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Fermion-mediated long-range interactions of bosons in the one-dimensional 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 in addition to bosonic Mott insulating (MI), superfluid (SF), and charge density-wave phases (CDW) a yet unreported 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 an effective fermion-mediated long-range interaction between bosons with alternating sign.

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Ultracold 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 the interaction with fermions has been predicted to allow the bosons under certain conditions to enter the a supersolid phase (SS), where CDW and off-diagonal long-range order coexist [11–13].

In the present Rapid Communication 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 [11,14,15], resulting in 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 to be 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 μ_B is the bosonic chemical potential and J_B the corresponding hopping amplitude. At double half filling, i.e., $\varrho_F = \varrho_B = \frac{1}{2}$, 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 yet unreported phase with coexistence between spatially separated Mott-insulator and CDW regions for noncommensurate boson filling. This phase which is absent for a pure boson model with nearest-neighbor interaction [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 Ref. [13] using quantum Monte Carlo simulations. In Ref. [13], numerical evidence was given that a SS only exists if the filling of the spin-polarized fermions is exactly one half and the system is doped with extra bosons away from half filling.

Mixtures of ultracold bosons and spin-polarized fermions in optical lattices are well described by the Bose-Fermi-Hubbard Hamiltonian [18,19]

$$\hat{H} = -J_B \sum_j (\hat{b}_j^\dagger \hat{b}_{j+1} + \hat{b}_{j+1}^\dagger \hat{b}_j) + \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1) - J_F \sum_j (\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j) + V \sum_j \hat{n}_j \hat{m}_j, \quad (1)$$

where $\hat{b}^\dagger, \hat{b}$ $(\hat{c}^\dagger, \hat{c})$ are bosonic (fermionic) creation and annihilation operators and $\hat{n}$ $(\hat{m})$ 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, i.e., on average one half fermion per site, we have plotted in Fig. 1 the phase diagram for the bosons obtained by numerical DMRG simulations ($L \geqslant 256$ sites) and exact diagonalization (ED) for $J_F = 10$, $V = 1.25$. In addition to the MI and SF phases expected from the pure bosonic model, the phase diagram displays a CDW phase at double half filling ($\varrho_F = \varrho_B = 1/2$). Exact diagonalization ($L = 12$ sites and periodic boundaries) is used for very small J_B to avoid

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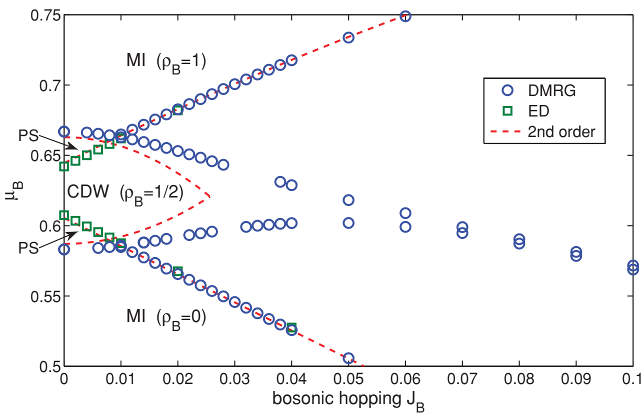

FIG. 1. (Color online) Boundaries of the incompressible MI phases and the CDW phase for half fermion filling $\varrho_F = 1/2$, $J_F = 10$, and $V = 1.25$ obtained by (open boundary) DMRG and for small values of J_B by (periodic boundary) ED. For the DMRG data, only those data points are used which do not show pinning to the boundary resembling the infinite system case. 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 second-order perturbation theory based on the effective bosonic model.

effects of boundary conditions. Furthermore, a novel phase is visible for the case of noncommensurate 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 persits 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 Fig. 1 on a quantitative level. In the limit of fast fermions one

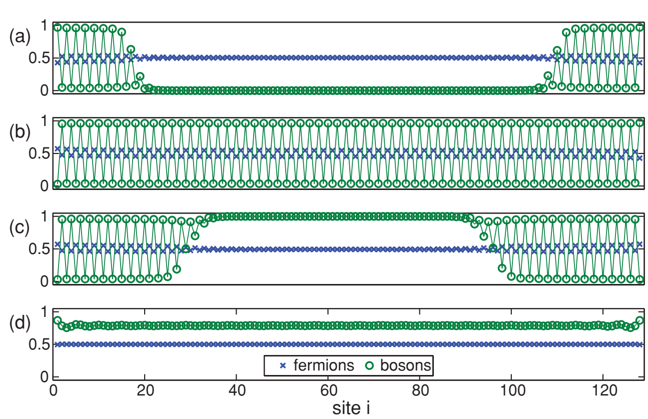

FIG. 2. (Color online) Densities of bosons and fermions corresponding to the different regions in the boson phase diagram Fig. 1 for a lattice of length $L = 128$ and open boundary conditions. The boson number N_B is (a) 19, (b) 64, (c) 96, and (d) 101. The plots (a), (b), and (c) are taken at $J_B = 0.01$ and (d) at $J_B = 0.07$. While (b) displays the gaped CDW, (a) and (c) show the PS phase. (d) is outside of the parameter regime with a CDW.

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 $\mu_B \to \mu_B - \varrho_F V$. And 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 average density $\tilde{n}_j$ of bosons. Thus $\hat{H}_{\rm F} = -J_F \sum_j (\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j) + V \sum_j \tilde{n}_j \hat{m}_j$ is the fermionic Hamiltonian and $\hat{H}_{\rm I} = V \sum_j (\hat{n}_j - \tilde{n}_j)\,\hat{m}_j$ the interaction.

To formally eliminate the fast fermions we follow standard techniques as presented in Ref. [11,14]. Since the fermionic hopping is the fastest process we obtain approximately an instantaneous long-range interaction which results in the effective bosonic Hamiltonian

$$\hat{H}_{\rm B}^{\rm eff} = \hat{H}_{\rm B} + V \sum_j (\hat{n}_j - \tilde{n}_j)\,\langle \hat{m}_j \rangle_{\rm F}$$

$$+ \sum_j \sum_{l=-\infty}^{\infty} g_l (\hat{n}_j - \tilde{n}_j)(\hat{n}_{j+l} - \tilde{n}_{j+l}), \qquad (2)$$

where $g_l = -i \frac{V^2}{2\hbar} \int_{-\infty}^{\infty} d\tau \,\langle\langle \mathcal{T} \hat{m}_j(\tau) \hat{m}_{j+l}(0) \rangle\rangle_{\rm F}$. $\mathcal{T}$ denotes time-ordering, and $\langle\langle \hat{m}_j \hat{m}_{j+l} \rangle\rangle = \langle \hat{m}_j \hat{m}_{j+l} \rangle - \langle \hat{m}_j \rangle \langle \hat{m}_{j+l} \rangle$ is the density-density correlation of the fermions. The couplings g_l describes a long-range density-density interaction between the bosons separated by l lattice sites.

In the case of free fermions, i.e., ignoring the back-action of bosons (i.e., setting $\tilde{n}_j \equiv 0$), fermionic correlations and couplings g_l can easily be calculated. For $\varrho_F = 1/2$, 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 ϱ_F they oscillate with period $1/\varrho_F$ which is typical for induced interactions of the Ruderman-Kittel-Kasuya-Yosida (RKKY) type [20–22]. The oscillation of the interaction is the origin of the formation of charge density waves. For $\varrho_F = 1/2$ 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 of this transition is, however, important, e.g., to address existence conditions of a supersolid phase. Therefore it is necessary to renormalize the effective interaction. This is done here by taking into account the back action of the bosons through the mean-field potential in $\hat{H}_F$. Since for $\varrho_F = 1/2$ the bosonic system is driven into a CDW with period 2, a good ansatz is $\tilde{n}_j = \frac{1}{2}[1 + (-1)^j \eta]$, where $\eta = \eta(J_B)$ is the amplitude of the density oscillation with $\eta|_{J_B=0} = 1$. In general η is treated as a free parameter and can be determined self-consistently by a minimization of the Hamiltonian. For the following calculations it turns out to be more convenient to introduce a parameter a proportional to η as $a = \eta V/(4\sqrt{2\pi} J_F)$.

Solving the free fermion problem in the periodic potential $V\widetilde{n}_j$ yields

$$g_l(a) = -\frac{V^2}{8\pi^2 J_F} \int_0^\pi \int_0^\pi \mathrm{d}\xi \mathrm{d}\xi' \times \frac{\cos(\xi l)\cos(\xi' l)}{\sqrt{\cos^2(\xi)+a^2} + \sqrt{\cos^2(\xi')+a^2}} \times \left(1 + \frac{\cos(\xi)}{\sqrt{\cos^2(\xi)+a^2}}\right)\left(1 - \frac{\cos(\xi')}{\sqrt{\cos^2(\xi')+a^2}}\right). \tag{3}$$

Similarly one finds for the fermionic density

$$\langle \hat{m}_j \rangle = \tfrac{1}{2}[1 - (-1)^j \eta_F], \tag{4}$$

with $\eta_F = \frac{4a}{\pi\sqrt{1+a^2}} K[\frac{1}{1+a^2}]$ and $K[x]$ being the complete elliptic integral of the first kind. This equation along with

$$\langle \hat{n}_j \rangle = \tfrac{1}{2}[1 + (-1)^j \eta] = \widetilde{n}_j \tag{5}$$

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 ($\langle \hat{m}_j \rangle = \frac{1}{2}$).

For a first test of the validity of the effective theory we have plotted in the inset of 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 and 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.

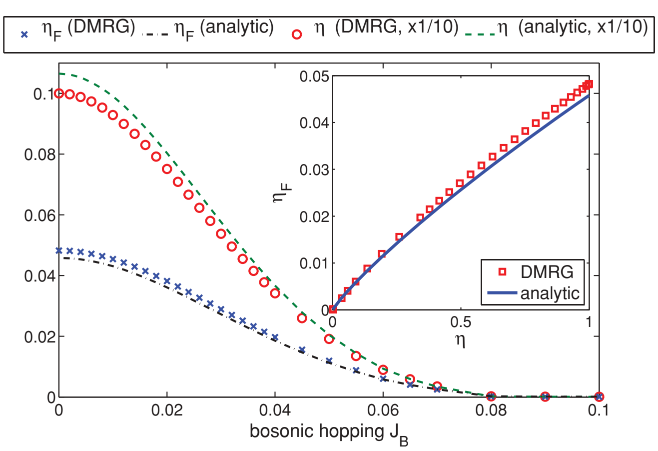

FIG. 3. (Color online) CDW amplitudes (points) of bosons and fermions for double half filling as function of normalized boson hopping. (Dash-dotted line) Analytic estimate of the fermionic amplitude η_F from the bosonic data. (Dashed line) Analytic estimate of the bosonic amplitude η from the fermionic data. One recognizes a reasonable agreement between the numerical data and the analytic estimate, where it should be kept in mind that the underlying perturbation theory gets better for $\eta \to 0$, i.e., for increasing J_B.

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 [23]. 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, i.e., the energy to add (remove) a boson to (from) the system. With this, the chemical potentials for bosonic filling ϱ_B are given by $\mu^{\pm}_{\varrho_B} = \pm(E(\varrho_B L \pm 1) - E(\varrho_B L))$, where $E(N)$ is the ground state energy for a given number of bosons N. At $J_B = 0$, this is straight forward to calculate since the ground state distribution of the bosons in the lattice is trivial and the variation parameter η is fixed to unity.

For $J_B > 0$ we apply degenerate perturbation theory in second order [24], where there is a local correction of the ground state energy for all numbers of particles, as well as second-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

$$\mu^{\pm}_{\frac{1}{2}} = \frac{V}{2} \pm V\,\eta_F \pm g_0(a) - \beta_{\pm} J_B^2. \tag{6}$$

Similarly one finds for the chemical potential corresponding to unity and zero filling

$$\mu^-_1 = \frac{V}{2} - g_0(0) + 2J_B - \alpha J_B^2, \tag{7}$$

$$\mu^+_0 = \frac{V}{2} + g_0(0) - 2J_B. \tag{8}$$

Here η_F and $g_0(a)$ are taken for $\eta \equiv 1$ ($J_B = 0$) because of the perturbative treatment starting from $J_B = 0$. The derivation of the constants α and $\beta_{\pm}$ is lengthy but straightforward and their explicit form is unwieldy and not shown here. 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 $\mu^+_{\frac{1}{2}}|_{J_B=0} > \mu^-_1|_{J_B=0}$, $\mu^-_{\frac{1}{2}}|_{J_B=0} < \mu^+_0|_{J_B=0}$. Thus there exists a region where the chemical potential is not monotonous in the boson number which 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 nearest-neighbor interaction due to the absence of the fermion induced mean-field potential $V\eta_F$. Only if the bosonic hopping exceeds a certain critical value, given by the crossing of the curves $\mu^{\pm}_{\frac{1}{2}}$ with μ^-_1 or, respectively, μ^+_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.

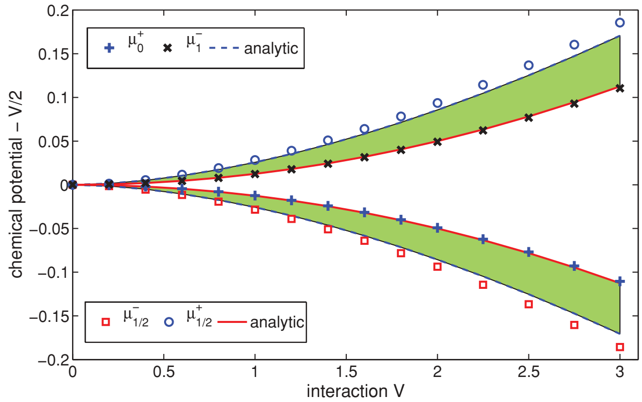

FIG. 4. (Color online) Boundaries (shifted by $V/2$) of incompressible MI and CDW phases for half fermion filling $\varrho_F = 1/2$ at vanishing bosonic hopping $J_B = 0$ with varying interaction V. Curves are the analytic results and the data points are obtained by DMRG (CDW phase, $L = 128$) and ED (MI lobes, periodic boundaries with infinite size scaling). The shaded region depicts the coexistence phase between MI and CDW with $\mu_0^+ > \mu_{\frac{1}{2}}^-$ and $\mu_{\frac{1}{2}}^+ > \mu_1^-$.

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. Furthermore, 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 Eqs. (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 $J_B^{\mathrm{CDW}} = 0.025$ beyond which the CDW ceases to exist for $J_F = 10$ and $V = 1.25$. Whether 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 $J_B = 1$. The critical values $J_B^{\mathrm{PS}} \approx 0.01$ 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 mediate a long-range density-density interaction which is of alternating sign for $\varrho_F = 1/2$. 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 were obtained from an analytic model and verified by numerical DMRG simulations. The effective model also gives a simple understanding and quantitative description of a 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 [25,26].

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[1] A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A **68**, 023606 (2003).
[2] M. Lewenstein, L. Santos, M. A. Baranov, and H. Fehrmann, Phys. Rev. Lett. **92**, 050401 (2004).
[3] K. Günter, T. Stoferle, H. Moritz, M. Kohl, and T. Esslinger, Phys. Rev. Lett. **96**, 180402 (2006).
[4] S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock, and K. Bongs, Phys. Rev. Lett. **96**, 180403 (2006).
[5] A. Mering and M. Fleischhauer, Phys. Rev. A **77**, 023601 (2008).
[6] K. V. Krutitsky, M. Thorwart, R. Egger, and R. Graham, Phys. Rev. A **77**, 053609 (2008).
[7] L. Pollet, M. Troyer, K. Van Houcke, and S. M. A. Rombouts, Phys. Rev. Lett. **96**, 190402 (2006).
[8] L. Mathey, D.-W. Wang, W. Hofstetter, M. D. Lukin, and E. Demler, Phys. Rev. Lett. **93**, 120404 (2004).
[9] E. Pazy and A. Vardi, Phys. Rev. A **72**, 033609 (2005).
[10] F. Hébert, F. Haudin, L. Pollet, and G. G. Batrouni, Phys. Rev. A **76**, 043619 (2007).
[11] H. P. Büchler and G. Blatter, Phys. Rev. Lett. **91**, 130404 (2003).
[12] I. Titvinidze, M. Snoek, and W. Hofstetter, Phys. Rev. Lett. **100**, 100401 (2008).
[13] F. Hébert, G. G. Batrouni, X. Roy, and V. G. Rousseau, Phys. Rev. B **78**, 184505 (2008).
[14] H. P. Büchler and G. Blatter, Phys. Rev. A **69**, 063603 (2004).
[15] R. M. Lutchyn, S. Tewari, and S. Das Sarma, Phys. Rev. B **78**, 220504(R) (2008).
[16] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
[17] T. D. Kühner, S. R. White, and H. Monien, Phys. Rev. B **61**, 12474 (2000).
[18] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[19] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[20] M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954).
[21] T. Kasuya, Prog. Theor. Phys. **16**, 45 (1956).
[22] K. Yosida, Phys. Rev. **106**, 893 (1957).
[23] J. K. Freericks and H. Monien, Phys. Rev. B **53**, 2691 (1996).
[24] D. J. Klein, J. Chem. Phys. **61**, 786 (1974).
[25] A. Hubener, M. Snoek, and W. Hofstetter, Phys. Rev. B **80**, 245109 (2009).
[26] T. Keilmann, I. Cirac, and T. Roscilde, Phys. Rev. Lett. **102**, 255304 (2009).