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Supersolids in one-dimensional Bose-Fermi mixtures

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Using quantum Monte Carlo simulations, we study a mixture of bosons and fermions loaded on an optical lattice. With simple on-site repulsive interactions, this system can be driven into a solid phase. We dope this phase and, in analogy with pure bosonic systems, identify the conditions under which the bosons enter a supersolid phase, i.e., exhibit at the same time charge density-wave and superfluid order. We perform finite-size scaling analysis to confirm the presence of a supersolid phase and discuss its properties, showing that it is a collective phase that also involve phase coherence of the fermions.

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The supersolid (SS) phase in which superfluid and solid order coexist was first examined in ^{4}He systems more than 50 years ago.[1] The presence of a SS phase was conclusively demonstrated in several lattice models such as variants of the bosonic Hubbard model. However, this phase has not been unambiguously observed experimentally and, with the recent progress in low-temperature physics, the search for experimental evidence of a SS phase has been reinvigorated.

In solid helium, a nonclassical reduction in the moment of inertia was observed in torsional oscillator measurements.[2,3] This reduction is due to the appearance of a superfluid fraction in the material and has been first interpreted as a sign of a SS phase. However, several experimental[4–6] and numerical studies[7–9] suggested that this superfluid behavior was, in fact, due to the presence of nonlocal defects in the system (grain boundaries for examples) along which superfluid currents exist. The presence of a bulk supersolid phase thus appears to be questionable in these systems.

Another promising approach for finding a SS phase emerged in the context of cold atoms loaded on optical lattices. Such systems, being well described by bosonic Hubbard models, are a good starting point to look for supersolids. However, the conditions necessary for supersolids to appear in these models are not easily achieved in real experiments; one generally observes a direct solid-superfluid transition[10] or a coexistence of superfluid and solid (in the case of a first-order phase transition).[11] Supersolids are stabilized in these models by specific long-range interactions[12–18] or long-range hopping terms.[19] Engineering precisely the values of the interaction as a function of distance appears to be tricky to achieve.

Recently Bose-Fermi mixtures have been introduced as a way to study the physics of fermions, using sympathetic cooling with the bosons to reach very low temperatures.[20,21] However, several theoretical studies[22–27] have shown that such mixtures loaded on optical lattices have a rich phase diagram where collective phases of fermions and bosons appear. Interestingly, with simple repulsive on-site interactions between fermions and bosons, the system can be driven into a solid phase where density-wave order develops.[25] In this paper, we will study the doping of such a solid phase and see under what conditions it could be driven into a bosonic supersolid phase. Other recent studies suggested the presence of SS behavior in Bose-Fermi mixtures.[28–31] Our study is performed on the translationally invariant system, in other words in the absence of a confining trap. The results are expected to be valid for the experimental system with a trap via the use of the local density approximation (LDA). In this approximation, the trap potential is treated as a local chemical potential and the phase of the system is expected to be locally that of the uniform system with the same chemical potential. The LDA has been shown to give an accurate mapping of the phases of the uniform system onto those of the trapped one.[32]

The paper is organized as follows. In Sec. I, we introduce the model and discuss the solid phase which is the starting point of our study. In Sec. II, we explore the different ways of doping this system and determine which one could lead to a supersolid phase. Finally, in Sec. III, we perform finite-size scaling analysis of physical quantities to verify if the supersolid phase persists in the thermodynamic limit.

I. SOLID PHASE IN THE BOSE-FERMI HUBBARD MODEL

We study a one-dimensional Hubbard model for a mixture of bosons and polarized (spinless) fermions. The Hamiltonian is given by

$$\mathcal{H} = \sum_{r=1}^{L} (-t_{\mathrm{b}} b^{\dagger}_{r+1} b_r - t_{\mathrm{f}} f^{\dagger}_{r+1} f_r + \mathrm{h.c.}) + \sum_{r=1}^{L} \left(U_{\mathrm{bb}} \frac{n^{\mathrm{b}}_r (n^{\mathrm{b}}_r - 1)}{2} + U_{\mathrm{bf}} n^{\mathrm{b}}_r n^{\mathrm{f}}_r \right), \tag{1}$$

where $b^{\dagger}_r$ (b_r) creates (destroys) a boson on site r, while $f^{\dagger}_r$ and f_r are the corresponding operators for fermions. The first term in Eq. (1) describes tunneling of bosons and fermions between neighboring sites, with different associated energies t_{b} and t_{f}. In the following, the energy scale is fixed by choosing $t_{\mathrm{b}}=1$. n^{b}_r and n^{f}_r are the bosonic and fermionic number operators at site r, and U_{bb} and U_{bf} are the boson-boson and boson-fermion contact repulsion terms. L is the total number of sites in a one-dimensional chain.

We will be mostly interested in the behavior of bosons and will, therefore, study the bosonic Green's function $G_{\mathrm{b}}(R)$ which measures phase correlations

$$G_b(R) = \frac{1}{L}\sum_{r=1}^{L} \langle b_{r+R}^{\dagger} b_r + b_r^{\dagger} b_{r+R}\rangle \tag{2}$$

as well as the boson superfluid density $\rho_s = \langle W^2 L\rangle/(2\beta t_b)$ where W is the winding number[33] and β the inverse temperature. The density-density correlation function

$$D_b(R) = \frac{1}{L}\sum_{r=1}^{L} [\langle n_{r+R}^{b} n_r^{b}\rangle - \langle n_{r+R}^{b}\rangle\langle n_r^{b}\rangle] \tag{3}$$

and its Fourier transform, the structure factor $S_b(k)$, give information on possible solid density-wave order.

We study this model using two different versions of the worm algorithm: the canonical worm (CW) (Refs. 34 and 35) algorithm (CW) and the directed stochastic Green's function (DSGF) (Refs. 36 and 37) algorithm. The CW method, which is very efficient for measurement of equal time Green's functions, has to be modified to include simultaneous updates of bosons and fermions to allow the study of mixtures.[38] However, this algorithm sometimes becomes inefficient for large system sizes ($L>20$), especially failing to sample different winding numbers which is necessary to calculate the superfluid density.[33] In those cases, we used the DSFG which explores a much larger configuration space and thus allows more efficient fluctuations of the winding number and the measure of ρ_s. The two algorithms gave results in agreement for other quantities in the range of sizes we used.

This model was widely studied in the special case where the total number of particles equals the number of sites $N_b + N_f = L$ where $N_{b(f)}$ is the number of bosons (fermions).[24,38] For large enough values of the repulsions, double occupancy of sites is forbidden and one can describe the system in terms of a pseudo-spin-1/2 $\sigma_r^z = n_r^b - n_r^f = \pm 1$.[22,23] The Hamiltonian can then be mapped, in the low energy limit, into an effective Heisenberg Hamiltonian

$$\mathcal{H}_{\text{eff}} = \sum_r J_{xy}(\sigma_r^x\sigma_{r+1}^x + \sigma_r^y\sigma_{r+1}^y) + \sum_r J_z\sigma_r^z\sigma_{r+1}^z, \tag{4}$$

where $J_{xy} = -t_b t_f/U_{bf}$ and $J_z = (t_b^2 + t_f^2)/(2U_{bf}) - t_b^2/U_{bb}$. When $J_z > |J_{xy}|$, the pseudospin system enters a Néel antiferromagnetic phase along the z axis.[39] In terms of bosons, this antiferromagnetic order corresponds to a density-wave order with alternating occupied and empty sites (see Fig. 1). Green's function, $G_b(R)$, decays exponentially indicating the absence of phase coherence. This phase persists in the thermodynamic limit at zero temperature (see Fig. 1, inset).

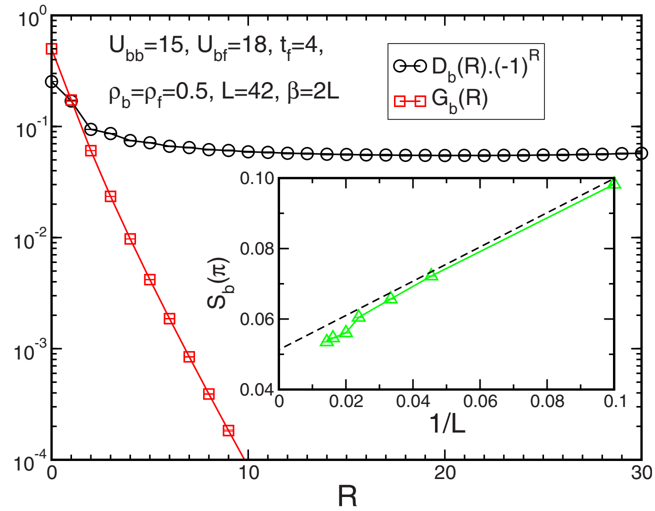

FIG. 1. (Color online) Density-density correlation $D_b(R)$ (multiplied by $(-1)^R$)and Green's function $G_b(R)$ for the bosons in the solid ordered phase. Inset: finite-size behavior of the bosonic structure factor $S_b(\pi)$ for the same parameters and sizes ranging from $L=10$ to 70.

II. DOPING THE SOLID PHASE

A similar density wave ordered phase for $N_b = L/2$ is observed in a one-dimensional bosonic system with near-neighbor repulsion.[17] In this latter system, a supersolid phase can be present when the solid phase is doped by adding bosons. However, for a supersolid phase to appear, the interactions must be chosen so that the added bosons do not introduce defects in the previous solid order: they must preferentially come on sites already occupied by bosons. A mean-field argument yields that the repulsion between bosons located on neighboring sites must be greater than half the on-site repulsion U_{bb}.

Following this example, we consider a system where the repulsion between bosons, $U_{bb}=15$, is smaller than the boson-fermion repulsion $U_{bf}=18$. Starting from the solid phase obtained for $N_b = N_f = L/2$ and $t_f=4$,[25] we changed slightly the number of the different types of particles and observed how the solid order was modified (see Fig. 2).

We found that upon changing the number of fermions, some defects are introduced in the solid order, which are exposed by the characteristic beating in the density-density correlations (Fig. 2, top).[40] On the other hand, when one changes the number of bosons, the density-wave order of alternating empty and filled sites persists (Fig. 2, bottom). A surprising result is that this wave order is present even when the number of bosons is reduced below half-filling, unlike what happens in the purely bosonic model with near neighbor repulsion.[17]

Examining the bosonic structure factor $S_b(\pi)$ (Fig. 3), we observe that only the case $N_f = L/2$ leads to large $S_b(\pi)$ and therefore to the long-range density order necessary for the establishment of SS. We also observe in Fig. 3 that when the bosonic population is doped above or below half-filling, $S_b(\pi)$ drops but remains rather appreciable especially above half-filling. Finite-size scaling is required to establish if these nonvanishing values of $S_b(\pi)$ persist in the thermodynamic limit (see Sec. III).

As expected, quasi-long-range phase coherence is recovered as soon as the solid is doped away from half-filling (see Fig. 4) and the bosons become superfluid. This phase coherence is stronger when the system is doped above half-filling.

These results lead to the conclusion that a supersolid phase can only be found for $N_f = L/2$, where no defects are introduced in the solid order. Doping the bosons above half-filling provides the best candidate to observe a supersolid as both the structure factor and the phase coherence are larger

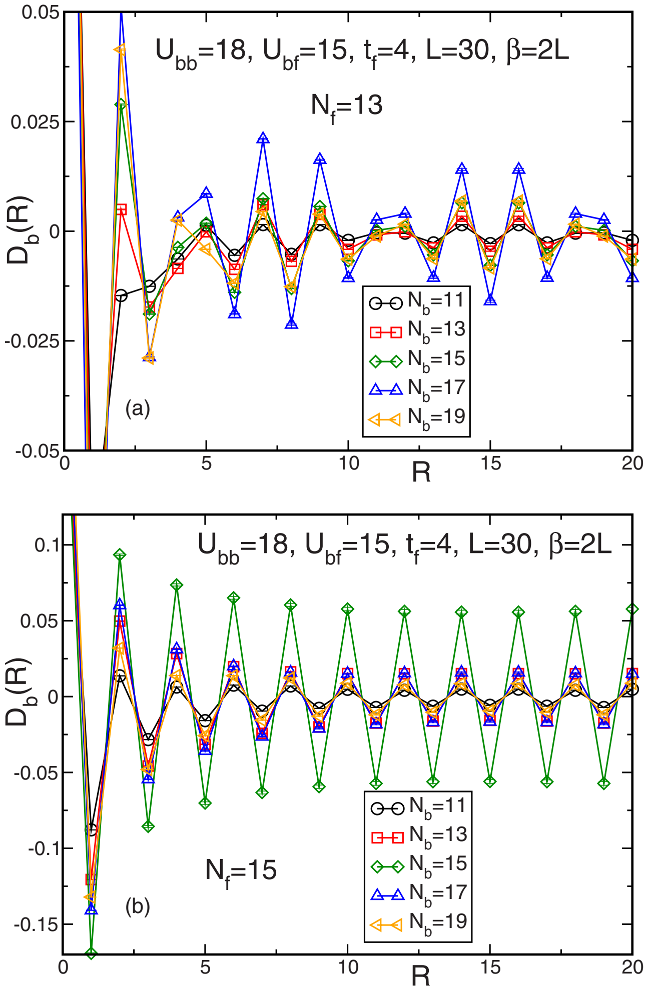

FIG. 2. (Color online) Density-density correlations for different boson fillings, N_{b}, and for two different fermion fillings, $N_{\mathrm{f}}=L/2-2$ and $N_{\mathrm{f}}=L/2$. In the first case (a), we observe the beating characteristic of the pseudospin phase at nonzero magnetization along z with a maximum when $N_{\mathrm{f}}+N_{\mathrm{b}}=L$. In the second case (b), we see a long-range order (or quasi-long-range) for the bosons.

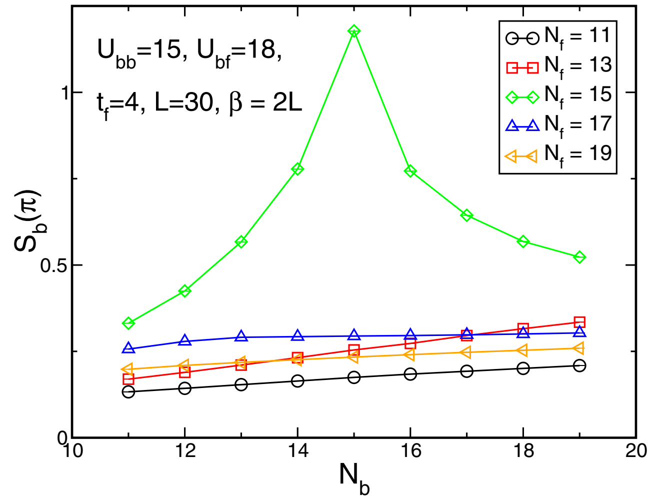

FIG. 3. (Color online) Structure factor $S_{\mathrm{b}}(\pi)$ as a function of the number of bosons N_{b} for different fermion fillings, N_{f}. The oscillations characterizing a density order only develop for $N_{\mathrm{f}}=L/2$.

in this case, but doping below half-filling could also yield to a supersolid phase. Finite-size analysis of the behavior of ρ_s and $S_{\mathrm{b}}(\pi)$ is needed to verify if the supersolid phase persists in the thermodynamic limit.

III. FINITE-SIZE ANALYSIS

In this system, the sizes that can be used in the finite-size scaling analysis are quite limited. In order to avoid sign problems, $N_{\mathrm{f}}=L/2$ must be odd. In addition, L cannot be very large in order for the simulation to converge in reasonable time. We used two different densities of bosons, $N_{\mathrm{b}}/L=0.4$ and 0.6 (one below and one above half-filling) which give an integer number of bosons for sizes $L=10,30,50\ldots$. When we could not obtain exactly these densities with the given constraints, we used the number of bosons that gives the closest density.

We first performed the finite-size analysis with the parameters used in the first part of this paper ($U_{\mathrm{bb}}=18$, $U_{\mathrm{bf}}=15$, $t_{\mathrm{f}}=4$) and above half-filling ($N_{\mathrm{b}}/L=0.6$). Figures 5 and 6 show that, for this case, the structure factor goes to zero in the thermodynamic limit while the superfluid density remains finite. This indicates that what appears to be a supersolid phase for small L is in fact a superfluid. Varying the different available parameters (U_{bb}, U_{bf}, t_{f}), we observed that increasing t_{f} increases noticeably the value of $S_{\mathrm{b}}(\pi)$, whereas varying the interaction did not yield similar variations. For $t_{\mathrm{f}}\geq 5$ (see Fig. 5) $S_{\mathrm{b}}(\pi)$ extrapolates to a finite value as L increases. This indicates that for these values of t_{f} the density-wave order survives in the thermodynamic limit when $N_{\mathrm{b}}=0.6L$ and $N_{\mathrm{f}}=L/2$.

In Fig. 6 we see that the superfluid density changes very little with L or t_{f}: ρ_s then goes to a finite value when $L\to\infty$. As mentioned above, obtaining precise values for ρ_s is difficult but, on the other hand, Green's function, $G_{\mathrm{b}}(R)$, is

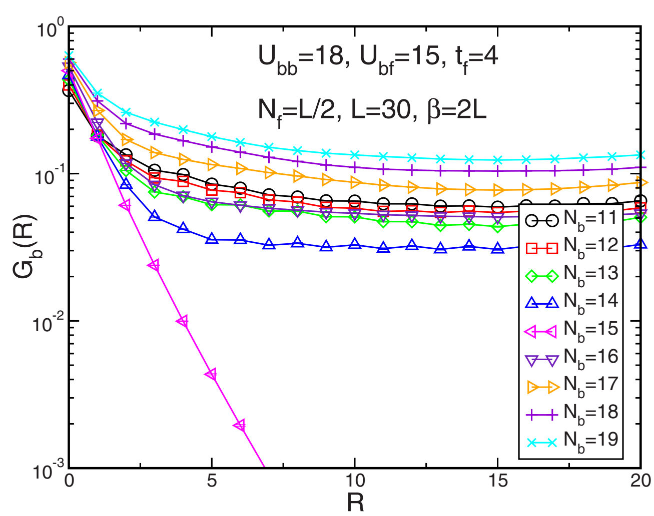

FIG. 4. (Color online) Phase correlation, $G_{\mathrm{b}}(R)$, for different boson fillings. There is always an algebraic decay characteristic of a superfluid in one dimension, except at double half-filling in the solid phase.

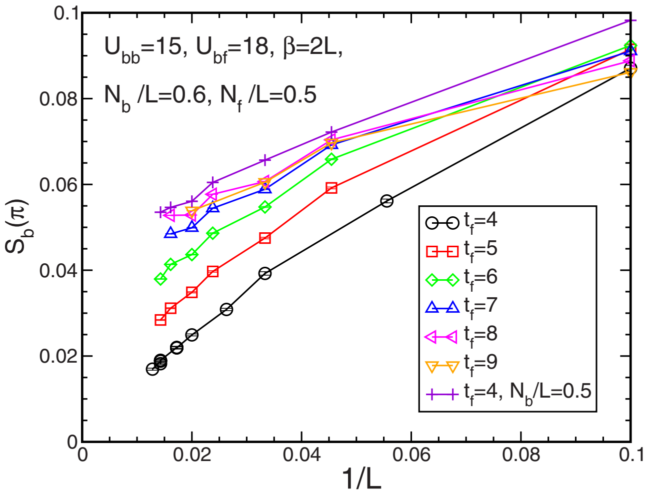

FIG. 5. (Color online) Finite-size scaling of the structure factor $S_{\rm b}(\pi)$ for different values of the hopping parameter $t_{\rm f}$. The structure factor goes to zero in the large size limit for $t_{\rm f}=4$. For $t_{\rm f}>4$, in the range of sizes that are accessible, the structure factor is nonzero.

measured with very good statistical accuracy and can, therefore, also be used to characterize the nature of the phase coherence. Figure 7 shows that $G_{\rm b}(R)$ exhibits power-law decay for all the sizes and values of the fermion hopping parameter we have studied (for $N_{\rm b}=0.6L$), confirming the existence of a quasi condensate which leads to a superfluid behavior in the presence of long-range density order for the fermions.

This indicates the presence of a supersolid phase in this system for $t_{\rm f}\geq 5$, $U_{\rm bb}=18$, $U_{\rm bf}=15$, and $N_{\rm b}=0.6L$.

So far, we have concentrated on the behavior of the bosons. However, the supersolid phase we have exposed is necessarily a collective phase of fermions and bosons. To study the behavior of fermions or the collective behavior of

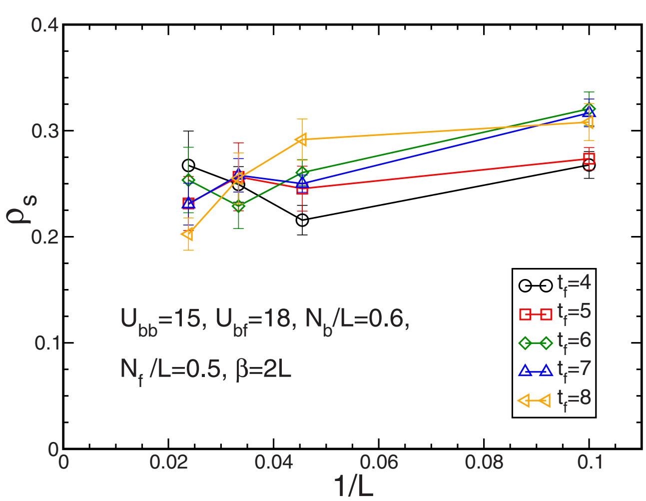

FIG. 6. (Color online) Finite-size scaling of the superfluid density ρ_s in the case where the system is doped above half-filling. Reliable results for this quantity are difficult to obtain for sizes larger than $L>42$. However, ρ_s shows very little variations when L or $t_{\rm f}$ vary and should then remain nonzero in the large L limit for all cases.

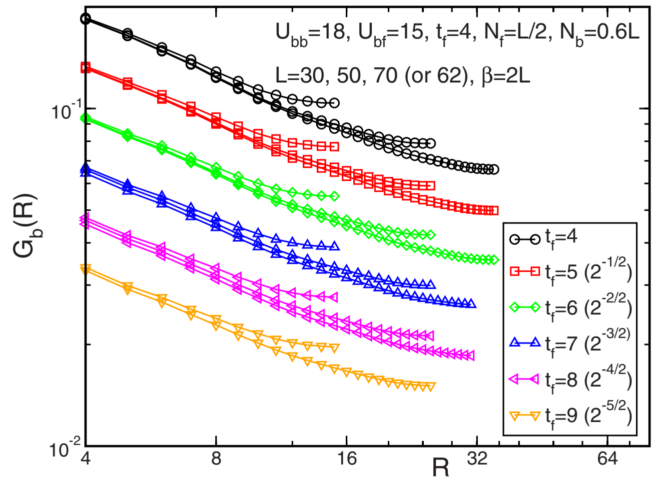

FIG. 7. (Color online) Finite-size scaling of Green's function $G_{\rm b}(R)$ for several values of the hopping parameter $t_{\rm f}$. $G_{\rm b}(R)$ always appears to decay algebraically. The curves have been multiplied by a factor indicated in the legend between parentheses.

fermions and bosons, we introduce Green's functions for fermions $G_{\rm f}$, boson-fermion pairs $G_{\rm bf}$, and boson-hole pairs $G_{\rm bh}$.

$$G_{\rm f}(R)=\frac{1}{L}\sum_{r=1}^{L}\langle f_{r+R}^{\dagger}f_r+f_r^{\dagger}f_{r+R}\rangle \tag{5}$$

$$G_{\rm bf}(R)=\frac{1}{L}\sum_{r=1}^{L}\langle f_{r+R}^{\dagger}b_{r+R}^{\dagger}b_r f_r+\text{h.c.}\rangle \tag{6}$$

$$G_{\rm bh}(R)=\frac{1}{L}\sum_{r=1}^{L}\langle f_{r+R}b_{r+R}^{\dagger}b_r f_r^{\dagger}+\text{h.c.}\rangle \tag{7}$$

Figure 8 shows that these Green's functions have alge-

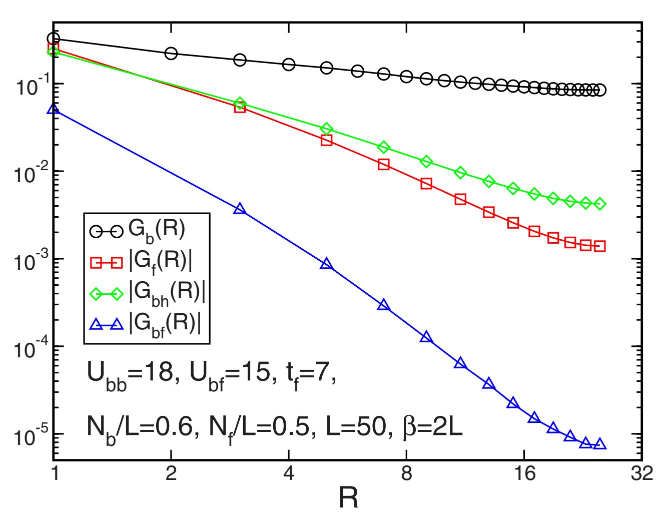

FIG. 8. (Color online) Green's functions for bosons, fermions, boson-fermion pairs, and boson-hole pairs in the candidate supersolid phase. All Green's functions have algebraic decay.

braic decay in the candidate supersolid phase. The dominant correlations are those of individual bosons; they have the slowest decay and the largest values. However, a description only in terms of bosons does not fully characterize this phase; we see that individual fermion, boson-hole, and boson-fermion pairs also have algebraic phase correlations and are also relevant degrees of freedom in the system. The boson-hole pairs have much stronger phase correlations than the boson-fermion pairs. This is to be expected since anticorrelated movement of bosons and fermions is a generic phenomenon in such mixtures with repulsive interactions.[22,25,41]

In a similar way to the case above half-filling, we performed finite-size scaling analysis when the system is doped below half-filling ($N_b/L=0.4$). We studied a case where the value of t_f is quite large ($t_f=7$), since we observed in the previous case that it improves the structure factor. We find that, as for the case above half-filling, the structure factor and the superfluid density both go to a finite value in the large L limit and that a supersolid phase is, therefore, thermodynamically stable (see Fig. 9). This behavior is different from what happens in the bosonic case with near-neighbor interactions where doping below half-filling leads to a superfluid with solitonlike quasiparticles.[17,40]

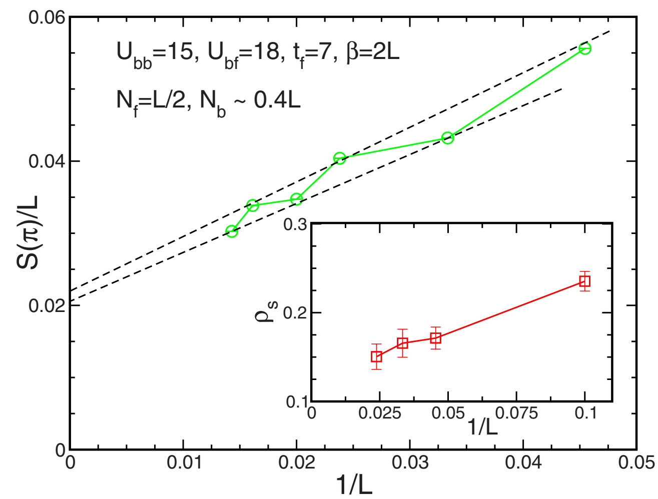

FIG. 9. (Color online) Finite-size scaling of the structure factor $S_b(\pi)$ below half-filling ($N_b/L=0.4$) for $t_f=7$. The structure factor goes to a nonzero value in the large size limit. The observed oscillations are due to the fact that we obtained exactly the desired density ($N_b/L=0.4$) only for $L=30$, 50, and 70.

IV. CONCLUSION

In this paper we have studied, using exact QMC simulations, the formation of supersolid phases in the ground state of Bose-Fermi mixtures on optical lattices. At double half-filling, $N_b=N_f=L/2$, and for sufficiently large t_f/t_b, the system exhibits long-range density order as exposed by $S_b(\pi)$.[25] Inspired by the behavior of the extended bosonic Hubbard model, which exhibits a supersolid phase above half-filling when the near-neighbor repulsion is large enough compared to the contact term,[12,17] we found that, similarly, when $U_{bf}>U_{bb}$ and the system is doped by adding bosons, the system enters a supersolid phase. It is important to keep in mind that this phase is a collective Bose-Fermi phase: the various Green's functions (boson-boson, fermion-fermion, and boson-fermion) we have presented demonstrate this clearly.

Surprisingly, we have also found that upon doping the system below half-filling for the bosons, we also obtain a stable supersolid phase. This is different from the behavior of the purely bosonic system.

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