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Mixtures of correlated bosons and fermions: Dynamical mean-field theory for normal and condensed phases

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We derive a dynamical mean-field theory for mixtures of interacting bosons and fermions on a lattice (BF-DMFT). The BF-DMFT is a comprehensive, thermodynamically consistent framework for the theoretical investigation of Bose-Fermi mixtures and is applicable for arbitrary values of the coupling parameters and temperatures. It becomes exact in the limit of high spatial dimensions d or coordination number Z of the lattice. In particular, the BF-DMFT treats normal and condensed bosons on equal footing and thus includes the effects caused by their dynamic coupling. Using the BF-DMFT we investigate two different interaction models of correlated lattice bosons and fermions, one where all particles are spinless (model I) and one where fermions carry a spin one-half (model II). In model I the local, repulsive interaction between bosons and fermions can give rise to an attractive effective interaction between the bosons. In model II it can also lead to an attraction between the fermions.

1 Introduction

Ultracold atoms in optical lattices are not only fascinating many-body systems *per se*, they also help to better understand interaction models and correlation phenomena in condensed matter physics [1, 2]. Indeed, the high tunability of experimental parameters in these systems allows to explore the properties of correlated fermions and bosons in parameter regimes which are not accessible in condensed matter systems provided by nature [2]. For example, precise measurements of the effects of strong disorder on interacting bosons have now become possible [3]. Similarly, important insights can be expected from investigations of strongly disordered interacting fermions, for which detailed predictions exist [4–10]. Ultracold atoms in optical lattices may also be employed to realize entirely new physical systems, e.g., mixtures with an arbitrary relative concentration of lattice fermions and bosons [11–13].

Quantum many-body problems in the thermodynamic limit can almost never be solved exactly and thus require approximate investigation methods. During the last 20 years the dynamical mean-field theory (DMFT) has proved to be a reliable approximation scheme for correlated lattice fermions (electrons) in dimension $d = 3$ [14–17]. The bosonic counterpart of the DMFT – the B-DMFT – was developed only most recently [19]. The B-DMFT is a thermodynamically consistent, conserving and non-perturbative theoretical framework for the investigation of correlated bosons on a lattice. It is applicable for all physical parameters and becomes exact in the limit of high spatial dimensions d or lattice coordination number Z . The B-DMFT has the important property that it treats normal and condensed bosons on equal footing and

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thus includes the effects caused by their dynamic coupling [19]. This is in contrast to the seminal static mean-field theory of Fisher et al. [20], and the equivalent Gutzwiller approximation [21], which focus on the condensed bosons and treat normal bosons as immobile. Explicit results of the B-DMFT were so far obtained for the bosonic Falicov-Kimball model [19] and the bosonic Hubbard model [19, 22–24]. In this paper we extend the DMFT and B-DMFT and formulate a dynamical mean-field theory for *mixtures* of correlated lattice bosons and fermions. The theoretical framework derived in this way, referred to as BF-DMFT in the following, is a generalization of both the fermionic DMFT and the B-DMFT. It provides a set of self-consistency equations which are valid for arbitrary coupling parameters and temperatures, and which describe the static and dynamic properties of a system of mutually interacting lattice bosons and fermions. These BF-DMFT equations are exact in the limit $Z \rightarrow \infty$ and provide a comprehensive, non-perturbative approximation scheme for Bose-Fermi mixtures on lattices with finite Z . Similar to the B-DMFT the BF-DMFT derived here treats normal and (pair-)condensed particles on equal footing.

Since the BF-DMFT includes many-body correlations and the dynamic coupling between normal and condensed particles in a systematic way it extends earlier theoretical investigations of Bose-Fermi mixtures formulated in the continuum [25–30] and on lattices [31–45]. A dynamic coupling between fermions in Bose-Fermi mixtures was included by Titvinidze, Snoek, and Hofstetter [43] who treated fermions within DMFT and bosons within the Gutzwiller approximation. One of the most interesting questions in this context concerns the renormalization of the interaction between bosons and between fermions due to the interaction between bosons and fermions. Employing the many-body BF-DMFT formulated in this paper we find that the effective interactions between bosons and between fermions can indeed be *attractive*, and can thus lead to phase instabilities towards superfluid fermions or phase-separated bosons. This confirms and extends the range of validity of earlier investigations performed within a T-matrix approximation or the static mean-field Bogoliubov approximation [25–32, 37, 39–43, 45].

In Sect. 2 we introduce two models of correlated, spinless lattice bosons interacting with correlated lattice fermions without spin (model I) and with spin (model II). In Sects. 3 and 4 we derive the BF-DMFT self-consistency equations for these models and discuss some of their properties, e.g., the emergence of effective attractions between bosons due to the interaction with fermions, and *vice versa*.

2 Lattice models for mixtures of correlated bosons and fermions

In the following we consider two different models for correlated lattice bosons (b) and fermions (f) with local interactions. In the first model (model I) all particles or atoms are spinless. Such a system can be obtained experimentally by preparing a mixture where ^{40}K fermionic and ^{87}Rb bosonic atoms are in only one hyper-fine state [11–13]. This would correspond to the simplest Bose-Fermi mixture where all spin-dependent effects are absent. The Hamiltonian has the form

$$H_I = \sum_{ij} t_{ij}^b b_i^\dagger b_j + \sum_i \epsilon_i^b n_i^b + \frac{U_b}{2} \sum_i n_i^b (n_i^b - 1) + \sum_{ij} t_{ij}^f f_i^\dagger f_j + \sum_i \epsilon_i^f n_i^f + U_{bf} \sum_i n_i^b n_i^f, \quad (1)$$

where b_i, f_i (b_i^\dagger, f_i^\dagger) are annihilation (creation) operators on lattice site i for bosons and fermions, respectively, with number operators $n_i^b = b_i^\dagger b_i$ and $n_i^f = f_i^\dagger f_i$ and hopping amplitudes t_{ij}^b and t_{ij}^f . The interaction between bosons is denoted by U_b , and that between bosons and a fermion by U_{bf} . In model I there is no local fermion–fermion interaction because of the exclusion principle [46]. For generality we include local potentials $\epsilon_i^b, \epsilon_i^f$, acting on bosons and fermions, respectively. They can either be applied externally such as by a harmonic trap, or act intrinsically as in the case of an additional random potential.

In model II the bosons are still spinless, but the fermions now carry a spin one-half. Experimentally the ^{40}K fermionic atoms should then be prepared in two hyperstates with equal population, whereas the ^{87}Rb bosonic atoms should remain in one hyperfine state. In such a situation superfluidity of condensed Cooper

pairs also becomes possible. In this case the Hamiltonian takes the form

$$H_{\text{II}} = \sum_{ij} t_{ij}^b b_i^\dagger b_j + \sum_i \epsilon_i^b n_i^b + \frac{U_b}{2} \sum_i n_i^b (n_i^b - 1) \\ + \sum_{ij\sigma} t_{ij}^f f_{i\sigma}^\dagger f_{j\sigma} + \sum_{i\sigma} \epsilon_i^f n_{i\sigma}^f + \frac{U_f}{2} \sum_{\sigma} n_{i\sigma}^f n_{i\bar{\sigma}}^f + U_{bf} \sum_{i\sigma} n_i^b n_{i\sigma}^f, \quad (2)$$

where σ denotes the spin (or hyperfine state) of the fermions. In contrast to (1) model II contains also a local interaction U_f between fermions with the opposite spins.

We will now derive the self-consistent DMFT equations for model I in real space [49]. To this end we employ the cavity method [16] together with a scaling of the hopping amplitudes for fermions [14] and bosons [19, 48].

3 Solution of model I within dynamical mean-field theory

In the DMFT approach the local, site-diagonal Green functions are of particular interest. The local one-particle bosonic Green functions are defined as

$$\mathbf{G}_i^b(\tau) \equiv -\langle T_\tau \mathbf{b}_i(\tau) \mathbf{b}_i^\dagger(0) \rangle_{S_i} \equiv - \begin{pmatrix} \langle T_\tau b_i(\tau) b_i^\dagger(0) \rangle_{S_i} & \langle T_\tau b_i(\tau) b_i(0) \rangle_{S_i} \\ \langle T_\tau b_i^\dagger(\tau) b_i^\dagger(0) \rangle_{S_i} & \langle T_\tau b_i^\dagger(\tau) b_i(0) \rangle_{S_i} \end{pmatrix}, \quad (3)$$

where we use the Nambu notation to incorporate the off-diagonal, anomalous Green functions in the case of Bose-Einstein condensed bosons [50, 51], and T_τ represents the time ordering operator [52]. The Nambu spinor operators for bosons are defined by

$$\mathbf{b}_i = \begin{pmatrix} b_i \\ b_i^\dagger \end{pmatrix} \quad \text{and} \quad \mathbf{b}_i^\dagger = (b_i^\dagger, b_i). \quad (4)$$

To characterize the bosons completely we also have to consider the order parameter of the BEC phase, i.e., the condensate wave function, given by

$$\Phi_i(\tau) \equiv \langle \mathbf{b}_i(\tau) \rangle_{S_i}. \quad (5)$$

The square of the absolute value of $\Phi_i(\tau)$ yields the number of bosons in the condensate at site i , i.e.

$$n_i^{\text{BEC}} = \langle b_i^\dagger(\tau) \rangle_{S_i} \langle b_i(\tau) \rangle_{S_i} = \frac{1}{2} |\Phi_i(\tau)|^2. \quad (6)$$

The equilibrium condensate density is expected to be independent of time. This still allows for a time-dependence of the phase of $\Phi_i(\tau)$. The local, site diagonal one-particle fermionic Green function is defined by

$$G_i^f(\tau) \equiv -\langle T_\tau f_i(\tau) f_i^\dagger(0) \rangle_{S_i}. \quad (7)$$

The local functions defined above are determined by the local action S_i which will be derived next.

Using the path integral formalism [53] the exact grand canonical partition function for the lattice Bose-Fermi mixture is obtained from

$$Z = \int D[b] \int D[f] e^{-S[b,f]}, \quad (8)$$

where the action $S[b, f]$ is given by

$$S[b, f] = \int_0^\beta d\tau \left\{ \sum_i [b_i^*(\tau)(\partial_\tau - \mu_b)b_i(\tau) + f_i^*(\tau)(\partial_\tau - \mu_f)f_i(\tau)] + H_I[b, f] \right\}. \quad (9)$$

Here μ_b and μ_f are the chemical potentials of bosons and fermions, respectively, and $\beta = 1/k_B T$ is the inverse temperature. In the cavity method [16] we select a single lattice site i_0 and split $S[b, f]$ into three contributions:

$$S[b, f] = S_{i_0}[b, f] + \Delta S_{i_0}[b, f] + S_{i \neq i_0}[b, f]. \quad (10)$$

Here the first term,

$$S_{i_0}[b, f] = \int_0^\beta d\tau \left\{ b_{i_0}^*(\tau)(\partial_\tau - \mu_b + \epsilon_{i_0}^b)b_{i_0}(\tau) + f_{i_0}^*(\tau)(\partial_\tau - \mu_f + \epsilon_{i_0}^f)f_{i_0}(\tau) + \frac{U_b}{2}n_{i_0}^b(\tau)(n_{i_0}^b(\tau) - 1) + U_{bf}n_{i_0}^b(\tau)n_{i_0}^f(\tau) \right\}, \quad (11)$$

corresponds to the action for a separated site i_0 . The second term,

$$\Delta S_{i_0}[b, f] = \int_0^\beta d\tau \sum_{j \neq i_0} (t_{i_0 j}^b b_{i_0}^* b_j + t_{j i_0}^b b_j^* b_{i_0} + t_{i_0 j}^f f_{i_0}^* f_j + t_{j i_0}^f f_j^* f_{i_0}), \quad (12)$$

is due to hopping processes between site i_0 and all other sites, and the third term, $S_{i \neq i_0}[b, f]$, represents the remaining parts of the action. In the next step we expand the exponential function with respect to $\Delta S_{i_0}[b, f]$ and perform the functional integrals with respect to the complex variables b_i and Grassmann variables f_i with $i \neq i_0$. The resulting expression for the partition function contains infinitely many correlation functions with different numbers of operators. Within DMFT we need to keep only terms with a single b_{i_0} operator as well as pairs of bosonic or fermionic operators. These terms are then re-exponentiated according to the linked cluster theorem [16, 19]. This approximation becomes exact in the limit of infinite dimensions d or coordination numbers Z , provided the hopping amplitudes for fermions, t_{ij}^f , [14] and bosons, t_{ij}^b , [19, 48] are appropriately scaled with d or Z . In this limit the self-energies are diagonal in lattice indices, i.e., $\Sigma_{ij}^{b,f}(\tau) = \Sigma_i^{b,f}(\tau)\delta_{ij}$. As a result one obtains a sum of three local DMFT actions for the lattice site i_0 as

$$S_{i_0} = S_{i_0}^b + S_{i_0}^f + S_{i_0}^{bf}. \quad (13)$$

Here

$$S_{i_0}^b = \frac{1}{2} \int_0^\beta d\tau \mathbf{b}_{i_0}^*(\tau) \left(\partial_\tau \sigma_3 - (\mu_b - \epsilon_{i_0}^b) \mathbf{1} \right) \mathbf{b}_{i_0}(\tau) + \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \mathbf{b}_{i_0}^*(\tau) \Delta_{i_0}^b(\tau - \tau') \mathbf{b}_{i_0}(\tau') + \frac{U_b}{2} \int_0^\beta d\tau n_{i_0}^b(\tau)(n_{i_0}^b(\tau) - 1) + \int_0^\beta d\tau \sum_{j \neq i_0} \kappa_{i_0 j} \mathbf{b}_{i_0}^*(\tau) \Phi_j(\tau) \quad (14)$$

is the action for bosons coupled to a reservoir of normal and condensed lattice bosons [19],

$$S_{i_0}^f = \int_0^\beta d\tau f_{i_0}^*(\tau) \left(\partial_\tau - \mu_f + \epsilon_{i_0}^f \right) f_{i_0}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' f_{i_0}^*(\tau) \Delta_{i_0}^f(\tau - \tau') f_{i_0}(\tau') \quad (15)$$

is the action for spinless fermions coupled to a reservoir of normal lattice bosons and

$$S_{i_0}^{bf} = U_{bf} \int_0^\beta d\tau n_{i_0}^b(\tau) n_{i_0}^f(\tau) \quad (16)$$

is the action describing the coupling between bosons and fermions at site i_0 . There is no coupling of fermions to condensed bosons since this coupling is described by disconnected correlation functions. The symbol $\mathbf{1}$ denotes a 2×2 unit matrix, and σ_3 is the Pauli matrices with ± 1 on the diagonal. The factor $1/2$ is added because in the Nambu representation the number of degrees of freedom is doubled [50]. We will now discuss the physical meaning of the quantities $\Delta_{i_0}^b$, $\Delta_{i_0}^f$ and κ_{i_0j} appearing in (14) and (15), and how they are determined.

The quantities $\Delta_{i_0}^b$ and $\Delta_{i_0}^f$ describe the resonant broadening of quantum-mechanical states on lattice site i_0 . They may be interpreted as a hybridization of bosons and fermions, respectively, on site i_0 with the surrounding bosonic or fermionic reservoirs and are given by

$$\Delta_{i_0}^b(i\nu_n) = - \sum_{ij \neq i_0} t_{i_0i}^b \tilde{G}_{ij}^b(i\nu_n) t_{ji_0}^b \quad (17)$$

and

$$\Delta_{i_0}^f(i\omega_n) = - \sum_{ij \neq i_0} t_{i_0i}^f \tilde{G}_{ij}^f(i\omega_n) t_{ji_0}^f. \quad (18)$$

Here $\nu_n = 2n\pi/\beta$ and $\omega_n = (2n+1)\pi/\beta$ are even (bosons) and odd (fermions) Matsubara frequencies, respectively. The tilde denotes cavity Green functions which are determined for a lattice where the site i_0 is removed. Nevertheless, using Eqs. (17,18) the hybridization functions can be expressed by local correlation functions only. Namely, since the self-energies are diagonal in the lattice indices and the cavity Green functions are related to the full Green functions by

$$\tilde{G}_{ij}^b(i\nu_n) = G_{ij}^b(i\nu_n) - G_{ii_0}^b(i\nu_n) G_{i_0i_0}^b(i\nu_n)^{-1} G_{i_0j}^b(i\nu_n), \quad (19)$$

and

$$\tilde{G}_{ij}^f(i\omega_n) = G_{ij}^f(i\omega_n) - G_{ii_0}^f(i\omega_n) G_{i_0i_0}^f(i\omega_n)^{-1} G_{i_0j}^f(i\omega_n), \quad (20)$$

one can derive [54] the corresponding local Dyson equations and express the hybridization functions by the self-energies and the local Green functions as

$$G_{i_0}^b(i\nu_n)^{-1} + \Sigma_{i_0}^b(i\nu_n) = i\nu_n \sigma_3 + (\mu_b - \epsilon_{i_0}^b) \mathbf{1} - \Delta_{i_0}^b(i\nu_n), \quad (21)$$

and

$$G_{i_0}^f(i\omega_n)^{-1} + \Sigma_{i_0}^f(i\omega_n) = i\omega_n + \mu_f - \epsilon_{i_0}^f - \Delta_{i_0}^f(i\omega_n). \quad (22)$$

To close the set of the DMFT equations we employ the Dyson equation for the lattice Green functions, where the exact self-energies are replaced by the local ones, i.e.,

$$G_{ij}^b(i\nu_n) = \left[(i\nu_n \sigma_3 + \mu_b \mathbf{1} - \Sigma_i(i\nu_n)) \delta_{ij} - t_{ij}^b \mathbf{1} \right]^{-1}, \quad (23)$$

and

$$G_{ij}^f(i\omega_n) = \left[(i\omega_n + \mu_f - \Sigma_i(i\omega_n)) \delta_{ij} - t_{ij}^f \right]^{-1}. \quad (24)$$

The self-consistent solution is reached when the local Green functions (3) and (7) are identical to the corresponding diagonal elements of the Green functions obtained from the Dyson Eqs. (23) and (24).

The scaled hopping amplitudes κ_{i_0j} appearing in Eq. (14) need to be determined such that in the non-interacting ($U_b = 0$) case the linear Gross-Pitaevski equation

$$\frac{1}{2} \left(\partial_\tau \sigma_3 - (\mu_b - \epsilon_{i_0}^b) \mathbf{1} \right) \Phi_{i_0}(\tau) + \frac{1}{2} \int_0^\beta d\tau' \Delta_{i_0}^b(\tau - \tau') \Phi_{i_0}(\tau') + \sum_{j \neq i_0} \kappa_{i_0j} \Phi_j(\tau) = 0 \quad (25)$$

is satisfied for a given lattice [55].

The real-space formulation presented here can be employed to study mixtures of bosons and fermions on a lattice in the presence of external potentials. It allows for the appearance of phases with diagonal long-range order, phase separation, and BEC. We note that when the external potentials are random, one also has to specify the average over the disorder [5–7]. In the absence of external potentials ($\epsilon_i^{b,f} = 0$) there is usually no need for a formulation in real-space since the lattice Dyson equations can be written as a Hilbert transform over the momenta. However, even for $\epsilon_i^{b,f} = 0$ a real-space formulation is more suitable when one wants to describe phase separation or incommensurate long-range order, e.g., stripe formation.

3.1 Effective attraction between bosons mediated by their interaction with fermions

Due to the absence of local fermion–fermion interactions the DMFT action for model I is bilinear in Grassmann variables. Therefore they can be integrated out yielding an effective local action for the interacting bosons. The local partition function reads

$$Z_{i_0} = \int D[b] e^{-S_{i_0}^b[b] + \ln \text{Det}[M_{i_0}^b]},$$

where the matrix elements of the operator $M_{i_0}^b$ in Matsubara frequency space have the form

$$\begin{aligned} [M_{i_0}^b]_{nm} &\equiv \left[(\partial_\tau - \mu_f + \epsilon_{i_0}^f + U_{bf} n_{i_0}^b(\tau)) \delta_{\tau, \tau'} + \Delta_{i_0}^f(\tau - \tau') \right]_{nm} \\ &= \left[-i\omega_n - \mu_f + \epsilon_{i_0}^f + \Delta_{i_0}^f(\omega_n) \right] \delta_{nm} + \frac{U_{bf}}{\sqrt{\beta}} n_{i_0}^b(\omega_n - \omega_m). \end{aligned} \quad (26)$$

Apparently the local interaction between bosons and fermions U_{bf} gives rise to a complicated effective dynamics of the bosons. Indeed, even if the interaction between the bosons is neglected ($U_b = 0$) the effective *bosonic action* is not bilinear. We will now show that this corresponds to a nontrivial effective interaction between the bosons. To this end we expand the logarithm of the determinant as

$$\begin{aligned} \ln \text{Det}[M^b] &= \text{Tr} \ln[M^b] = \text{Tr} \ln[-(\mathcal{G}^f)^{-1} + M_1^b] \\ &= \text{Tr} \ln[-(\mathcal{G}^f)^{-1}] - \sum_{m=1}^{\infty} \frac{1}{m} \text{Tr}[\mathcal{G}^f M_1^b]^m, \end{aligned} \quad (27)$$

where we make use of the Weiss Green function

$$\mathcal{G}_{i_0}^f(\omega_n) = \frac{1}{i\omega_n + \mu_f - \epsilon_{i_0}^f - \Delta_{i_0}^f(\omega_n)}. \quad (28)$$

By keeping only the first two terms one obtains the Random Phase Approximation (RPA), which takes into account bubble diagrams for fermions plus fermionic Hartree contributions. The effective bosonic action is then found as

$$\tilde{S}_{i_0}^b \approx S_{i_0}^b + \frac{U_{bf}}{\sqrt{\beta}} \sum_n \mathcal{G}_{i_0}^f(\omega_n) n_{i_0}^b(\nu_m = 0) - \frac{U_{bf}^2}{2} \sum_n n_{i_0}^b(\nu_n) \Pi_{i_0}^f(\nu_n) n_{i_0}^b(-\nu_n), \quad (29)$$

where we introduced the fermionic polarization (bubble) function

$$\Pi_{i_0}^f(\nu_n) \equiv -\frac{1}{\beta} \sum_m \mathcal{G}_{i_0}^f(\omega_m) \mathcal{G}_{i_0}^f(\omega_m + \nu_n). \quad (30)$$

The first-order term in U_{bf} is the Hartree contribution and leads to a renormalization of the bosonic chemical potential. The second-order term describes a frequency dependent (retarded) local interaction between

bosons due to presence of the fermions. The static component of the polarization function is equal to the fermionic local density of states $N_{i_0}^f$ at the Fermi level, i.e., $\Pi_{i_0}^f(\nu_n = 0) = N_{i_0}^f(\mu)$. Therefore the effective static interaction between the bosons is given by $U_b^{\text{eff}} = U_b - U_{bf}^2 N_{i_0}^f(\mu)$, which becomes attractive for $U_b < U_{bf}^2 N_{i_0}^f(\mu)$. The bosonic subsystem then becomes unstable against phase separation or the formation of bosonic molecules. It is interesting to note that this effective attraction between the bosons originates from their interaction with the fermions. This effective attraction is a very general quantum mechanical effect. Namely, it arises from second-order perturbation theory for the same reason that the second-order contribution to the ground-state energy is always negative. This negative sign implies an attraction, unless higher order corrections invert the sign of the effective interaction. Diagrammatically one may interpret this as an interaction between bosons due to the exchange of virtual fermions. The effective attraction between bosons is complementary to the well-known mediation of an effective attraction between fermions through the exchange of virtual bosons, e.g., phonons. This corroborates earlier results on the effective interaction between bosons [25–32, 37, 39–43, 45].

3.2 Immobile fermions: Falicov-Kimball limit of model I

In the case of immobile fermions, i.e., $t_{ij}^f = 0$ (atomic limit), model I reduces to a Falicov-Kimball like model [19, 56] for Bose-Fermi mixtures. The number of fermions on each site is then conserved and can be used to characterize many-body states. The local partition function takes the form

$$Z_{i_0} = \sum_{n_{i_0}=0,1} e^{\beta(\mu_f - \epsilon_{i_0}^f)n_{i_0}} \int D[b] e^{-S_{i_0}^b - U_{bf} n_{i_0}^f \int_0^\beta d\tau n_{i_0}^b(\tau)}. \quad (31)$$

Similar expressions can be derived for bosonic correlation functions. Although the fermions are immobile they are still thermodynamically coupled to the bosons. This is expressed by the annealed (rather than quenched) average over different possible configurations of fermions on the lattice. In other words, due to the fluctuations around the microscopic equilibrium configurations the systems probes different configurations of fermions and, for a given temperature and other external parameters, realizes the optimal configuration. In particular, on a bipartite lattice and at low enough temperatures the fermions can be long-range ordered with a checker board structure. Therefore the $t_{ij}^f = 0$ (Falicov-Kimball) limit of model I differs from an Anderson disorder model, where fermions are *fixed* at random lattice sites which are independent of temperature or other parameters.

For $t_{ij}^f = 0$ model I can have several different solutions. In particular, a sufficiently strong repulsion between bosons and fermions, U_{bf} , will cause a splitting of the bosonic band into two subbands. In this limit, and for a homogeneous system with boson density \bar{n}^b satisfying $\bar{n}^b + \bar{n}^f \in \mathbb{N}$, where \bar{n}^f is the density of fermions, a change of the interaction U_b will lead to a transition from a superfluid to a Mott insulator. Namely, for large values of U_{bf} the lattice sites occupied by fermions are inaccessible for bosons, thereby increasing the effective density of bosons. This transition is an analog of the metal-insulator transition for fermions at non-integer densities in the presence of binary-alloy disorder [57]. Away from these special densities the ground state will be a superfluid. Since the condensation temperature T_{BEC} increases with the density of bosons we also expect T_{BEC} to increase with increasing U_{bf} . Indeed, for $U_b = 0$ the model is equivalent to the bosonic Falicov-Kimball model with immobile, hard-core bosons discussed in [19] where it was shown that the transition temperature T_{BEC} increases with increasing U_{bf} .

4 Solution of model II within dynamical mean-field theory

In the case of Bose-Fermi mixtures with spinful fermions described by model II, (2), condensation into a state with macroscopic quantum coherence is not restricted to bosons. Namely, fermions can undergo *pair condensation* provided $U_f < 0$, or if the effective boson-mediated attraction dominates over the bare repulsion $U_f > 0$ (see below). To include the possibility of fermionic superfluidity (or superconductivity

in the case of charged fermions) within the DMFT we employ the Nambu formalism also for fermions. To this end we define Nambu spinor fermion operators

$$\mathbf{f}_i = \begin{pmatrix} f_{i\sigma} \\ f_{i\bar{\sigma}}^\dagger \end{pmatrix} \quad \text{and} \quad \mathbf{f}_i^\dagger = (f_{i\sigma}^\dagger, f_{i\bar{\sigma}}) \quad (32)$$

and the local fermionic one-particle Green function

$$\mathbf{G}_i^f(\tau) \equiv -\langle T_\tau \mathbf{f}_i(\tau) \mathbf{f}_i^\dagger(0) \rangle_{S_i} \equiv - \begin{pmatrix} \langle T_\tau f_{i\sigma}(\tau) f_{i\sigma}^\dagger(0) \rangle_{S_i} & \langle T_\tau f_{i\sigma}(\tau) f_{i\bar{\sigma}}(0) \rangle_{S_i} \\ \langle T_\tau f_{i\bar{\sigma}}^\dagger(\tau) f_{i\sigma}^\dagger(0) \rangle_{S_i} & \langle T_\tau f_{i\bar{\sigma}}^\dagger(\tau) f_{i\bar{\sigma}}(0) \rangle_{S_i} \end{pmatrix}. \quad (33)$$

For bosons all relevant Green functions and the BEC order parameter are the same as in model I.

To derive the DMFT equations for model II in real space we again employ the cavity method and proceed as before. As a result we find the following local DMFT action at site i_0

$$S_{i_0} = S_{i_0}^b + S_{i_0}^f + S_{i_0}^{bf}, \quad (34)$$

where

$$\begin{aligned} S_{i_0}^b = & \frac{1}{2} \int_0^\beta d\tau \mathbf{b}_{i_0}^*(\tau) \left(\partial_\tau \boldsymbol{\sigma}_3 - (\mu_b - \epsilon_{i_0}^b) \mathbf{1} \right) \mathbf{b}_{i_0}(\tau) + \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \mathbf{b}_{i_0}^*(\tau) \boldsymbol{\Delta}_{i_0}^b(\tau - \tau') \mathbf{b}_{i_0}(\tau') \\ & + \frac{U_b}{2} \int_0^\beta d\tau n_{i_0}^b(\tau) (n_{i_0}^b(\tau) - 1) + \int_0^\beta d\tau \sum_{j \neq i_0} \kappa_{i_0 j} \mathbf{b}_{i_0}^*(\tau) \boldsymbol{\Phi}_j(\tau) \end{aligned} \quad (35)$$

is the action for bosons coupled to a reservoir of normal and condensed lattice bosons [19],

$$\begin{aligned} S_{i_0}^f = & \int_0^\beta d\tau \mathbf{f}_{i_0}^*(\tau) \left(\partial_\tau \mathbf{1} - (\mu_f - \epsilon_{i_0}^f) \boldsymbol{\sigma}_3 \right) \mathbf{f}_{i_0}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' \mathbf{f}_{i_0}^*(\tau) \boldsymbol{\Delta}_{i_0}^f(\tau - \tau') \mathbf{f}_{i_0}(\tau'), \\ & + \frac{U_f}{2} \int_0^\beta d\tau \sum_\sigma n_{i_0\sigma}^f(\tau) n_{i_0\bar{\sigma}}^f(\tau) \end{aligned} \quad (36)$$

is the action for spinful fermions coupled to a fermionic reservoir, and

$$S_{i_0}^{bf} = U_{bf} \int_0^\beta d\tau \sum_\sigma n_{i_0}^b(\tau) n_{i_0\sigma}^f(\tau) \quad (37)$$

is the action describing the coupling between bosons and fermions at site i_0 . The hybridization function matrices $\boldsymbol{\Delta}_{i_0}^b$ and $\boldsymbol{\Delta}_{i_0}^f$ are related to the local self-energies through the local Dyson equations

$$\mathbf{G}_{i_0}^b(i\nu_n)^{-1} + \boldsymbol{\Sigma}_{i_0}^b(i\nu_n) = i\nu_n \boldsymbol{\sigma}_3 + (\mu_b - \epsilon_{i_0}^b) \mathbf{1} - \boldsymbol{\Delta}_{i_0}^b(i\nu_n), \quad (38)$$

and

$$\mathbf{G}_{i_0}^f(i\omega_n)^{-1} + \boldsymbol{\Sigma}_{i_0}^f(i\omega_n) = i\omega_n \mathbf{1} + (\mu_f - \epsilon_{i_0}^f) \boldsymbol{\sigma}_3 - \boldsymbol{\Delta}_{i_0}^f(i\omega_n). \quad (39)$$

The set of self-consistent DMFT equations for the model II is closed by the Dyson equations for the bosonic and fermionic lattice Green functions with local self-energies

$$\mathbf{G}_{ij}^b(i\nu_n) = \left[(i\nu_n \boldsymbol{\sigma}_3 + \mu_b \mathbf{1} - \boldsymbol{\Sigma}_i(i\nu_n)) \delta_{ij} - t_{ij}^b \mathbf{1} \right]^{-1}, \quad (40)$$

and

$$\mathbf{G}_{ij}^f(i\omega_n) = \left[(i\omega_n \mathbf{1} + \mu_f \boldsymbol{\sigma}_3 - \boldsymbol{\Sigma}_i(i\omega_n)) \delta_{ij} - t_{ij}^f \mathbf{1} \right]^{-1}. \quad (41)$$

These equations yield the general DMFT solution for Bose-Fermi mixture on a lattice. They include the possibility for bosonic and fermionic superfluidity, phase separation, and the appearance of phases with diagonal long-range order.

4.1 Effective attraction between fermions mediated by the interaction with bosons

In model II the presence of fermions with a local interaction can lead to similar effects as those discussed in connection with model I, namely to an effective attraction between bosons, and band splitting in the Falicov-Kimball (atomic) limit where $t_{ij}^f = 0$. In particular, we will now discuss the situation where bosons influence the effective local interaction between fermions. For non-interacting bosons, $U_b = 0$, the local action is bilinear in the bosonic field which can therefore be integrated out analytically. We introduce a Bogoliubov shift of the complex bosonic field to remove the linear term in the bosonic part of the action as

$$b(\tau) \rightarrow \tilde{b}(\tau) + c(\tau), \quad b^*(\tau) \rightarrow \tilde{b}^*(\tau) + c^*(\tau). \quad (42)$$

Here $\tilde{b}(\tau)$ and $c(\tau)$ represent normal and condensed bosons, respectively. The local bosonic action then takes the form

$$S_{i_0}^b = \int_0^\beta d\tau \tilde{b}_{i_0}^*(\tau) \left(\partial_\tau - \mu_b + \epsilon_{i_0}^b + U_{bf} \bar{n}_{i_0}^f \right) \tilde{b}_{i_0}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' \tilde{b}_{i_0}^*(\tau) \Delta_{i_0}^b(\tau - \tau') \tilde{b}_{i_0}(\tau) \\ + \frac{\sum_{j \neq i_0} \kappa_{i_0 j} |\phi_j|}{\mu_b - \epsilon_{i_0}^b - U_{bf} \bar{n}_{i_0}^f - \Delta_{i_0}^b(\nu_n = 0)}, \quad (43)$$

where the last term describes the Bose-Einstein condensate, and the chemical potential for bosons is renormalized due to the interaction with the fermions by a Hartree-like term. The contribution describing the interaction between bosons and fermions is now expressed in terms of normal bosons \tilde{b} , i.e.,

$$S_{i_0}^{bf} = U_{bf} \int_0^\beta d\tau \tilde{b}_{i_0}^*(\tau) \tilde{b}_{i_0}(\tau) n_{i_0}^f(\tau). \quad (44)$$

In the next step we integrate out the normal bosons and thereby obtain the following partition function for fermions:

$$Z_{i_0}^f = \int D[f] e^{-S_{i_0}^f[f] - \ln \text{Det}[M_{i_0}^f]}. \quad (45)$$

Here the matrix elements of the operator $M_{i_0}^f$ in Matsubara frequency space have the form

$$\left[M_{i_0}^f \right]_{nm} = \left[(\partial_\tau - \mu_b + U_{bf} \bar{n}_{i_0}^f + \epsilon_{i_0}^b + U_{bf} \sum_\sigma n_{i_0\sigma}^f) \delta_{\tau\tau'} + \Delta_{i_0}^b(\tau - \tau') \right]_{nm} \\ = \left[-i\nu_n - \mu_b + U_{bf} \bar{n}_{i_0}^f - \epsilon_{i_0}^b + \Delta_{i_0}^b(\nu_n) \right] \delta_{nm} + \frac{U_{bf}}{\sqrt{\beta}} \sum_\sigma n_{i_0\sigma}^f (\nu_n - \nu_m). \quad (46)$$

Finally we introduce the Weiss Green function for local bosons

$$\mathcal{G}_{i_0}^b(\nu_n) = \frac{1}{i\nu_n + \mu_b - U_{bf} \bar{n}_{i_0}^f - \epsilon_{i_0}^b - \Delta_{i_0}^b(\nu_n)}, \quad (47)$$

and perform a Taylor expansion to second order in U_{bf} . The effective fermionic action then takes the form

$$\tilde{S}_{i_0}^f \approx S_{i_0}^f - \frac{U_{bf}}{\sqrt{\beta}} \sum_{n\sigma} \mathcal{G}_{i_0}^b(\nu_n) n_{i_0}^f(0) + \frac{U_{bf}^2}{2} \sum_{n\sigma\sigma'} n_{i_0\sigma}^f(\nu_n) \Pi_{i_0}^b(\nu_n) n_{i_0\sigma'}^f(-\nu_n),$$

where the bosonic polarization function is given by

$$\Pi_{i_0}^b(\nu_n) = \frac{1}{\beta} \sum_m \mathcal{G}_{i_0}^b(\nu_m) \mathcal{G}_{i_0}^b(\nu_m + \nu_n). \quad (48)$$

In the static limit this polarization function yields the local compressibility, $\Pi_{i_0}^b(\nu_n = 0) = -\partial \bar{n}_{i_0}^b / \partial \mu_b$, which must be positive for the system to be stable. The effective local interaction between fermions $U_f^{eff} = U_f - U_{bf}^2 \partial \bar{n}_{i_0}^b / \partial \mu_b$ becomes negative (attractive) for $U_f < U_{bf}^2 \partial \bar{n}_{i_0}^b / \partial \mu_b$. Hence a repulsive interaction between fermions and bosons can lead to an effective attraction between fermions. The fermionic subsystem then becomes unstable with respect to a condensation of Cooper pairs as is well-known from the theory of superconductivity [58].

5 Summary

We derived a comprehensive, thermodynamically consistent theoretical framework for the investigation of mixtures of correlated lattice bosons and fermions – the BF-DMFT. In analogy to its purely fermionic and bosonic counterparts the BF-DMFT becomes exact in the limit of high spatial dimensions d or coordination number Z . It may be employed to calculate the phase diagram and thermodynamics of mixtures of interacting lattice bosons and fermions in the entire range of microscopic parameters. As in the B-DMFT the BF-DMFT employs a different scaling of the hopping amplitude of bosons with Z , depending on whether the bosons are in the normal or the condensed phase. Thereby normal and condensed bosons are treated on equal footing. Namely, in the BF-DMFT the normal bosons retain their dynamics even in the limit $Z \rightarrow \infty$, such that the effects of the dynamic coupling between normal bosons and the condensate are fully included.

Using the self-consistency equations of the BF-DMFT we solved two different interaction models of correlated bosons and fermions: model I where all particles are spinless, and model II where fermions carry spin one-half. In the latter model a local interaction between fermions is present which leads to dynamical effects even in the limit of large Z . In model I we showed that the local interaction between bosons and fermions can give rise to an effective attraction between bosons. The bosonic subsystem is therefore unstable against phase separation or the formation of bosonic molecules. In the case of immobile fermions model I reduces to a Falicov-Kimball model for Bose-Fermi mixtures which can be solved in closed form. Model II has several different solutions depending on the interaction parameters and the density of bosons. In particular, the interaction between bosons and fermions can mediate an effective attractive local interaction not only between bosons but also between fermions. The latter leads to an instability with respect to Cooper pair formation as in superconductivity.

In conclusion, interaction effects in mixtures of bosons and fermions on a lattice can lead to a multitude of fascinating correlation phenomena, including the emergence of an effective attraction between bosons mediated by fermions and vice versa. Experiments with cold atoms in optical lattices will be able to test these predictions and lead to deep insights into the overall physical behavior of many-body systems with particles obeying different statistics.

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