrix eigenstates with the weight of the discarded states in the density matrix less than 1×10^{-6}. We compute various physical quantities to characterize the different phases. Some of these quantities have been calculated by us using the DMRG method to study related models [25,28]. We describe below the quantities which are most important for the characterization of the different phases.

In order to distinguish between gapped and gapless phases, we calculate the chemical potentials

$$\mu = (\mu^+ + \mu^-)/2, \tag{2}$$

where $\mu^+ = E(N+1,L) - E(N,L)$ and $\mu^- = E(N,L) - E(N-1,L)$. In Eq. (2), $E(L,N)$ is the ground-state energy of the system with L sites and N bosons.

The CDW order in the system can be quantified by calculating the structure factor, which is the Fourier transform of the density-density correlation function

$$S(k) = \frac{1}{L^2} \sum_{i,j} e^{ik(i-j)} \langle n_i n_j \rangle. \tag{3}$$

The BO phase is characterized by a nonzero value of the bond-order parameter

$$O_{\mathrm{BO}} = \frac{1}{L} \sum_i (-1)^i B_i, \tag{4}$$

where

$$B_i = \langle a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i \rangle. \tag{5}$$

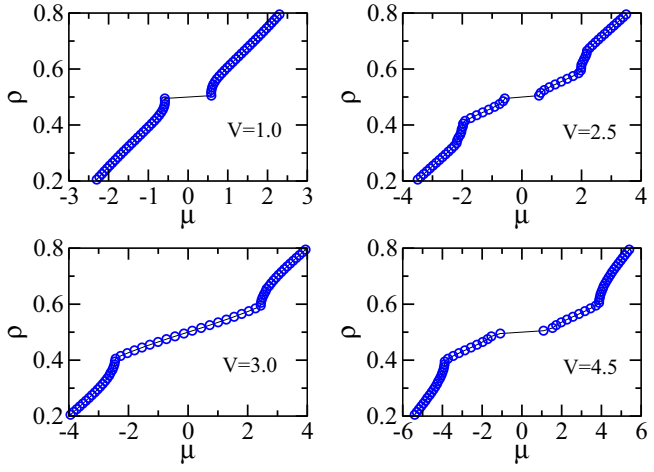

FIG. 3. (Color online) Plots of ρ vs μ for different values of V. The appearance of a plateau indicates an incompressible (gapped) phase. The length of the plateau measured along the μ direction gives the size of the gapped region in the phase diagram at a given V. At $V = 3.0$, which is where the direct transition from CDW to BO occurs at $\mu = 0$, the gap exists only very close to the transition point and hence there is no plateau.

III. RESULTS AND DISCUSSION

We first discuss how to obtain the signature of the gapless and gapped phases at incommensurate and commensurate densities, respectively. This is done by computing the chemical potential μ defined in Eq. (2) for various densities ρ. We start at a value of ρ far away from half filling and then dope the system to increase ρ gradually. Since the model considered is particle-hole symmetric, the signatures at densities above half filling are mirror reflections of those below half filling. The gapless-to-gapped transition can be seen in the ρ-μ plot as shown in Fig. 3. It can be seen that there exists a jump in μ as a function of ρ at $\rho = 0.5$ for different values of V. The corresponding length of the plateau in ρ decreases as $V \sim 3.0$, where the gap exists only very close to the transition between CDW and BO phases at $\mu = 0$ and again increases. The end points of the plateaus trace out the BO and CDW phases which are shown in Fig. 2. The BO and CDW phases are characterized by the finite bond-order parameter and density-wave structure factor as defined in Eqs. (4) and (3), respectively.

It is obvious from Fig. 3 that the compressibility $\partial\rho/\partial\mu$ is zero along the plateau and is finite on the shoulders around the plateau. However, it should be noted that there is a kink in the ρ vs μ plot for $V \geqslant 2.0$, where the chemical potential tends to saturate with respect to ρ and therefore the compressibility diverges. These kinks appear for all the values of $V \geqslant 2.0$ considered in our calculation. The divergent compressibility can be regarded as the signature of a phase transition which can be located from the kink position. This phase transition corresponds to the transition among the gapless phases, the SS, and the SF. Once, ρ is increased beyond the position of the kink, μ increases monotonically with ρ indicating a finite compressibility in the gapless SS phase. The kink positions which give us the phase boundaries between the gapless phases are shown in Fig. 2. Note that we cannot characterize the nature of these gapless phases (i.e., say whether they are SS or SF) from the above analysis. For

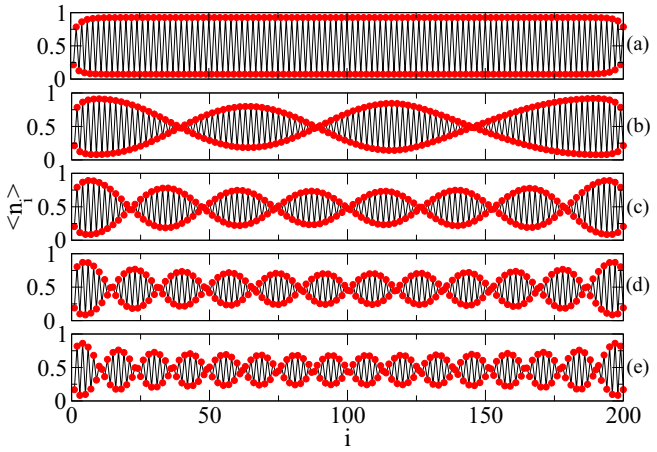

FIG. 4. (Color online) On-site number density $\langle n_i \rangle$ plotted as a function of site index i for different values of ρ with (a) $\rho = 0.50$, (b) $\rho = 0.49$, (c) $\rho = 0.48$, (d) $\rho = 0.47$, and (e) $\rho = 0.46$ for $V = 4.0$. It can be seen that while there is perfect CDW order at $\rho = 0.5$, there is a modulation over at a wave vector k_m that appears as one moves away from $\rho = 0.5$.

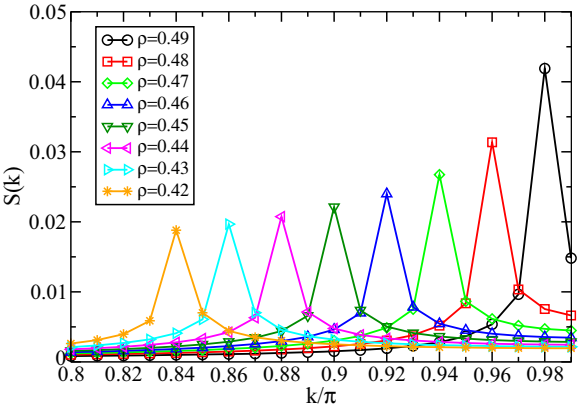

FIG. 5. (Color online) $S(k)$ vs k for different densities for $V = 4.0$. It can be seen that the location of the peak shifts away from $k = \pi$ as the filling ρ decreases for $\rho = 0.5$. The shift is found to be linear in ρ such that the modulation vector $k_m = 2\pi\rho$.

that we require calculation of the correct order parameters as well, which we discuss in the following sections. The CDW and BO phases which occur at $\mu = 0$ are gapped and thus one would expect them to remain robust to small changes in μ. Thus, we would expect the CDW and BO phases to appear as lobes (as seen in Fig. 2). To understand what happens as we move away from half filling, we calculate the density-density structure factor as defined in Eq. (3) and also look at the local density n_i as a function of lattice site i. It can be seen from Fig. 4 that there is a modulation of the density with wave vector k_m superimposed on the CDW order as the filling is changed from $\rho = 0.5$. We can quantify the dependence of k_m on ρ by plotting the density-density structure factor $S(k)$ as in Fig. 5. With a modulation k_m in the density, $S(k)$ has a peak at $k = \pi - k_m$, which can be seen as the peak shifts away from $k = \pi$ as ρ changes. Tracking the positions of the peaks yields $k_m = 2\pi\rho$. A similar feature has been studied before in a system of hard-core bosons in a zigzag ladder [29]. From Fig. 3, it can be seen that the state one obtains for $\rho \neq 0.5$, where the density modulation occurs, is a compressible (gapless) state and thus corresponds to a SS.

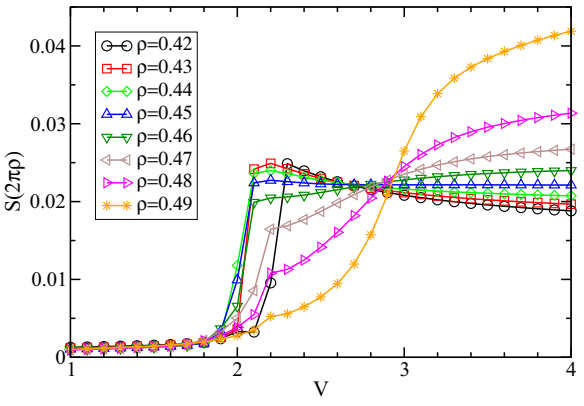

FIG. 6. (Color online) $S(k = 2\pi\rho)$ is plotted as a function of V for different ρ. The peak position drifts linearly with the filling fraction ρ. The modulation wave vector $k_m = 2\pi\rho$.

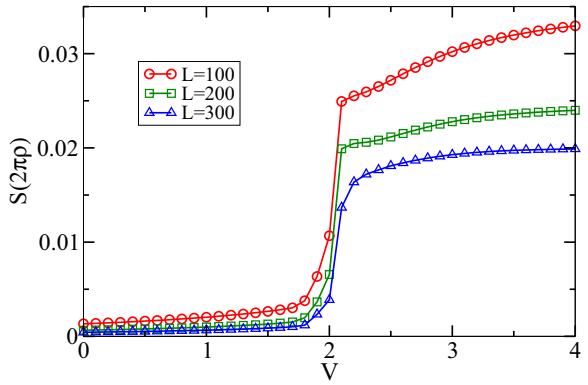

FIG. 7. (Color online) Plot of $S(\pi - k_m)$ vs V for $\rho = 0.46$ for different system sizes shows that there is a fairly steep jump at a particular value of V which does not appear to drift appreciably with increasing system size. However, the jump seems to become more gradual with increasing system size.

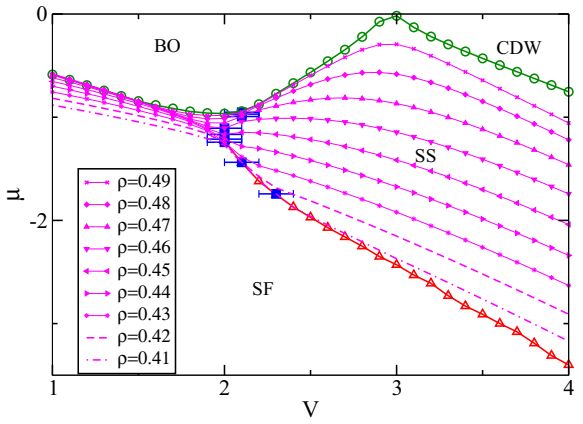

FIG. 8. (Color online) An enlarged view of the SS lobe and regions around it of the phase diagram of Fig. 2, with the lines of constant density marked.

However, it is a supersolid, where the charge ordering wave vector is dependent on the filling ρ.

The SS phase shares phase boundaries with the CDW, BO, and SF phases as can be seen from Fig. 2. The phase boundary between the SS and gapped CDW and BO phases is obtained by measuring the charge gap, which is zero in the SS phase but finite in the gapped phases. The other phase boundary between the SS and the SF phases cannot be obtained in this way since they are all gapless. To obtain this boundary we plot the peak value of the structure factor $S(\pi - k_m)$ as a function of V for different values of ρ as shown in Fig. 6. The value of $S(\pi - k_m)$ at each density as a function of V shows a fairly steep increase at a particular value of V. The value of V at which this happens does not drift appreciably with increasing system as shown in Fig. 7 although it appears steeper for smaller system sizes. The phase boundary obtained this way coincides with the one obtained from the positions of the kinks in the plots of Fig. 3 as discussed earlier. This validates this particular way of obtaining the phase boundary. The lines of constant density in the SS and SF phases of the phase diagram can be seen in Fig. 8.

The SF phase might be stabilized over a larger part of the phase diagram and be easier to detect if we choose a different set of parameters, say $|t'| < t$. As we have seen in our previous work, for such a choice of parameters, it is possible to obtain a regular superfluid phase even exactly at half filling [25] and it is quite likely that this phase will remain over a fairly large part of the phase diagram even when we move away from half filling. However, for these parameters, it is likely that the SS phase will occupy a smaller region of the phase diagram (see Fig. 8).

IV. CONCLUSIONS

We have studied a system of hard-core bosons in a one-dimensional optical lattice with frustrated next-nearest-neighbor hopping and nearest-neighbor interaction. Using the finite-size DMRG method we have obtained the ground-state phase diagram of this model and have shown that in addition to gapped CDW and BO phases, it also displays the regular SS phase, which has concurrent superfluid and CDW order.

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