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Boson Hubbard model with weakly coupled fermions

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Using an imaginary-time path integral approach, we develop the perturbation theory suited to the boson Hubbard model and apply it to calculate the effects of a dilute gas of spin-polarized fermions weakly interacting with the bosons. The full theory captures both the static and the dynamic effects of the fermions on the generic superfluid-insulator phase diagram. We find that, in a homogenous system described by a single-band boson Hubbard Hamiltonian, the intrinsic perturbative effect of the fermions is to generically suppress the insulating lobes and to enhance the superfluid phase.

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I. INTRODUCTION

The boson Hubbard model has long provided the paradigm for studying one of the simplest quantum phase transitions (QPTs), the superfluid to insulator transition (SIT) in a dilute gas of bosons. Most satisfactorily, recent experiments[1,2] using ultracold bosonic atoms confined to an optical lattice, which mimics the boson Hubbard model in a custom setting, demonstrated the existence of the SIT in a pristine disorder free boson-only system. By varying the effective $\frac{t}{U}$ of the ultracold atoms in optical lattices, where t is the boson nearest-neighbor hopping parameter and U is the on-site boson-boson repulsion, the researchers demonstrated the existence of the Mott-insulating (small $\frac{t}{U}$) and the superfluid (large $\frac{t}{U}$) states in the time-of-flight experiments.[1,2] At some intervening value of $\frac{t}{U}$, then, there should be a QPT separating the two states.[3,4]

An important theoretical question, which has received wide attention[5–11] in light of the recent experiments in the Bose-Fermi mixtures,[12,13] is what happens to the insulating and the superfluid phases when fermions are introduced to the bare boson Hubbard model. In the case of the bosons weakly interacting with spin-polarized fermions, which are away from half-filling, this question can be addressed analytically. While some of the earlier studies[5,10] concluded that the region occupied by the superfluid phase in the phase diagram is enhanced by fermions, more recent ones[11] concluded that the opposite is true because of an effect akin to the fermionic orthogonality catastrophe due to the dynamic effects. In this Rapid Communication, we address this question by developing a rigorous perturbation theory suited to the single-band boson Hubbard model, which captures both the static and the dynamic effects mediated by the fermions. Our conclusion is that, in a homogenous single-band system and in the absence of loss of cooling due to adding fermions, the fermions intrinsically shrink the area occupied by the Mott-insulating lobes (Fig. 1), thus generically enhancing the superfluid region. The overall effect is qualitatively in the same direction as in the effects of Ohmic dissipation in enhancing the superconducting phase coherence in Josephson junction arrays[14] or in granular superconductors.[15] If the Bose-Fermi interaction strength can be brought to the perturbative regime,[16] our predictions can be tested experimentally. Thus, our predictions can be tested experimentally. Furthermore, in light of our present analytical results (and the results in Refs. 5 and 10) it seems likely that the observed loss of superfluid coherence by adding fermions[12,13] should be attributed to the external factors, such as heating[17] and self-trapping of the bosons and fermions.[18] Hence, experiments which can avoid such effects (e.g., shallower lattices and lower boson filling factor have reduced boson self-trapping due to fermions[18]) are necessary to see the intrinsic effect—enhancement of the superfluidity—due to the fermions. We stress that the perturbation theory of the boson Hubbard model we develop, which deviates from the standard machinery[19] applicable to the free bosons, should have other important applications, e.g., the phase diagram of the boson Hubbard model in the presence of coupling to a dissipative Ohmic bath[20] or a second boson species. In general, our method, specifically Eqs. (12)–(14), can be taken over in any

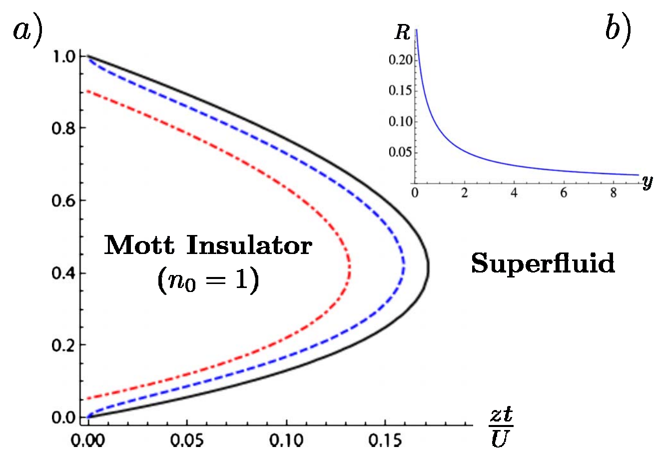

FIG. 1. (Color online) (a) Main panel: phase boundary of the boson Hubbard model with and without the fermions for the boson density n_0=1. Solid line describes the insulator-superfluid phase boundary without the fermions. The dashed line corresponds to the same phase boundary with the fermions present. The dashed-dotted line denotes the phase boundary in the static approximation. The regions near the degeneracy points (integer μ/U) are implicitly excluded from this figure (Ref. 22). Here we used $\frac{U}{4E_F}$=0.1 and $\frac{U_{FB}^2}{\Delta U}$=0.15. (b) Inset: the dependence of the function $R(y)$ on its argument.

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problem where Green's function of the boson Hubbard model has to be calculated in perturbation theory.

II. MODEL AND RESULTS

We consider a mixture of bosonic and spin-polarized fermionic atoms in an optical lattice. The Hamiltonian of the Bose-Fermi system is written as $H=H_B+H_F+H_{BF}$, with

$$H_B=\sum_i\left(\frac{U}{2}\hat{n}_i(\hat{n}_i-1)-\mu\hat{n}_i\right)-t\sum_{<ij>}(b_i^\dagger b_j+\text{H.c.}),\quad (1)$$

$$H_F=-t_F\sum_{<ij>}(c_i^\dagger c_j+\text{H.c.})-\mu_F\sum_i c_i^\dagger c_i,\quad (2)$$

$$H_{FB}=U_{FB}\sum_i \hat{n}_i(c_i^\dagger c_i-n_{Fi}^0).\quad (3)$$

Here $c_i^\dagger$ and $b_i^\dagger$ are the fermion and the boson creation operators on site i, $\hat{n}_i=b_i^\dagger b_i$ is the boson density operator, $U>0(U_{FB})$ describes the on-site boson-boson (boson-fermion) interaction, $t(t_F)$ corresponds to the hopping matrix element for the bosons (fermions), n_{Fi}^0 is the average density of the fermions, and $\mu=\mu_0-U_{FB}n_{Fi}^0$ and μ_F are chemical potentials for boson and fermions, respectively. Here μ_0 is the boson chemical potential without the fermions.

The partition function of the bare model (without the fermions) can be written in terms of an imaginary-time path integral over a complex scalar field $\psi(\mathbf{x},\tau)$,[3,4] where τ is the imaginary time. The action in terms of $\psi(\mathbf{x},\tau)$ takes the form of a ϕ^4 theory [see Eq. (9)]. In this description, the details of the bare Hamiltonian are hidden in the coefficients of the various terms of the action. For example, the coefficient, r, of the term $|\psi(\mathbf{x},\tau)|^2$ (see below) is determined by Green's function, $\langle T_\tau b_i(\tau)b_i^\dagger(0)\rangle$, of the bosons,[19] where $\langle\cdots\rangle$ denotes average with respect to the on-site part of the boson Hubbard Hamiltonian. In mean-field theory, $r=0$ gives the locus of the insulator $(r>0,\langle\psi(\mathbf{r},\tau)\rangle=0)$ to the superfluid $(r<0,\langle\psi(\mathbf{r},\tau)\rangle\neq 0)$ QPT, revealing the Mott-insulating lobes in the phase diagram.[3,4]

With fermions, a similar description of the partition function still holds, but now the boson Green's function must incorporate the perturbative effects of the boson-boson interaction *mediated* by the fermions. We stress that this mediated interaction is manifestly nonlocal in both space and time. Therefore, it is not obvious that this problem can be treated in an effective Weiss-type single-site theory as done in Ref. 11. The perturbative corrections to the boson Green's function cannot be calculated by using the standard diagrammatic machinery[19] either because the bare Hamiltonian is an interacting one and the interaction U has to be treated nonperturbatively. We solve this problem by noting that we can still calculate the needed correlation functions exactly by making use of the eigenstates of the number operators $\{n_i\}$. A modified linked-cluster theorem still holds which gets rid of all the divergences encountered in the perturbation theory. The locus of the equation, $r'=0$, where r' includes the perturbative corrections to the boson Green's function, provides the phase boundary between the superfluid and the insulating states. Our central result for the phase boundary is shown in Fig. 1. Below we give a summary of the methods and the calculations used to arrive at the results. The details of the calculations will be given elsewhere.[21]

III. SUMMARY OF THE METHODS

To the lowest order in U_{FB}, the effect of the fermions on the constituent bosons is a trivial shift of the boson chemical potential $\mu=\mu_0-U_{FB}n_{Fi}^0$. All the nontrivial effects appear in the second order in U_{FB}. By integrating out the fermions, the imaginary-time partition function becomes (we assume here zero temperature $T\to 0$)

$$Z=\int \mathfrak{D}b_i^*\mathfrak{D}b_i\exp(-S_{\text{eff}}[b_i^*,b_i]),\quad (4)$$

$$S_{\text{eff}}[b_i^*,b_i]=\int_0^\beta d\tau\left(\sum_i b_i^*\partial_\tau b_i+H_B\right)-\sum_{ij}\int_0^\beta d\tau_1\int_0^\beta d\tau_2 n_i(\tau_1)M_{ij}(\tau_1-\tau_2)n_j(\tau_2).\quad (5)$$

In the second order in U_{FB}, the integral over the fermion degrees of freedom gives rise to an effective nonlocal density-density interaction for the bosons with the function $M_{ij}(\tau_1-\tau_2)$ being

$$M_{ij}(\tau_1-\tau_2)=\frac{U_{FB}^2}{2}\langle\Delta n_{Fi}(\tau_1)\Delta n_{Fj}(\tau_2)\rangle.\quad (6)$$

In the frequency and momentum domain, $M_{\boldsymbol{q}}(\Omega_n)$ is proportional to the fermion polarization function and in two dimensions $M_{\boldsymbol{q}}(\Omega_n)$ is given by

$$M_{\boldsymbol{q}}(\Omega_n)=\frac{U_{FB}^2}{2\Delta}\left(1-\frac{|\nu_n|}{\sqrt{\nu_n^2+k^2}}\right).\quad (7)$$

Here, $\nu_n=\Omega_n/4E_F$ and $k=q/2k_F$, with E_F and k_F being the Fermi energy and the Fermi momentum, respectively. Δ is the fermion mean level spacing, $\Delta=1/\nu_F V$, with ν_F as the density of states at the Fermi level and V as the volume of the unit cell. Equation (7) is valid for $k<1$. Here, for simplicity, we consider a two-dimensional (2D) system. However, our qualitative conclusions hold for the three-dimensional (3D) case as well.[21]

Using the Hubbard-Stratonovich transformation with a complex scalar field $\psi_i(\tau)$, we integrate out the bosonic fields to write $Z=Z_0\int\mathfrak{D}\psi_i\mathfrak{D}\psi_i^*\exp(-S[\psi_i,\psi_i^*])$, where the action $S[\psi_i,\psi_i^*]$ is given by

$$S[\psi_i,\psi_i^*]=\int_0^\beta d\tau\sum_{i,j}\psi_i^*(\tau)w_{ij}^{-1}\psi_j(\tau)-\ln\left\langle\exp\left[\int_0^\beta d\tau\sum_i b_i(\tau)\psi_i^*(\tau)+\text{H.c.}\right]\right\rangle.\quad (8)$$

Here the matrix elements of the symmetric matrix, w_{ij}, are equal to t for the nearest neighbors and zero otherwise. The expectation value in Eq. (8) is taken with respect to the action $S_{\text{eff}}[b_i^*, b_i]$ (with $t=0$). By expanding $S[\psi,\psi^*]$ up to the fourth power of the field ψ and taking the continuum limit, we arrive at the action of an effective complex ψ^4 field theory,

$$\mathcal{S}[\psi,\psi^*] = \int d\boldsymbol{x}\left(c_1\psi^* \frac{\partial\psi}{\partial\tau} + c_2\left|\frac{\partial\psi}{\partial\tau}\right|^2 + c|\boldsymbol{\nabla}\psi|^2 + r|\psi|^2 + u|\psi|^4 \right) \tag{9}$$

with $\boldsymbol{x}=\{\boldsymbol{r},\tau\}$. The coupling constants c_1, c_2, c, r, and u are given by the correlation functions of the boson Hubbard model with $t=0$. In mean-field theory, the phase boundary between the superfluid and insulating states can be obtained by setting the coefficient r to zero,

$$r \propto \frac{1}{zt} + \int_{-\beta}^{\beta} d\tau \mathbf{G}_i(\tau) = 0, \tag{10}$$

where $\mathbf{G}_i(\tau)=-\langle T_\tau b_i(\tau) b_i^\dagger(0)\rangle$ is the single-site boson Green's function, which, in the presence of the fermions, should include the effective fermion-mediated density-density interaction. Without the fermions, this Green's function is given by[4]

$$G_i(i\omega_n) = \left[\frac{(n_0+1)}{i\omega_n - \delta E_p} - \frac{n_0}{i\omega_n + \delta E_h}\right], \tag{11}$$

where δE_p and δE_h are particle and hole excitation energies, $\delta E_p = U n_0 - \mu$ and $\delta E_h = \mu - U(n_0-1)$, and n_0 is the number of bosons per site minimizing the ground state energy. Thus, the problem is now reduced to the calculation of the on-site full boson Green's function by computing the corrections to Eq. (11). As we show below, this can be done perturbatively in U_{FB}.

The calculation of the perturbative corrections to the boson Green's function is nontrivial because the bare Hamiltonian, H_B (with $t=0$), is not quadratic in the boson operators. Therefore, one cannot use the standard diagrammatic techniques[19] because Wick's theorem does not hold. To make progress, we write the corrections to Green's function using the cumulant expansion

$$\langle\langle T_\tau b_i(\tau) b_i^\dagger(0)\rangle\rangle = \langle T_\tau b_i(\tau) b_i^\dagger(0)\rangle + \sum_{jl}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \times M_{jl}(\tau_1-\tau_2) K_{ijl}(\tau,\tau_1,\tau_2), \tag{12}$$

where $\langle\langle\cdots\rangle\rangle$ denotes Green's function which includes the perturbative corrections. In the Mott-insulating state, it is convenient to calculate the correlation function $K_{ijl}(\tau,\tau_1,\tau_2)$ in the second quantized representation,

$$K_{ijl}(\tau,\tau_1,\tau_2) = \langle T_\tau b_i(\tau) b_i^\dagger(0) n_j(\tau_1) n_l(\tau_2)\rangle - \langle T_\tau b_i(\tau) b_i^\dagger(0)\rangle \times \langle T_\tau n_j(\tau_1) n_l(\tau_2)\rangle. \tag{13}$$

Given that the on-site part of the boson Hubbard Hamiltonian conserves the number of bosons, the correlation functions above can be calculated exactly using the particle-number eigenstates.[21] The terms in $K_{ijl}(\tau,\tau_1,\tau_2)$ contributing to static and dynamic screening are given by

$$\begin{aligned} K_{ijl}(\tau,\tau_1,\tau_2) = {} & \Theta(\tau)\Theta(\tau_1)\Theta(\tau_2)\Theta(\tau-\tau_1)\Theta(\tau-\tau_2) \\ & \times[(\delta_{ij}+\delta_{il})n_0(n_0+1) + \delta_{ij}\delta_{il}(n_0+1)] \\ & \times\exp(-\delta E_p\tau) + \Theta(-\tau)\Theta(-\tau_1) \\ & \times\Theta(-\tau_2)\Theta(\tau_1-\tau)\Theta(\tau_2-\tau) \\ & \times[-(\delta_{ij}+\delta_{il})n_0^2 + \delta_{ij}\delta_{il}n_0]\exp(\delta E_h\tau) + \cdots . \end{aligned} \tag{14}$$

It is important to note that $K_{ijl}(\tau,\tau_1,\tau_2)$ is irreducible and cannot be factored into the product of the bare Green's functions, as would have been possible if Wick's theorem were applicable.

We now proceed to calculate the effects of the fermions by first approximating $M_{\boldsymbol{q}}(\Omega_n)$ in Eq. (7) by the constant piece, $M_{\boldsymbol{q}}(\Omega_n) \sim \frac{U_{FB}^2}{2\Delta}$ (static approximation, see also Refs. 5 and 11). By substituting the corresponding expression for M_{jl}, $M_{jl}(\tau_1-\tau_2) = \frac{U_{FB}^2}{2\Delta}\delta_{lj}\delta(\tau_1-\tau_2)$, into Eq. (12), and carrying out the imaginary-time integrals, we find the following expression for Green's function at zero frequency:[22]

$$\mathbf{G}_i(0) = -\frac{n_0+1}{\delta E_p}\left[1 + \frac{U_{FB}^2(1+2n_0)}{2\Delta\,\delta E_p}\right] - \frac{n_0}{\delta E_h}\left[1 + \frac{U_{FB}^2(1-2n_0)}{2\Delta\,\delta E_h}\right]. \tag{15}$$

Alternatively, we could substitute the static on-site form of $M_{ij}(\tau_1-\tau_2)$ directly into the action [Eq. (5)] and calculate Green's function exactly. It is easy to see that, in the static approximation, the mobile fermions simply renormalize μ and U of the bare boson Hubbard Hamiltonian H_B: $U \to U - U_{FB}^2/\Delta$ and $\mu \to \mu + U_{FB}^2/2\Delta$. The exact Green's function, thus, can simply be obtained by substituting these renormalized parameters in Eq. (11). After expanding the result to the second order in U_{FB}, the resulting expression exactly matches[21] that in Eq. (15). This validates the correctness of our perturbation theory. Using Eq. (10) one can see that, in the static approximation, the fermions markedly shrink the area of the Mott-insulating lobes in the phase diagram (see Fig. 1).

The static screening approximation for $M_{\boldsymbol{q}}(\Omega_n)$ does not, however, take into account the important retardation effects[11] and the spatially nonlocal nature of the interaction kernel in Eq. (6). By substituting the full expression for $M_{ij}(\tau_1-\tau_2)$ into Eq. (12), doing the imaginary-time integrals, as well as carrying out the summation over j and l, we obtain the following expression for the boson Green's function at zero frequency,

$$\mathbf{G}_i(0) = -\frac{n_0+1}{\delta E_p}\left[1 + \frac{U_{FB}^2}{\Delta\,\delta E_p}R\left(\frac{\delta E_p}{4E_F}\right)\right] - \frac{n_0}{\delta E_h}\left[1 + \frac{U_{FB}^2}{\Delta\,\delta E_h}R\left(\frac{\delta E_h}{4E_F}\right)\right]. \tag{16}$$

Here we introduced the dimensionless function $R(y)$,

$$R(y) = \frac{4}{\pi^2}\int_0^1 kdk\int_0^\infty d\nu\left[1-\frac{|\nu|}{\sqrt{k^2+\nu^2}}\right]\frac{y}{\nu^2+y^2}$$
$$= \frac{4}{\pi^2}\left[\frac{\pi}{4}+y-\frac{\pi}{2}y^2+y\sqrt{y^2-1}\,\sec(y)\right]. \qquad (17)$$

The inset of Fig. 1 depicts the behavior of the monotonic function $R(y)$ as a function of its argument. As follows from Eq. (16), the importance of the fermion renormalization effects is determined by the ratio of $\delta E_{p/h}$ and E_F. When the fermion density is small, i.e., $\delta E_{p/h}/E_F \gg 1$, the corrections to Green's function are suppressed since $R(y\gg 1)\to 0$. In the opposite limit, $\delta E_{p/h}/E_F \ll 1$, the function $R(y\ll 1)\sim 1$, and thus, for a given value of U_{FB}, the effects of the fermions on the bosons are more pronounced. Finally, using Eqs. (10) and (16), we calculate the phase diagram on the $(\mu - t)$ plane as shown in Fig. 1. We emphasize that the net effect of the fermions is to suppress the Mott-insulating lobes and enhance the superfluidity.

The above result is consistent with numerical calculation in Ref. 10 and is in disagreement with the conclusions of Ref. 11. We note that the correctness of our formalism for the perturbative evaluation of Green's function (in the static screening approximation) was confirmed independently [see the discussion after Eq. (15)]. The generalization of the scheme to the dynamical screening is straightforward and amounts to only taking the frequency and momentum integrals, mandated by Eq. (12). Thus, we are able to calculate the perturbative effects to the boson Hubbard model of an arbitrary time- and space-dependent interaction kernel. In contrast, it is not obvious that a spatially nonlocal interaction kernel, such as that in Eq. (6), can be properly treated in the Weiss-type self-consistent mean-field theory employed in Ref. 11. Note also that the function $M_{\boldsymbol{q}}(\Omega_n)$ is positive definite for all momenta and frequencies. Therefore, the net effect of the full interaction kernel is qualitatively similar to its constant piece (the static approximation), even though the latter significantly overestimates the suppression of the insulating phase. Thus, our qualitative conclusions should be valid for 3D systems as well.[21] We note that the sign of the phase boundary shift can be predicted from the sign of the fermion density-density correlation function, while the magnitude of the corrections to the phase diagram depends on the microscopic details such as the ratio of $\delta E_{p/h}$ and E_F as follows from Eqs. (16) and (17). Finally, we emphasize that, near the degeneracy points, where the excitation energy $\delta E_{p/h}$ is smaller than U_{FB}^2/Δ, our perturbation theory breaks down [see Eqs. (15) and (16)]. Thus, the effect of fermions on the boson Hubbard phase diagram near these points is an open question.

IV. CONCLUSION

In summary, we develop a framework for carrying out the perturbation theory for the boson Hubbard model and use it to calculate the effects of a dilute gas of spin-polarized fermions weakly interacting with the bosons. The full theory captures both the static and the important dynamic effects of the fermions on the constituent bosons. We find that within single-band boson Hubbard model the net effect of the fermions is to inherently suppress the Mott-insulating lobes and enhance the superfluid phase in the generic Bose-Hubbard phase diagram.

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