Ultra-cold atomic gases in light induced periodic potentials have become an important experimental testing ground for concepts of many-body physics since they allow the realization of precisely controllable model Hamiltonians with widely tunable parameters. A system which has attracted particular interest in the recent past is a mixture of bosons and spin-polarized fermions in a deep lattice potential, described by the Bose-Fermi-Hubbard model (BFHM) [1, 2]. Mixing lattice bosons with fermions, Günther et al. [3] and Ospelkaus et al. [4] observed an unexpected reduction of bosonic superfluidity which triggered a number of theoretical and experimental studies on the influence of fermions on boson superfluidity. In the limit of small fermion mobility the phase diagram can be well understood by mapping to the purely bosonic Hubbard system with binary disorder [5, 6]. For increasing fermionic hopping amplitudes a number of new phenomena emerge [7], including polaronic phases [8] and density waves [9, 10]. Furthermore under certain conditions bosons can enter the a supersolid phase (SS), where CDW and off-diagonal long-range order coexist [11, 12, 14].

In the present paper we study the 1D BFHM in the limit of large fermion hopping which allows for a rather comprehensive understanding of the existing phases and their origin in particular in the case of half filling of the spin-polarized fermions. In the large hopping limit the fermions can be formally integrated out [11, 13, 15] resulting in an oscillating mean-field potential as well as a long-range density-density interaction between the bosons. This interaction has alternating sign if the fermion filling is commensurate with the lattice which is the origin of the 4k_F CDW. In the thermodynamic limit it is however formally divergent and needs to be renormalized which is done here by taking into account the back-action of the bosons to the fast fermions. The resulting effective boson model allows an analytic and quantitative prediction of the \((\mu_B - J_B)\) phase diagram, where \(\mu_B\) is the bosonic chemical potential and \(J_B\) the corresponding hopping amplitude. At double-half filling, i.e. \(q_F = q_B = 1/2\), we identify an incompressible CDW phase and study its transition to a SF with increasing \(J_B\) both using analytic results from the effective model and numerical simulations based on DMRG [16]. DMRG simulations also show the presence of a novel phase with coexistence between spatially separated Mott-insulator and CDW regions for non-commensurate boson filling. This phase which is absent for an extended Bose-Hubbard model [17] can be well explained within the effective model and is shown to exist for all values of the boson-fermion interaction. As the effective theory describes the appearance of a density wave on a quantitative level it is expected to explain also the conditions for the existence of a SS found in [14] using quantum Monte Carlo simulations. Numerical evidence was given [14] that a SS exists only if the filling of spin-polarized fermions is exactly one half but that of bosons is non-commensurate and if the boson-fermion repulsion exceeds that of the bosons. The emergence of a finite superfluid fraction from the effective model will be discussed at a different place [18].

Mixtures of ultracold bosons and spin-polarized fermions in optical lattices are well described by the Bose-Fermi-Hubbard Hamiltonian [19, 20]

\[
\hat{H} = -J_B \sum_{j} (\hat{b}_j^\dagger \hat{b}_{j+1} + \hat{b}_{j+1}^\dagger \hat{b}_j) + \frac{U}{2} \sum_{j} \hat{n}_j (\hat{n}_j - 1) - J_F \sum_{j} (\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j) + V \sum_{j} \hat{n}_j \hat{n}_j,
\]

where \(\hat{b}_j^\dagger, \hat{b} (\hat{c}_j^\dagger, \hat{c})\) are bosonic (fermionic) creation and annihilation operators and \(\hat{n}_j (\hat{n}_j)\) the corresponding number operators. Here, the bosonic (fermionic) hopping amplitude is given by \(J_B (J_F)\), and \(U (V)\) accounts for the intra- (inter-) species interaction energy. In the following we consider the limit of large fermionic hopping, i.e. we assume \(J_F \gg U, |V|, J_B\) and the energy scale is set by \(U = 1\).

In this limit of large fermionic hopping the physics of the BFHM is well captured by the bosonic phase diagram alone. Considering the most interesting case of half filling of the spin-polarized fermions, we have plotted in figure 1 the phase diagram for the bosons obtained numerically by DMRG simulations and exact diagonalization (ED) for \(J_F = 10, V = 1.25\). Besides the MI and SF phases expected from the pure bosonic model, the phase diagram displays a CDW phase at double-half filling \((q_F = q_B = 1/2)\). Exact diagonalization is used for very small \(J_B\) to avoid boundary

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**Fermion mediated long-range interactions of bosons in the 1D Bose-Fermi-Hubbard model**

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The ground-state phase diagram of mixtures of spin polarized fermions and bosons in a 1D periodic lattice is discussed in the limit of large fermion hopping and half filling of the fermions. Numerical simulations performed with the density matrix renormalization group (DMRG) show besides bosonic Mott insulating (MI), superfluid (SF), and charge-density-wave phases (CDW) a novel phase with spatial separation of MI and CDW regions. We derive an effective bosonic theory which allows for a complete understanding and quantitative prediction of the bosonic phase diagram. In particular the origin of CDW phase and the MI-CDW phase separation is revealed as the interplay between fermion-induced mean-field potential and long range interaction with alternating sign.

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effects. Furthermore a novel phase is visible for the case of non-commensurate boson filling in which spatially separated regions of bosonic Mott insulators and density waves coexist (phase separation, PS). Figure 2 shows numerical results for the density cuts from within the corresponding phases. We note that while the pinning of the CDW to the boundaries is a result of the open boundary conditions required for DMRG, the phase separation persists for large systems and was verified for small systems using periodic boundary conditions.

In the following we derive an effective bosonic model which provides an understanding of the phase diagram in figure 1 on a quantitative level. In the limit of fast fermions one could expect that their main influence is through a mean field contribution, which according to eq. (1) amounts to a simple shift of the bosonic chemical potential \( \mu_B \to \mu_B - g_{F} V \). Indeed the two Mott lobes in fig. 1 are symmetrically located around \( \mu = \frac{1}{2} V \). To explain the CDW and PS phases one needs however an effective description beyond the mean-field level. In order to adiabatically eliminate the fast fermions we first separate the fermion Hamiltonian. As will be seen later on it is essential to take into account the back action of bosons to the fermions.

To do this we incorporate in the fermion Hamiltonian the interaction with a mean field potential given by a yet undetermined density \( \bar{n}_j \) of bosons. Thus \( \hat{H}_F = -J_F \sum_j \left( c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + V \sum_j \bar{n}_j \hat{m}_j \) is the fermionic Hamiltonian and \( \hat{H}_1 = V \sum_j (\hat{n}_j - \bar{n}_j) \hat{m}_j \) the interaction. We start from the S-matrix \( \hat{S} = T \exp \left\{ -\frac{i}{\hbar} \int_0^\infty d\tau H_1(\tau) \right\} \) of the full system with \( \hat{H}_1(\tau) = e^{-\frac{i}{\hbar} (\hat{H}_1 - \hat{H}_1^\dagger)\tau} \hat{H}_1 e^{\frac{i}{\hbar} (\hat{H}_1 - \hat{H}_1^\dagger)\tau} \) and trace out the fermions exactly using a cumulant expansion \( [21] \). Since the characteristic time scale of fermionic correlations is of order \( 1/J_F \) and thus much shorter than any other time scale in the system, a Markov approximation can be used, replacing two-time bosonic operators by equal time operators, i.e. \( \int d\tau \int d\tau' \langle \hat{n}_j(\tau) \hat{n}_{j+d}(\tau') \rangle_F \to \int d\tau \langle \hat{n}_j(\tau) \hat{n}_{j+d}(\tau) \rangle_F \int d\tau' \langle \hat{n}_j(\tau') \hat{n}_{j+d}(\tau') \rangle \). This leads to an effective Hamiltonian for the bosons

\[
\hat{H}_B^{\text{eff}} = \hat{H}_B + V \sum_j (\hat{n}_j - \bar{n}_j) \langle \hat{m}_j \rangle_F 
+ \sum_{j} \sum_{l=-\infty}^{\infty} g_l (\hat{n}_j - \bar{n}_j)(\hat{n}_{j+l} - \bar{n}_{j+l}),
\]

where \( g_l = -\frac{V^2}{2\pi} \int_0^\infty d\tau \langle \langle T \hat{m}_j(\tau) \hat{m}_{j+l}(0) \rangle \rangle_F \). \( T \) denotes time-ordering. One recognizes a fermion-induced mean-field potential proportional to \( \langle \hat{m}_j \rangle_F \). The couplings \( g_l \) describes a long-range density-density interaction between the bosons separated by \( l \) lattice sites. The mean-field potential and the density-density interaction are the only interaction terms emerging in the effective theory since higher order moments in the cumulant expansion vanish.

In the case of free fermions, i.e. ignoring the back-action of bosons \( \langle \hat{n}_j = 0 \rangle \), fermionic correlations and couplings \( g_l \) can easily be calculated. For \( g_F = 1/2 \), \( g_l \) scales asymptotically as \( g_l \sim (-1)^l / l \), i.e. has a long-range character and alternating sign. For a general fermion density \( g_F \) they oscillate with period \( 1/g_F \), which is typical for induced interactions of the RKKY type \([22-24]\). The oscillation of the interaction is the origin of the formation of charge density waves. For \( g_F = 1/2 \) the interaction energy is minimized if the bosons occupy sites with distance 2. An effective theory with coupling constants resulting from free fermions has however a fundamental problem: As \( g_l \sim 1/l \) the boson-boson interaction energy diverges logarithmically with the total length of the lattice. This would result in an incompressible CDW for any value of the bosonic hopping \( J_B \). Thus such a theory completely fails to describe the transition from a CDW phase to a bosonic superfluid. An accurate description

FIG. 1: (Color online) Boundaries of the incompressible MI phases and the CDW phase for half fermion filling \( g_F = 1/2 \), \( J_F = 10 \), and \( V = 1.25 \) obtained by DMRG and for small values of \( J_B \) by ED. One recognizes partial overlap between MI and CDW phase for small values of \( J_B \) indicating regions of spatial phase separation (PS) between MI and CDW. The dashed lines are results from the 2nd order perturbation theory based on the effective bosonic model.

FIG. 2: (Color online) Densities of bosons and fermions corresponding to the different regions in the boson phase diagram fig. 1 for a lattice of length \( L = 128 \) and open boundary conditions. The boson number \( N_B \) is (a) 19, (b) 64, (c) 96, and (d) 101. The plots (a,b,c) are taken at \( J_B = 0.01 \) and (d) at \( J_B = 0.07 \). While (b) displays the gaped CDW, (a) and (c) shows the PS phase. (d) is outside of the parameter regime with a CDW.
Similarly one finds for the fermionic density
\[ \langle \hat{\eta} \rangle = \frac{1}{2} \left[ 1 - (-1)^j \eta F \right], \]  
with \( \eta F = \frac{4a}{\pi \sqrt{1 + a^2}} K \left[ \frac{1}{1 + a^2} \right] \) and \( K[x] \) being the complete elliptic integral of the first kind. This equation along with
\[ \langle \hat{n}_j \rangle = \frac{1}{2} \left[ 1 + (-1)^j \eta \right] = \bar{n}_j \]
gives the density distributions of fermions and bosons for double-half filling, i.e. in the CDW phase, as function of the variational parameter \( a \). In the limit \( a \to 0 \) the above expressions reduces to the free fermion case \( \langle \hat{\eta} \rangle = \frac{1}{2}, \langle \hat{n}_j \rangle = \bar{n}_j \). To provide a first test of the validity of the effective theory we have plotted in Fig. 3 the ratio of the amplitudes of the bosonic and fermionic density waves obtained from the data in fig. 1 along with the prediction from eqs. (4) and (5). Note that this ratio is exactly fixed by the effective theory and independent on the variational parameter \( a \). One recognizes a very good agreement. Also shown in Fig. 3 are the amplitudes of bosonic and fermionic density waves respectively as function of bosonic hopping \( J_B \) obtained numerically as well as from the effective theory using the numerical data of the other species as input. It can be seen, that the renormalized effective theory fits quite well with the numerical results.

Using the effective Hamiltonian, (2) we will now derive an analytic approximation to the phase diagram of the full BFHM using a strong-coupling expansion valid for small values of \( J_B \) [26]. Since we are mainly interested in the boundaries of the incompressible lobes, we will calculate them in the canonical ensemble from the energies of the relevant states as a function of the bosonic hopping amplitude \( J_B \). The upper (lower) boundary is given by the bosonic particle-hole gap. With this, the chemical potentials for bosonic filling \( \varrho_B \) are given by \( \mu_{\varrho_B}^\pm = \pm (E(\varrho_B L \pm 1) - E(\varrho_B L)) \), where \( E(N) \) is the ground state energy for a given number of bosons \( N \). At \( J_B = 0 \), this is straightforward to calculate since the ground state distribution of the bosons is trivial and the variation parameter \( \eta \) is fixed to unity.

For \( J_B > 0 \) we apply degenerate perturbation theory in 2nd order using Kato’s expansion [25]. In second order, there is a local correction of the ground state energy for all numbers of particles, as well as 2nd order two-site hopping processes connecting the states within the ground state manifold in the case of an additional (absent) boson. Incorporating this, the upper and lower chemical potentials for the CDW phase can be expressed in a simple analytic form as
\[ \mu_{\varrho_B}^\pm = \frac{V}{2} \pm V \eta_F \pm g_0(a) - \beta_\pm J_B^2 . \]  

Similarly one finds for the chemical potential corresponding to unity and zero filling
\[ \mu_1^- = \frac{V}{2} - g_0(0) + 2J_B - \alpha J_B^2, \]
\[ \mu_0^+ = \frac{V}{2} + g_0(0) - 2J_B. \]  

Here \( \eta_F \) and \( g_0(a) \) are taken for \( \eta \equiv 1 \) (\( J_B = 0 \)) because of the perturbation expansion. The derivation of \( \alpha \) and \( \beta_\pm \) is lengthy but straight forward. Their explicit form will be given along with other details elsewhere [18]. One finds in particular \( \beta_+ > 0 > \beta_- \). Note that \( V \eta_F \) is positive irrespective
of the sign of $V$ and is larger in magnitude than both $g_0(0)$ and $g_0(a)$. With this one can see that $\mu_1^+|_{J_B=0} > \mu_2^-|_{J_B=0}$, $\mu_2^-|_{J_B=0} < \mu_0^+|_{J_B=0}$. Thus there exists a region where the chemical potential is not monotonous in the boson number. This explains the coexistence of MI and CDW in the PS phases found numerically in fig. 1. The long-range character of the fermion mediated interaction together with the fermion-induced mean-field potential prefers extended, spatially homogeneous regions of a commensurate CDW. Extra bosons will be pushed out and form an incompressible Mott insulator region. Such a phase does not exist in purely bosonic systems with extended interactions due to the absence of the fermion induced mean-field potential $V \eta_F$. If the bosonic hopping exceeds a certain critical value, given by the crossing of the curves $\mu_0^+$ with $\mu_1^-$ or respectively $\mu_0^-$ the minimization of kinetic energy by equally distributing the particle is larger than the loss in interaction energy due to the fermion mediated interaction.

In fig. 4 we have plotted the chemical potentials for zero bosonic hopping as function of the interaction strength $V$ defining the boundaries of the Mott insulating phases with zero and unity filling as well as the lower and upper boundaries of the CDW phase with half filling of bosons. One recognizes that phase separation between MI and CDW exists for all values of the boson-fermion interaction $V$. Once again there is a rather good agreement between full numerics and effective theory, which provides another test for its validity.

The phase boundaries for $J_B > 0$ obtained from the analytic results for the chemical potentials in eqns. (6) to (8) are shown in fig. 1 as dashed lines. Although the precise form of the CDW lobe is not correctly reproduced (as expected for the strong-coupling perturbation approach), the qualitative agreement is remarkable. The strong coupling approximation yields a critical value of $J_{\text{CDW}}^{\text{PS}} = 0.025$ beyond which the CDW ceases to exist for $J_F = 10$ and $V = 1.25$. Whether or not the CDW gap vanishes at a finite value of $J_B$ is however unclear. Our numerics indicates that a very small gap may persist even for values of $J_B = 1$ and may not close at for $J_B < J_F$. The critical values $J_{\text{PS}}^{\text{PS}} \approx 0.01$ for the PS region obtained from the effective model agrees however rather well with the numerical data.

In summary we developed an effective model for a mixture of bosons and spin polarized fermions in a periodic lattice in the limit of large fermion hopping. This model reveals the physical origin of the incompressible CDW phase and provides a simple quantitative description. The fast fermions cause a mean-field potential and mediate a long-range density-density interaction which is of alternating sign for $g_F = 1/2$. In order to accurately describe the conditions for the existence of a CDW renormalization effects due to the back-action of the bosons need to be taken into account. The density wave amplitudes where obtained from an analytic model and verified by numerical DMRG simulations. The effective model also gives a simple understanding and quantitative description of a novel phase where spatially separated regions of a maximum amplitude CDW and a MI coexist. The effective model is expected to provide a means for predicting and understanding conditions for the existence of a SS phase in Bose-Fermi mixtures and other mass imbalanced two-species models.

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