Rotationally invariant slave bosons for strongly correlated superconductors

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We extend the rotationally invariant formulation of the slave-boson method to superconducting states. This generalization, building on the recent work by Lechermann *et al.* [Phys. Rev. B **76**, 155102 (2007)], allows to study superconductivity in strongly correlated systems. We apply the formalism to a specific case of strongly correlated superconductivity, as that found in a multiorbital Hubbard model for alkali-doped fullerides, where the superconducting pairing has phonic origin, yet it has been shown to be favored by strong correlation owing to the symmetry of the interaction. The method allows to treat on the same footing the strong correlation effects and the interorbital interactions driving superconductivity, and to capture the physics of strongly correlated superconductivity, in which the proximity to a Mott transition favors the superconducting phenomenon.

I. INTRODUCTION

The theoretical description of strongly correlated systems and of the prototypical models introduced to understand their behavior plays a central role in modern many-body theory. Even if the number of materials of interest in which the mutual interaction between electrons has been identified as relevant is now countless, there is no doubt that the main trigger for the development of the correlated-electron field has been the discovery of high-temperature superconductivity in doped correlated insulators such as the copper oxides. Yet, the link between strong correlation and high-temperature superconductivity has not been established unambiguously, which prompts for theoretical methods able to describe the superconducting phenomenon in the presence of strong electron correlations.

One of the main reasons why strongly correlated systems and their properties are, at the same time, interesting and hard to solve is that they are intrinsically out of weak-coupling regimes, where a perturbative expansion can be performed. Starting from an uncorrelated system and imagining to continuously increase the degree of correlation, the relevance of local repulsion gradually introduces constraints to the electronic motion, leading eventually to the localization of the carriers (Mott transition). Thus a proper method for correlated electrons should be able to introduce local constraints onto an otherwise uncorrelated state, that would be naturally delocalized, i.e., spatially unconstrained.

A popular strategy which formally implements this point of view is based on slave bosons.[1,2] Within these approaches, the Hilbert space is enlarged to include, besides fermionic degrees of freedom associated to Landau quasiparticles, suitable extra degrees of freedom of bosonic character which are typically related to local states. The auxiliary (slave) degrees of freedom are then treated in a mean-field approximation, leading to an effective low-energy theory for the quasiparticles. The high-energy physics can only be recovered introducing fluctuations in the fields describing the auxiliary particles.[3] We can see this strategy as a way to enforce a local point of view, which is expected to be correct in very strong coupling, starting from delocalized noninteracting

states. In its most popular version, introduced by Kotliar and Ruckenstein,[2] one defines one boson for each local configuration (namely, $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$), and the equivalence between the physical Hilbert space and the new extended space is enforced by imposing constraints which, as we shall discuss below, imply that the local configurations should be coherently labeled by the fermionic and bosonic degrees of freedom, and that precisely one boson should be present on each lattice site.

Yet, as thoroughly discussed in Ref. 4, the standard four-boson representation[2] for the single-band Hubbard model, as well as its simplest generalizations to multiorbital models,[5] are not suitable to handle arbitrary forms of the interaction Hamiltonian, characterized by terms which cannot be put in the form of density-density interactions, such as exchange interactions associated to the Hund's rule coupling. Furthermore, even for pure density-density interactions, the Kotliar-Ruckenstein approach still remains inadequate to handle charge-symmetry-breaking order parameters such as the superconducting one in the Hubbard model. Slave-boson approaches to superconductivity in the Hubbard model have indeed mostly used the approximately equivalent strong-coupling *t-J* model and have been based on specific assumptions.[6]

The first attempt in overcoming the inadequacy of Kotliar-Ruckenstein's representation was made by Li *et al.*,[7] who proposed a spin-rotation invariant slave-boson formulation of the single-band Hubbard model, while in Ref. 8 Frésard and Wölfle introduced a more general representation for single-band models, in which spin and charge degrees of freedom are treated on the same footing and rotational invariance involves both spin and particle-hole transformations. Although the formalism presented by these authors refers only to a four-state system with the slave-boson fields labeled in correspondence with the specific SU(2)⊗SU(2) generators of spin and particle-hole rotations, it already has all the ingredients required for describing systems with local superconducting pairing. Such method has been indeed applied to the single-band attractive Hubbard model in Ref. 9. Developing the ideas of these pioneering works in a more systematic way, Lechermann *et al.*[4] finally built a completely basis-independent slave-boson formalism, suitable to de-

scribe, within a generic multiorbital model, any arbitrary form of local interaction. As it is found for Kotliar-Ruckenstein's approach, it is worth mentioning that, at mean-field level, such formalism turns out to be equivalent[10] to analogous extensions of the Gutzwiller approach.[11,12]

While the possibility of extending the formalism to superconducting states is mentioned in Ref. 4, the explicit derivation is limited to normal solutions, imposing no charge-symmetry breaking. In the present work, instead, we lift this restriction and consider explicitly the more general case of full rotational invariance under any local transformation of the electronic degrees of freedom and we apply the formalism to solve a three-orbital model which has been proposed to describe alkali-doped fullerides.[13,14] Besides its relevance to the fullerides, the model has important properties that led us to choose it as an optimal benchmark for our method. The model has indeed been shown to present "strongly correlated superconductivity,"[13] i.e., the enhancement of phonon-mediated superconductivity in the proximity of a Mott transition. The key of the phenomenon is that a small attraction which involves orbital and spin degrees of freedom is not screened when charge fluctuations are frozen by strong correlations. This leads to an enhancement of superconductivity since the unscreened attraction now acts on strongly renormalized quasiparticles with a larger effective density of states. This effect has been identified using dynamical mean-field theory (DMFT),[15] which fully takes into account local quantum fluctuations, but it has not been reproduced by ordinary slave-boson methods due to the difficulties in treating interactions which are not of the charge-charge form, such as those driving superconductivity in the model we are dealing with. In this light, the model is an ideal test ground of the ability of the rotationally invariant slave-boson method in accurately treating general forms of interactions. On the other hand, the model has only local (on-site) interactions, which simplifies the approach.

The paper is organized as follows. In Sec. II we introduce the rotationally invariant slave-boson method for models with local superconducting pairing. In Sec. III we present the multiorbital model used for the description of fullerenes, illustrating the way it can be solved by means of the slave-boson approach. In Sec. IV we present the results obtained with our method and finally Sec. V is dedicated to concluding remarks and perspectives.

II. THE GENERAL FORMALISM

In this section we will explicitly extend the rotationally invariant slave-boson formalism introduced by Lechermann *et al.*[4] to the possibility of describing superconducting states. To facilitate the reading and the comparison with the formalism of Ref. 4, whenever possible we shall use the same notation for corresponding quantities.

A. Motivations

Without entering in details, we shall first provide a brief reminder on slave-boson formulations, in order to face the difficulties encountered with noninvariant approaches such as Kotliar-Ruckenstein's one.

In a generic multiorbital model the local Hilbert space of electronic states is defined as the set of all the possible "atomic" configurations at a given lattice site (for simplicity, we will drop site indices throughout this section); a natural choice for the basis set of this space is provided by the 2^M Fock states

$$|n\rangle \equiv (d_1^\dagger)^{n_1} \cdots (d_M^\dagger)^{n_M}|\text{vac}\rangle, \quad [n_\alpha = 0,1] \qquad (1)$$

where $\alpha = 1, \dots, M$ are the local-orbital species and $d_\alpha^\dagger$ the corresponding electron-creation operators. A slave-boson representation is then constructed by mapping the local Hilbert space $\mathcal{H}$ (e.g., the Fock states $|n\rangle$) onto an "enlarged" Hilbert space $\underline{\mathcal{H}}$ generated by the tensor products of boson operators $\phi_\mu^\dagger$ and auxiliary fermion operators $f_\alpha^\dagger$

$$\mathcal{H}{:}\{|n\rangle\} \mapsto \underline{\mathcal{H}}{:}\left\{\prod_\mu (\phi_\mu^\dagger)^{N_\mu}|\text{vac}\rangle \otimes |n\rangle_f\right\}.$$

In the above expression $|n\rangle_f$ refers to the Fock states generated by the auxiliary fermions $f_\alpha^\dagger$, which correspond to quasiparticle (QP) degrees of freedom: their presence ensures the possibility of describing Fermi-liquid properties within the auxiliary-fields representation (note that the orbital basis for quasiparticle degrees of freedom may not coincide, in general, with that of the physical electron operator $d_\alpha^\dagger$). On the other hand, an arbitrary number of auxiliary bosons ϕ_μ, for each species μ, can in principle be present in the enlarged Hilbert space, unless some constraints, which characterize the specific form of the slave-boson representation, are imposed to its states. In other words, a given representation is defined by the way in which the auxiliary states are selected out of the enlarged space $\underline{\mathcal{H}}$ in order to represent uniquely the original physical states $|n\rangle$

$$|n\rangle \mapsto |\underline{n}\rangle,$$

$$|\underline{n}\rangle \equiv \sum_{\{N_\mu\},m} K(n,\{N_\mu\},m)\prod_\mu (\phi_\mu^\dagger)^{N_\mu}|\text{vac}\rangle \otimes |m\rangle_f. \qquad (2)$$

Needless to say, the choice of a specific representation K, apart from being consistent with the above uniqueness assumption, must also provide some simplifications in the (local) interaction Hamiltonian: the whole purpose of introducing auxiliary bosons is indeed the possibility of writing local interactions as a sum of quadratic terms in the boson fields, at the expense of a larger number of degrees of freedom and a more complex structure of hopping terms.

In multiorbital generalization of Kotliar-Ruckenstein's approach, 2^M boson fields $\phi_\mu \equiv \phi_n$ are introduced in correspondence with the original Fock states $|n\rangle$, and the representation of such states in the enlarged Hilbert space reads

$$|\underline{n}\rangle \equiv \phi_n^\dagger|\text{vac}\rangle \otimes |n\rangle_f. \qquad (3)$$

The "physical states" in $\underline{\mathcal{H}}$ are therefore those states containing exactly one boson and whose quasiparticle content $|n\rangle_f$ matches the Fock configuration associated to the boson field ϕ_n. From Eq. (3) it should be evident the noninvariant nature of this representation under rotations of the quantization basis. Consider, in fact, an SU(M) rotation of the orbital indices[16]

$$d_\alpha^\dagger = \sum_\beta U_{\alpha\beta} \tilde{d}_\beta^\dagger, \quad f_\alpha^\dagger = \sum_\beta U_{\alpha\beta} \tilde{f}_\beta^\dagger. \tag{4}$$

This rotation will induce a corresponding unitary transformation on both physical and QP Fock states, $|n\rangle = \sum_m \mathcal{U}(U)_{nm}|\tilde{m}\rangle$, so that the representation of physical states would now read

$$|\underline{\tilde{m}}\rangle = \sum_{nm'} (\mathcal{U}_{mn}^\dagger \phi_n^\dagger \mathcal{U}_{nm'})|\text{vac}\rangle \otimes |\tilde{m}'\rangle_{\tilde{f}} = \sum_{m'} \tilde{\phi}_{mm'}^\dagger |\text{vac}\rangle \otimes |\tilde{m}'\rangle_{\tilde{f}}. \tag{5}$$

In the new orbital basis, therefore, the slave-boson representation does not retain its original form, and more specifically the definite relation between physical states and their quasiparticle content no longer holds. As discussed in Ref. 8, indeed, only disentangling physical and quasiparticle degrees of freedom it becomes possible to formulate rotationally invariant slave-boson representations.

As a consequence of its basis-dependent nature, Kotliar-Ruckenstein's approach can be applied only to systems whose local Hamiltonian can be written, in an appropriate basis, in terms of purely orbital-density operators $\hat{n}_\alpha = d_\alpha^\dagger d_\alpha$,

$$H_{\text{loc}} = \sum_\alpha \epsilon_\alpha^0 \hat{n}_\alpha + \sum_{\alpha\beta} W_{\alpha\beta} \hat{n}_\alpha \hat{n}_\beta, \tag{6}$$

i.e., when the Fock states $|n\rangle$ are eigenstates of H_{loc}. In this case, the representation of H_{loc} in the enlarged Hilbert space can be easily written as a free-boson Hamiltonian

$$\underline{H}_{\text{loc}} = \sum_n E_n \phi_n^\dagger \phi_n, \tag{7}$$

with $E_n = \sum_\alpha \epsilon_\alpha^0 n_\alpha + \sum_{\alpha\beta} W_{\alpha\beta} n_\alpha n_\beta$. We remark, however, that the definite relation imposed between quasiparticle degrees of freedom and the (physical) Fock content of boson fields inhibits the development of those spontaneous symmetry-breaking order parameters that cannot be expressed in terms of orbital-density operators (e.g., superconductivity, magnetization perpendicular to the spin-quantization axis, etc.).

B. Representation of physical states

The electron Hamiltonian for a generic multiorbital model with purely local interactions is given by

$$H = H_{\text{kin}} + \sum_i H_{\text{loc}}[i], \tag{8}$$

$$H_{\text{kin}} = \sum_{\mathbf{k}} \sum_{\alpha\beta} \epsilon_{\alpha\beta}(\mathbf{k}) d_{\mathbf{k}\alpha}^\dagger d_{\mathbf{k}\beta}, \tag{9}$$

where all the local terms, including the chemical potential and the orbital energy levels, are included in H_{loc}, so that $\sum_{\mathbf{k}} \epsilon_{\alpha\beta}(\mathbf{k}) = 0$.

In comparison to the Sec. II A, we choose here, as the basis set for the (physical) local Hilbert space, a generic set of states $\{|A\rangle\}$ (not necessarily Fock states) that are eigenstates of the local particle-number operator $\hat{n}^{(d)} = \sum_{\alpha=1}^M d_\alpha^\dagger d_\alpha$, with eigenvalues N_A. Eventually, among these sets, we can choose the eigenstates $\{|\Gamma\rangle\}$ of the local Hamiltonian since

H_{loc} commutes with the local number operator. The basis set for quasiparticle states, instead, is still given by the Fock states $|n\rangle_f$ generated by the auxiliary fermion operators $f_\alpha^\dagger$.

As discussed previously in pointing out the limitations of Kotliar-Ruckenstein's approach, the key ingredient in constructing rotationally invariant slave-boson representations is to disentangle physical and quasiparticle degrees of freedom.[4] Therefore, we introduce a set of auxiliary boson fields $\phi_\mu \equiv \phi_{An}$ associated, in principle, to each pair $(|A\rangle, |n\rangle_f)$ of physical and quasiparticle states, without assuming any *a priori* relation between those states in the enlarged Hilbert-space representation. Depending on the phases one takes into account, however, there exist some limitations in the possible $\mathcal{H}$ states $\phi_{An}^\dagger|\text{vac}\rangle \otimes |n\rangle_f$ which can figure in the representation of a physical state $|A\rangle$

$$|\underline{A}\rangle \propto \sum_n \phi_{An}^\dagger|\text{vac}\rangle \otimes |n\rangle_f. \tag{10}$$

Indeed, if we limit to normal phases as in Ref. 4, it is sufficient to consider, for a given state $|A\rangle$, only those states $|n\rangle_f$ which have exactly the same number of particles of $|A\rangle$; in other words, physical states with a definite number of electrons are represented by a superposition of auxiliary states characterized by the same number of quasiparticles. On the other hand, when allowing for the spontaneous breaking of particle-number conservation, as in superconducting states, we need to consider, for each state $|A\rangle$, all the Fock states $|n\rangle_f$ characterized by

$$\left[\sum_{\alpha=1}^M n_\alpha - N_A\right](\text{mod } 2) = 0,$$

i.e., all the 2^{M-1} quasiparticle states with the same statistics of $|A\rangle$. While the former representation is invariant only under rotations of the QP basis that are block diagonal in the quasiparticle occupation number $\sum_{\alpha=1}^M n_\alpha$, the latter is invariant under a larger class of QP rotations, represented by all the unitary transformations that preserve the statistics of quasiparticle states: in such representation, the quasiparticle number operator is no longer a conserved quantity and its expectation value does not correspond to any physical observable as particle-hole transformations may change its value.

The explicit representation of $|A\rangle$ will then read, in the fully invariant formalism

$$|\underline{A}\rangle \equiv \frac{1}{\sqrt{2^{M-1}}} \sum_n \phi_{An}^\dagger|\text{vac}\rangle \otimes |n\rangle_f \tag{11}$$

with the sum running over the 2^{M-1} QP Fock states whose particle-number parity equals that of $|A\rangle$. It is worthwhile to remark that the above representation cannot be further enlarged, including, for example, in the definition of $|\underline{A}\rangle$, the remaining quasiparticle states with opposite statistics. This, in fact, would lead to unphysical results such as nonvanishing expectation values of odd numbers of fermion operators.

Constraints

In order to characterize uniquely the physical states among all the states of the enlarged Hilbert space $\mathcal{H}$, it is

necessary and sufficient that the selected states satisfy, as operator identities, the following constraints:

$$\sum_{An} \phi_{An}^{\dagger} \phi_{An} = 1, \tag{12}$$

$$\sum_{A} \sum_{nn'} \phi_{An}^{\dagger} \phi_{An'} \langle n'|f_{\alpha}^{\dagger} f_{\alpha'}|n \rangle = f_{\alpha}^{\dagger} f_{\alpha'}, \tag{13}$$

$$\sum_{A} \sum_{nn'} \phi_{An}^{\dagger} \phi_{An'} \langle n'|f_{\alpha}^{\dagger} f_{\alpha'}^{\dagger}|n \rangle = f_{\alpha}^{\dagger} f_{\alpha'}^{\dagger}. \tag{14}$$

The first two types of constraints are already present in the normal-phase formalism of Lechermann *et al.*:[4] the first equation, indeed, limits the physical subspace of $\mathcal{H}$ to one-boson states only while the second set of constraints ensures the rotational invariance of Eq. (11) under QP rotations that preserve quasiparticle number. On the other hand, the last set of constraints promotes the rotational invariance to particle-hole rotations, enabling the nonconservation of quasiparticle number.

It is worthwhile to remark that, for single-band models ($M=2$), the above equations reduce to the same set of constraints characterizing the $SU(2) \otimes SU(2)$ spin-charge invariant formalism introduced in Refs. 8 and 9, as long as the appropriate changes in notation are made. For this purpose, Ref. 9 provides a useful link between our notation and the one presented in Ref. 8. A more compact form of Eqs. (12)–(14) will be derived in Sec. II D, where we shall relate the role of constraints to the gauge group structure of the slave-boson representation.

C. Physical electron operator

The representation of the physical electron-creation operator in the enlarged Hilbert space is defined by

$$\underline{d}_{\alpha}^{\dagger}|\underline{B}\rangle = \sum_{A} \langle A|d_{\alpha}^{\dagger}|B\rangle|\underline{A}\rangle. \tag{15}$$

When the constraints Eqs. (12)–(14) are satisfied exactly, its expression in terms of bosons and quasiparticle operators reads

$$\underline{d}_{\alpha}^{\dagger} = \frac{1}{M} \sum_{AB,nm,\beta} \langle A|d_{\alpha}^{\dagger}|B\rangle \phi_{An}^{\dagger} \phi_{Bm} [\langle n|f_{\beta}^{\dagger}|m\rangle f_{\beta}^{\dagger} + \langle n|f_{\beta}|m\rangle f_{\beta}] \tag{16}$$

with the normalization factor $1/M$ coming from the following relation:

$$\sum_{p,\beta} [\langle n|f_{\beta}^{\dagger}|p\rangle f_{\beta}^{\dagger}|p\rangle + \langle n|f_{\beta}|p\rangle f_{\beta}|p\rangle] = M|n\rangle. \tag{17}$$

We can thus summarize the nondiagonal relation between physical and quasiparticle degrees of freedom in the form

$$\underline{d}_{\alpha}^{\dagger} = R_{\alpha\beta}^{(p)}[\phi]^* f_{\beta}^{\dagger} + R_{\alpha\beta}^{(h)}[\phi] f_{\beta} \tag{18}$$

(summation over repeated indices is implied), where we have defined the R-matrix operators as

$$R_{\alpha\beta}^{(p)}[\phi]^* = \frac{1}{M} \sum_{AB,nm} \langle A|d_{\alpha}^{\dagger}|B\rangle \phi_{An}^{\dagger} \phi_{Bm} \langle m|f_{\beta}|n\rangle, \tag{19}$$

$$R_{\alpha\beta}^{(h)}[\phi] = \frac{1}{M} \sum_{AB,nm} \langle A|d_{\alpha}^{\dagger}|B\rangle \phi_{An}^{\dagger} \phi_{Bm} \langle m|f_{\beta}^{\dagger}|n\rangle. \tag{20}$$

In the above expressions, we have taken advantage of the reality of the matrix elements between Fock states, $\langle n|f_{\beta}|m\rangle = \langle m|f_{\beta}^{\dagger}|n\rangle$, in order to guarantee the correct transformation properties of the R operators under the gauge group transformations discussed in Sec. II D.

At the saddle-point level, on the other hand, when the boson fields are treated as probability amplitudes and the constraints are satisfied only on average, the expression of $\underline{d}_{\alpha}^{\dagger}$ must be modified,[2] in order to recover the correct normalization of transition amplitudes in the noninteracting limit. For this purpose, it is easier to define the physical electron operator in the orbital basis $\{\lambda\}$ in which the quasiparticle and quasihole density matrices are diagonal

$$\hat{\Delta}_{\alpha\beta}^{(p)} \equiv \sum_{Anm} \phi_{An}^* \phi_{Am} \langle m|f_{\alpha}^{\dagger} f_{\beta}|n\rangle = \sum_{\lambda} U_{\alpha\lambda} \xi_{\lambda} U_{\lambda\beta}^{\dagger}, \tag{21}$$

$$\hat{\Delta}_{\alpha\beta}^{(h)} \equiv \sum_{Anm} \phi_{An}^* \phi_{Am} \langle m|f_{\beta} f_{\alpha}^{\dagger}|n\rangle = \sum_{\lambda} U_{\alpha\lambda} (1 - \xi_{\lambda}) U_{\lambda\beta}^{\dagger}, \tag{22}$$

where $\xi_{\lambda} = \sum_{An} |\Omega_{An}|^2 n_{\lambda}$ is the probability to find the system in a state such that $n_{\lambda} = 1$, i.e., with a quasiparticle in the orbital λ (note that $\sum_{An} |\Omega_{An}|^2 = 1$). In these expressions, the quasiparticle operators referred to the new orbitals are related to the old ones by the unitary transformation

$$f_{\alpha}^{\dagger} = \sum_{\lambda} U_{\alpha\lambda} \psi_{\lambda}^{\dagger} \tag{23}$$

while the boson fields transform with the corresponding rotation of the Fock states (summation over repeated indices is implied)

$$|n\rangle_f = \mathcal{U}(U)_{nm}|m\rangle_{\psi}, \quad \phi_{An} = \mathcal{U}(U)_{nm} \Omega_{Am}. \tag{24}$$

In such basis, the transition amplitude between states with $n_{\lambda} = 0$ in the initial [final] configuration, and $n_{\lambda} = 1$ in the final [initial] one, must be normalized by the factor $1/\sqrt{\xi_{\lambda}(1-\xi_{\lambda})}$, yielding the following expression for the physical electron operator:

$$\underline{d}_{\alpha}^{\dagger} = \sum_{AB,nm,\lambda} \frac{\langle A|d_{\alpha}^{\dagger}|B\rangle \Omega_{An}^* \Omega_{Bm}}{\sqrt{\xi_{\lambda}[\Omega](1 - \xi_{\lambda}[\Omega])}}$$
$$\times [\langle n|\psi_{\lambda}^{\dagger}|m\rangle \psi_{\lambda}^{\dagger} + \langle n|\psi_{\lambda}|m\rangle \psi_{\lambda}]. \tag{25}$$

Rotating back to the original basis, we finally get, for the saddle-point expressions of the R matrices

$$R_{\alpha\beta}^{(p)}[\phi]^* = \sum_{AB,nm,\gamma} \langle A|d_{\alpha}^{\dagger}|B\rangle \phi_{An}^* \phi_{Bm} \langle m|f_{\gamma}|n\rangle M_{\gamma\beta},$$

$$R^{(h)}_{\alpha\beta}[\phi] = \sum_{AB,nm,\gamma} \langle A|d^\dagger_\alpha|B\rangle \phi^*_{An} \phi_{Bm} \langle m|f^\dagger_\gamma|n\rangle M_{\beta\gamma}, \quad (26)$$

where

$$M_{\gamma\beta} = \left[\frac{1}{2}(\hat{\Delta}^{(p)}\hat{\Delta}^{(h)} + \hat{\Delta}^{(h)}\hat{\Delta}^{(p)}) \right]^{-1/2}_{\gamma\beta} \quad (27)$$

is the particle-hole symmetrized version of the normalization factor, expressed in the original basis.

D. Functional integral representation

The partition function of a generic multiorbital Hamiltonian (8) can be formally written, in terms of auxiliary fields, as

$$\mathcal{Z} = \int \mathcal{D}[f,f^\dagger]\mathcal{D}[\{\phi\},\{\mathcal{A}\}]e^{-\int_0^\beta d\tau \mathcal{L}(\tau)}, \quad (28)$$

where we have introduced, along with slave bosons and auxiliary fermions, a set of Lagrange multiplier fields $\{\mathcal{A}_i(\tau)\}$ that allow to enforce, at each lattice site i and imaginary-time value τ, the constraints Eqs. (12)–(14). The Lagrangian functional entering the above expression reads

$$\mathcal{L}(\tau) = \sum_i (\phi^\dagger_{An,i}\partial_\tau \phi_{An,i} + f^\dagger_{\alpha,i}\partial_\tau f_{\alpha,i} + \underline{H}_{\text{const}}[i] + \underline{H}_{\text{loc}}[i]) + \underline{H}_{\text{kin}}$$

$$(29)$$

(except for lattice sites, summation over repeated indices is always implied throughout this section), where $\underline{H}_{\text{loc}}$ and $\underline{H}_{\text{kin}}$ are, respectively, the representatives of the local and kinetic part of the Hamiltonian (8) in the enlarged Hilbert space, while $\underline{H}_{\text{const}}$ contains the constraint interactions between auxiliary fields and Lagrange multipliers.

In order to derive the expressions of the Hamiltonian terms in Eq. (29), and thereby identify the underlying symmetry group of the Lagrangian, it is convenient to collect all the local fermionic degrees of freedom (either physical or auxiliary) into a $2M$-component Nambu-Gor'kov spinor

$$\Xi_i \equiv \begin{pmatrix} \{d_{\alpha,i}\} \\ \{d^\dagger_{\alpha,i}\} \end{pmatrix}, \quad \Psi_i \equiv \begin{pmatrix} \{f_{\alpha,i}\} \\ \{f^\dagger_{\alpha,i}\} \end{pmatrix}.$$

In such formalism, the representation of physical electrons in terms of bosons and quasiparticles Eq. (18) is simply written as $\Xi_i = \mathbf{R}_i\Psi_i$, where the local $2M \times 2M$ matrix operator

$$\mathbf{R}_i \equiv \mathbf{R}[\phi_i] = \begin{pmatrix} \mathbf{R}^{(p)}[\phi_i] & \mathbf{R}^{(h)}[\phi_i]^* \\ \mathbf{R}^{(h)}[\phi_i] & \mathbf{R}^{(p)}[\phi_i]^* \end{pmatrix} \quad (30)$$

is defined in terms of the boson fields $\phi_{An,i}$ associated to the corresponding site i (note that, to lighten the notation, site indices were omitted in previous sections). The representation of the kinetic Hamiltonian is then readily obtained as

$$\underline{H}_{\text{kin}} = \sum_{ij} t^{\alpha\beta}_{ij} \underline{d}^\dagger_{\alpha,i} \underline{d}_{\beta,j} = \frac{1}{2}\sum_{ij} \Xi^\dagger_i \tilde{\mathbf{t}}_{ij}\Xi_j = \frac{1}{2}\sum_{ij} \Psi^\dagger_i \mathbf{R}^\dagger_i \tilde{\mathbf{t}}_{ij}\mathbf{R}_j\Psi_j,$$

$$(31)$$

$$\tilde{\mathbf{t}}_{ij} = \begin{pmatrix} \mathbf{t}_{ij} & 0 \\ 0 & -\mathbf{t}^*_{ij} \end{pmatrix}, \quad (32)$$

$\mathbf{t}_{ij}$ being the real-space hopping matrix, whose Fourier transform gives the band dispersion matrix $\boldsymbol{\epsilon}(\mathbf{k})$ defined in Eq. (9).

On the other hand, the local terms of the model Hamiltonian, which may include any kind of on-site interaction between (physical) electrons, are represented, within the enlarged Hilbert space, by a purely quadratic boson Hamiltonian

$$\underline{H}_{\text{loc}}[i] = \langle A|H_{\text{loc}}|B\rangle \phi^\dagger_{An,i}\phi_{Bn,i} = E_\Gamma \phi^\dagger_{\Gamma n,i}\phi_{\Gamma n,i}, \quad (33)$$

where the physical states $\{|\Gamma\rangle\}$ denote the eigenstates of H_{loc}.

1. Gauge invariance

In order to discuss the symmetry structure of the Lagrangian Eq. (29), we begin to notice that the auxiliary-fields Hamiltonian $\underline{H} = \underline{H}_{\text{kin}} + \Sigma_i \underline{H}_{\text{loc}}[i]$ is invariant under the following gauge transformations:

$$\Psi_i(\tau) \to \mathbf{U}_i(\tau)\Psi_i(\tau), \quad (34)$$

$$\phi_{An,i}(\tau) \to e^{i\xi^0_i(\tau)}\mathcal{U}[\mathbf{U}]_{nn'}\phi_{An',i}(\tau). \quad (35)$$

The unitary matrix $\mathbf{U}_i(\tau)$ in Eq. (34) represents an arbitrary $SO(2M)$ rotation of quasiparticle operators acting independently on each site, and it is conveniently parameterized as

$$\mathbf{U}_i(\tau) = e^{i\xi^a_i(\tau)\mathbf{T}^a}, \quad (36)$$

the $\mathbf{T}^a$ matrices being a $2M$-dimensional representation of the $M(2M-1)$ group generators. We note, however, that such matrices are not expressed in the usual form of an orthogonal group generator (namely, as purely imaginary antisymmetric matrices) but are instead of the form

$$\mathbf{T}^a = \begin{pmatrix} \mathbf{T}^a_{\text{H}} & \mathbf{T}^a_{\text{A}} \\ -(\mathbf{T}^a_{\text{A}})^* & -(\mathbf{T}^a_{\text{H}})^* \end{pmatrix}, \quad (37)$$

with $\mathbf{T}^a_{\text{H}}$ and $\mathbf{T}^a_{\text{A}}$ denoting, respectively, $M \times M$ Hermitian and antisymmetric matrices. In other words, the $2M$-dimensional Nambu spinors do not transform with real orthogonal matrices under $SO(2M)$ rotations, even though they clearly form a real representation of the gauge group

$$\Psi^\dagger_i = \Psi^T_i \mathcal{E}, \quad (38)$$

$$\mathbf{U}^*_i = \mathcal{E}\mathbf{U}_i\mathcal{E}, \quad (39)$$

$$\mathcal{E} = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}. \quad (40)$$

The transformation law of the boson fields, on the other hand, is characterized by the unitary transformation of Fock states $|n\rangle \to \mathcal{U}[\mathbf{U}]_{nn'}|n'\rangle$ that is associated to the $SO(2M)$ rotation of quasiparticle operators, plus an additional $U(1)$ factor $e^{i\xi^0_i(\tau)}$ under which the Nambu spinors are neutral. Following the exponential parameterization of $\mathbf{U}_i(\tau)$, we can then similarly write

$$\mathcal{U}[\mathbf{U}]_{nn'} = [e^{i\xi_i^a(\tau)\mathcal{J}^a}]_{nn'}, \tag{41}$$

where $\mathcal{J}_{nn'}^a$ are the SO(2M) group generators expressed in the Fock-space representation.

While the gauge invariance of $\underline{H}_{\text{loc}}[i]$ follows immediately from its definition Eq. (33), in the case of $\underline{H}_{\text{kin}}$ we still need to establish the transformation properties of the $\mathbf{R}_i$ operators, defined in Eq. (30). These, however, can be readily obtained by writing such operators directly in terms of the physical and auxiliary Nambu spinors, in matrix notation

$$\mathbf{R}_i = \frac{1}{M}\langle A|\Xi|B\rangle \phi_{An,i}^\dagger \phi_{Bm,i}\langle m|\Psi^\dagger|n\rangle, \tag{42}$$

$$\mathbf{R}_i(\tau) \to \mathbf{R}_i(\tau)\mathbf{U}_i^\dagger(\tau). \tag{43}$$

The above transformation law ensures the gauge invariance of the physical electron operator $\Xi_i = \mathbf{R}_i\Psi_i$ and hence of the whole kinetic Hamiltonian (31). In the discussion of the gauge invariance of the Lagrangian Eq. (29), we are thus left with the time-derivatives and constraints terms, whose transformation properties are closely related to each other. The time-derivative terms, in fact, are clearly not invariant under the transformations Eqs. (34) and (35), which generate inhomogeneous terms proportional to the time derivatives of the rotation parameters (e.g., $\partial_\tau\xi_i^a$ and $\partial_\tau\xi_i^0$). Such terms, however, can be reabsorbed by a corresponding inhomogeneous transformation of the Lagrange multiplier fields[8,17] (which may be regarded as "gauge bosons") making the whole Lagrangian gauge invariant.

To show how this mechanism works, we rewrite the $M^2 + M(M-1)$ local constraints Eqs. (13) and (14) in the following way:

$$\phi_{An,i}^\dagger \phi_{An',i}\langle n'|\Psi^\dagger\mathbf{T}^a\Psi|n\rangle = \Psi_i^\dagger\mathbf{T}^a\Psi_i, \tag{44}$$

where we have made use of the "orthogonality" between the SO(2M) $\mathbf{T}^a$ matrices. It is then straightforward (though somewhat lengthy) to verify that the Fock-space generators $\mathcal{J}_{nn'}^a$, introduced in Eq. (41), are represented by

$$\mathcal{J}_{nn'}^a = -\frac{1}{2}\langle n'|\Psi^\dagger\mathbf{T}^a\Psi|n\rangle \tag{45}$$

(in other words, the above matrices provide a faithful representation of the SO(2M) Lie algebra) so that we can finally write:

$$\underline{H}_{\text{const}}[i] = \mathcal{A}_i^a\left(\frac{1}{2}\Psi_i^\dagger\mathbf{T}^a\Psi_i + \phi_{An,i}^\dagger\mathcal{J}_{nn'}^a\phi_{An',i}\right) + \mathcal{A}_i^0(\phi_{An,i}^\dagger\phi_{An,i} - 1). \tag{46}$$

Together with the time-derivative terms, the above interactions may be arranged in "covariant derivatives" acting on the auxiliary fields (fermions and bosons)

$$\frac{1}{2}\Psi_i^\dagger D_\tau\Psi_i = \frac{1}{2}\Psi_i^\dagger[\partial_\tau + \mathcal{A}_i^a\mathbf{T}^a]\Psi_i, \tag{47}$$

$$\phi_{An,i}^\dagger D_\tau\phi_{An,i} = \phi_{An,i}^\dagger[(\partial_\tau + \mathcal{A}_i^0)\delta_{nn'} + \mathcal{A}_i^a\mathcal{J}_{nn'}^a]\phi_{An',i}, \tag{48}$$

where the role of gauge fields is played by the Lagrange multipliers $\mathcal{A}_i^a$ and $\mathcal{A}_i^0$. It is then easily checked that the Lagrangian

$$\mathcal{L} = \sum_i\left[\phi_{An,i}^\dagger D_\tau\phi_{An,i} + \frac{1}{2}\Psi_i^\dagger D_\tau\Psi_i + \underline{H}_{\text{loc}}[i] - \mathcal{A}_i^0\right] + \underline{H}_{\text{kin}} \tag{49}$$

is indeed invariant under the $SO(2M) \otimes U(1)$ gauge group, provided the Lagrange multipliers transform as gauge fields in the adjoint representation[18]

$$\mathcal{A}_i^0 \to \mathcal{A}_i^0 - i\partial_\tau\xi_i^0(\tau), \tag{50}$$

$$\mathcal{A}_i^a\mathbf{T}^a \to \mathbf{U}_i(\tau)[\mathcal{A}_i^a\mathbf{T}^a + \partial_\tau]\mathbf{U}_i^\dagger(\tau). \tag{51}$$

Note that the transformation law of $\mathcal{A}_i^a\mathbf{T}^a$ induces a corresponding transformation of $\mathcal{A}_i^a\mathcal{J}_{nn'}^a$, that has exactly the same structure of Eq. (51) with the $\mathbf{U}_i$ matrix replaced by $\mathcal{U}[\mathbf{U}]_{nn'}$. More precisely, both transformation laws descend from that of the Lagrange multiplier field $\mathcal{A}_i^a(\tau)$, which for infinitesimal rotations transforms as

$$\mathcal{A}_i^a \to \mathcal{A}_i^a + f^{abc}\mathcal{A}_i^b\xi_i^c - i\partial_\tau\xi_i^a + \mathcal{O}(\xi^2), \tag{52}$$

f^{abc} being the structure constants of the group.

Finally, it is worth mentioning that for $M=2$ (single-band models) the orthogonal group SO(4) is locally isomorphic to $SU(2) \otimes SU(2)$ so that the gauge group structure of the present formalism reduces to that of the spin-charge invariant formalism of Ref. 8.

2. Gauge fixing

As discussed in Ref. 8, the gauge invariance of the functional-integral representation causes Eq. (28) to contain integration over spurious degrees of freedom, namely, the physically equivalent field configurations connected to each other by gauge group trajectories. It is thus necessary to impose a "gauge fixing" condition that removes the integration over the unphysical degrees of freedom, as it is usually done in gauge-field theories.[19]

We choose to work in the so-called "radial gauge,"[20] in which the complex boson fields are represented through real amplitudes and complex phase fields. In this representation, the $SO(2M) \otimes U(1)$ gauge transformations allow to remove $M(2M-1)+1$ phase variables so that a corresponding number of boson fields can be reduced to purely real amplitudes with no phase fluctuations. The boson fields that remain fully complex, on the other hand, continue to display some phase dynamics, which is responsible for the incoherent features of the spectrum[21] (e.g., lower and upper Hubbard bands).

It is beyond our purpose to enter into the formal details of the radial gauge representation, thoroughly derived in Ref. 17. Nevertheless, it is worthwhile to observe, here, that such gauge fixing procedure allows to avoid Elitzur's theorem,[22] which would prevent the slave bosons to acquire a nonzero

expectation value, making therefore legitimate the use of the saddle-point approximation.

E. Saddle-point approximation

The saddle-point approximation of the functional integral Eq. (28) is obtained by considering the slave bosons and Lagrange multipliers as static variables, corresponding to the time averages of these fields. Moreover, we will assume a homogeneous spatial structure of the saddle-point solution so that we can finally set: $\phi_{An,i}(\tau) \mapsto \varphi_{An}$, $\mathcal{A}_i^a(\tau) \mapsto \mathcal{A}^a$, and $\mathcal{A}_i^0(\tau) \mapsto \mathcal{A}^0$.

In such approximation, all the bosonic amplitudes φ_{An} are assumed to have a constant phase, in contrast to the radial gauge representation, where we are allowed to remove (fix) a limited number of complex phases (namely, $M(2M-1)+1$). The phase fluctuations of those fields that remain intrinsically complex are thus ruled out, precluding the possibility of describing the high-energy physics of a given model. The low-energy features, on the other hand, will be suitably described in terms of coherent Landau-Bogoliubov quasiparticles, providing a Fermi-liquid description of metallic and superconducting states.

At the saddle point, the free-energy per site $\Omega = -(1/\beta N)\ln \mathcal{Z}$ is obtained as the (minimum) stationary value of the following free-energy functional:

$$\Omega[\{\varphi\},\{\mathcal{A}\}] = -\frac{1}{\beta N}\ln \mathcal{Z}_f - \mathcal{A}^0 + \sum_{ABnm} \varphi_{An}^*[\langle A|H_{\mathrm{loc}}|B\rangle \delta_{nm}$$
$$+ (\mathcal{A}^0 \delta_{nm} + \mathcal{A}^a \mathcal{J}_{nm}^a)\delta_{AB}]\varphi_{Bm}, \quad (53)$$

where N is the total number of sites and $\mathcal{Z}_f$ represents the Gaussian integral over the auxiliary fermions

$$\mathcal{Z}_f = \int \mathcal{D}\Psi \exp\left[-\frac{1}{2}\int_0^\beta d\tau \sum_{ij} \Psi_i^\dagger(\delta_{ij}D_\tau + \mathbf{R}^\dagger \tilde{\mathbf{t}}_{ij}\mathbf{R})\Psi_j\right]$$
$$= \int \mathcal{D}\Psi \exp\left\{-\frac{1}{2}\int_0^\beta d\tau \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger[\partial_\tau + \mathbf{h}(\mathbf{k})]\Psi_{\mathbf{k}}\right\}. \quad (54)$$

In the last expression, $\mathbf{h}(\mathbf{k})$ denotes the momentum-space quasiparticle energy matrix

$$\mathbf{h}(\mathbf{k}) = \mathbf{R}^\dagger[\varphi]\begin{pmatrix} \boldsymbol{\epsilon}(\mathbf{k}) & 0 \\ 0 & -\boldsymbol{\epsilon}(-\mathbf{k})^* \end{pmatrix}\mathbf{R}[\varphi] + \mathcal{A}^a \mathbf{T}^a. \quad (55)$$

To evaluate the functional integral in Eq. (54), we note that, up to irrelevant constants, $\mathcal{Z}_f^2 = \det[\partial_\tau + \mathbf{h}(\mathbf{k})]$, so that we can write

$$\ln \mathcal{Z}_f = \frac{1}{2}\ln \det[\partial_\tau + \mathbf{h}(\mathbf{k})] = \frac{1}{2}\sum_{\mathbf{k}} \mathrm{tr} \ln[1 + e^{-\beta \mathbf{h}(\mathbf{k})}].$$
$$(56)$$

The saddle-point equations are then obtained by setting to zero all the partial derivatives of the free-energy functional Eq. (53) with respect to the slave-boson amplitudes and Lagrange multipliers. For practical calculations, however, it is useful to consider a different basis set for the $M(2M-1)$ Lagrange multipliers $\mathcal{A}^a$, belonging the adjoint representa-

tion of SO($2M$). In place of them, in fact, we can equivalently use the set of independent matrix elements of $\mathcal{A}^a\mathbf{T}^a$, parameterized as follows:

$$\mathcal{A}^a\mathbf{T}^a = \begin{pmatrix} \boldsymbol{\Lambda} & \boldsymbol{\Pi} \\ -\boldsymbol{\Pi}^* & -\boldsymbol{\Lambda}^* \end{pmatrix},$$

$$\Lambda_{\alpha\beta} = \Lambda_{\beta\alpha}^*,$$

$$\Pi_{\alpha\beta} = -\Pi_{\beta\alpha}. \quad (57)$$

With this choice, the saddle-point equations can be derived without knowing the explicit expressions of the $\mathbf{T}^a$ matrices, differentiating the free-energy functional directly with respect to $\Lambda_{\alpha\beta}$ and $\Pi_{\alpha\beta}$. To this end, we note that $\Omega[\{\varphi\},\{\mathcal{A}\}]$ can be easily expressed in terms of the new set of Lagrange multipliers by means of the following relation:

$$\mathcal{A}^a\mathcal{J}_{nn'}^a = -\frac{1}{2}\langle n'|\Psi^\dagger(\mathcal{A}^a\mathbf{T}^a)\Psi|n\rangle$$

$$= -\frac{1}{2}[\Lambda_{\alpha\beta}\langle n'|(f_\alpha^\dagger f_\beta - f_\beta f_\alpha^\dagger)|n\rangle$$
$$+ \Pi_{\alpha\beta}\langle n'|f_\alpha^\dagger f_\beta^\dagger|n\rangle + \Pi_{\alpha\beta}^*\langle n'|f_\beta f_\alpha|n\rangle]. \quad (58)$$

F. Green's functions and observables

After solving the saddle-point equations, we can finally obtain the expressions for the quasiparticle and physical electron propagators, conveniently written here in Nambu notation. For quasiparticles, the propagator is defined as

$$\mathbf{D}_f(\mathbf{k},\tau) = -\langle T\Psi_{\mathbf{k}}(\tau)\Psi_{\mathbf{k}}^\dagger(0)\rangle = \begin{bmatrix} \mathbf{G}_f(\mathbf{k},\tau) & \mathbf{F}_f^\dagger(\mathbf{k},-\tau) \\ \mathbf{F}_f(\mathbf{k},\tau) & -\mathbf{G}_f^T(-\mathbf{k},-\tau) \end{bmatrix},$$
$$(59)$$

where $G_f(\mathbf{k},\tau)_{\alpha\beta} = -\langle Tf_{\mathbf{k}\alpha}(\tau)f_{\mathbf{k}\beta}^\dagger(0)\rangle$ and $F_f(\mathbf{k},\tau)_{\alpha\beta} = -\langle Tf_{-\mathbf{k}\alpha}^\dagger(\tau)f_{\mathbf{k}\beta}^\dagger(0)\rangle$ are the normal and anomalous quasiparticle Green's functions. Following Eq. (54), we can then readily write the quasiparticle inverse propagator as

$$\mathbf{D}_f^{-1}(\mathbf{k},\omega) = \omega - \mathbf{h}(\mathbf{k}). \quad (60)$$

The physical electron propagator, on the other hand, is defined by

$$\mathbf{D}_d(\mathbf{k},\tau) = -\langle T\Xi_{\mathbf{k}}(\tau)\Xi_{\mathbf{k}}^\dagger(0)\rangle, \quad (61)$$

where $\Xi_{\mathbf{k}}^\dagger \equiv (\{d_{\mathbf{k}\alpha}^\dagger\},\{d_{-\mathbf{k}\alpha}\})$ is the Nambu spinor containing the physical degrees of freedom, represented in terms of slave-boson amplitudes and quasiparticles by $\Xi_{\mathbf{k}} = \mathbf{R}[\varphi]\Psi_{\mathbf{k}}$. The expression for the inverse physical propagator is thus written as

$$\mathbf{D}_d^{-1}(\mathbf{k},\omega) = [\mathbf{R}^\dagger]^{-1}[\omega - \mathbf{h}(\mathbf{k})]\mathbf{R}^{-1}. \quad (62)$$

Using the corresponding expression for the "bare" physical propagator

$$\mathbf{D}_{d0}^{-1}(\mathbf{k},\omega) = \omega - [\tilde{\boldsymbol{\epsilon}}_0 + \tilde{\boldsymbol{\epsilon}}(\mathbf{k})], \quad (63)$$

$$\tilde{\boldsymbol{\epsilon}}_0 + \tilde{\boldsymbol{\epsilon}}(\mathbf{k}) = \begin{pmatrix} \boldsymbol{\epsilon}_0 + \boldsymbol{\epsilon}(\mathbf{k}) & 0 \\ 0 & -[\boldsymbol{\epsilon}_0 + \boldsymbol{\epsilon}(-\mathbf{k})]^* \end{pmatrix} \quad (64)$$

($\boldsymbol{\epsilon}_0$ represents the one-body part of H_{loc}), we can then find the saddle-point approximation for the self-energy

$$\boldsymbol{\Sigma}_d(\omega) = \mathbf{D}_{d0}^{-1} - \mathbf{D}_d^{-1} = \omega(1 - [\mathbf{R}\mathbf{R}^\dagger]^{-1}) - \tilde{\boldsymbol{\epsilon}}_0$$
$$+ [\mathbf{R}^\dagger]^{-1} \begin{pmatrix} \boldsymbol{\Lambda} & \boldsymbol{\Pi} \\ -\boldsymbol{\Pi}^* & -\boldsymbol{\Lambda}^* \end{pmatrix} \mathbf{R}^{-1}. \quad (65)$$

The cancellation of the k dependence, in the above equation, follows from the definition of the QP energy matrix, Eq. (55). Indeed, this form of the self-energy is just the one we would expect from the saddle-point (mean-field) approximation, which freezes spatial and dynamical fluctuations. From the linear term in ω, one readily obtains the matrix of quasiparticle spectral weights

$$\mathbf{Z} = \left[1 - \frac{\partial \boldsymbol{\Sigma}_d}{\partial \omega}\right]_{\omega=0}^{-1} = \mathbf{R}\mathbf{R}^\dagger. \quad (66)$$

We conclude this formal section by writing the representation, in the enlarged Hilbert space, of the local physical density operator, whose expectation value defines the average number of electrons per site

$$\hat{\underline{n}}^{(d)} = \sum_\alpha \underline{d}_\alpha^\dagger \underline{d}_\alpha = \sum_A N_A \sum_n \phi_{An}^\dagger \phi_{An}. \quad (67)$$

As mentioned previously, we remark that this expression differs substantially from that for the local quasiparticle density

$$\sum_\alpha f_\alpha^\dagger f_\alpha = \sum_{An} \sum_\alpha n_\alpha \phi_{An}^\dagger \phi_{An}, \quad (68)$$

which is not a physical quantity and depends from the choice of the QP basis set. More generally, the representation of any (local) two-particle physical operator may be easily obtained in terms of boson operators only: for particle-hole operators we find

$$\underline{d}_\alpha^\dagger \underline{d}_\beta = \sum_{AB} \langle A | d_\alpha^\dagger d_\beta | B \rangle \sum_n \phi_{An}^\dagger \phi_{Bn} \quad (69)$$

while for particle-particle operators we have

$$\underline{d}_\alpha^\dagger \underline{d}_\beta^\dagger = \sum_{AB} \langle A | d_\alpha^\dagger d_\beta^\dagger | B \rangle \sum_n \phi_{An}^\dagger \phi_{Bn}. \quad (70)$$

III. APPLICATION TO THE THREE-ORBITAL MODEL FOR FULLERIDES

A. The model

In this section we present an explicit application of the rotationally invariant slave-boson approach. To this aim we have chosen a three-orbital Hubbard-type model that has been used to understand the role of strong correlations in alkali-doped fullerides. The physics of alkali-doped fullerene systems A_nC_{60} represents an optimal playground in understanding the key role of strong correlations on high-temperature superconductors: indeed, these systems display a

relatively high T_c compared to ordinary Bardeen-Cooper-Schrieffer (BCS) superconductors, and, similarly to what is found in cuprate systems, the enhancement of T_c seems to be closely related to the proximity of a Mott-insulating phase.[13,14,23] Although the nature of the pairing mechanism is most likely different from that characterizing cuprate superconductors, in fullerene systems being due to ordinary electron-phonon (vibron) interaction,[24] and in spite of the different symmetry of the order parameter (s wave in fullerides), the phase diagram as a function of the intermolecular separation in these systems presents strong similarities to that of cuprates as a function of doping,[23] providing an independent example of the key role of electronic correlations in enhancing superconductivity.

The local Hamiltonian describing the C_{60}^{n-} molecular ion, assuming rotational invariance within the threefold degenerate level t_{1u} hosting the valence electrons provided by the alkali metals, can be written, for a generic site i, as

$$H_{\mathrm{loc}}[i] = \frac{U}{2}\hat{n}_i^2 - J_{\mathrm{H}}\left[2\mathbf{S}_i \cdot \mathbf{S}_i + \frac{1}{2}\mathbf{L}_i \cdot \mathbf{L}_i + \frac{5}{6}(\hat{n}_i - 3)^2\right] + H_{\mathrm{JT}}, \quad (71)$$

where the three terms represent, respectively, the global onsite Coulomb repulsion, Hund's rules splitting ($J_{\mathrm{H}} > 0$) and the Jahn-Teller coupling between electrons and the vibrational modes (vibrons) of C_{60}. In the above expression, $\hat{n}_i = \sum_{a\sigma} d_{i,a\sigma}^\dagger d_{i,a\sigma}$ is the local electron-number operator ($a = 1,2,3$ labels the t_{1u} orbitals and $\sigma = \uparrow, \downarrow$ the spin components) while $\mathbf{S}_i$ and $\mathbf{L}_i$ are, respectively, the local spin and orbital angular-momentum operators

$$\mathbf{S}_i = \frac{1}{2} \sum_{a,\sigma\sigma'} d_{i,a\sigma}^\dagger \hat{\boldsymbol{\sigma}}_{\sigma\sigma'} d_{i,a\sigma'}, \quad (72)$$

$$\mathbf{L}_i = \sum_{ab,\sigma} d_{i,a\sigma}^\dagger \hat{\boldsymbol{\ell}}_{ab} d_{i,b\sigma}, \quad (73)$$

where $\hat{\boldsymbol{\sigma}}_{\sigma\sigma'}$ are the Pauli matrices and $\hat{\ell}_{bc}^{(a)} = i\varepsilon_{bac}$ the $O(3)$ group generators characterizing orbital rotations.

The Jahn-Teller Hamiltonian involves both electron and vibron field operators but if we are interested only in the electron dynamics we can formally integrate out the vibronic degrees of freedom obtaining an effective action for the electron operators only. If performed exactly, this procedure would clearly generate noninstantaneous (i.e., timedependent) interaction terms, preventing a purely electronic Hamiltonian formulation of the effective action; however, if we assume the vibronic frequencies to be much higher than the relevant electronic scales, we can take the antiadiabatic limit of the electron effective action, neglecting retardation effects and considering an instantaneous interaction term which preserves the symmetries of the original local Hamiltonian. While this approximation may be questionable for fullerides, it will not affect our claims since the neglect of retardation can only disfavor superconductivity, and analogous results have been obtained in a similar model that takes into account the phonon dynamics.[25] The Jahn-Teller interaction can then be reabsorbed in Hund's term and the result-

ing Hamiltonian is simply given by the first two terms of Eq. (71) with a renormalized Hund's coupling $J_H \mapsto -J = J_H - \frac{3}{4}E_{JT} < 0$, E_{JT} being the characteristic Jahn-Teller energy gain.[26] The net effect of the electron-vibron coupling is therefore that of reversing Hund's rules, favoring atomic configurations with low spin and orbital angular momentum. The inversion of the Hund's rule is experimentally confirmed by the low-spin state of both tetravalent[27] and trivalent[28] fullerides and by the presence of a spin gap.[29]

Given the local Hamiltonian for the C_{60}^{n-} molecular ion, the expression for a tight-binding electronic Hamiltonian describing A_nC_{60} solids will then read

$$H_{latt} = \sum_{ij,ab,\sigma} t_{ij}^{ab} d_{i,a\sigma}^\dagger d_{j,b\sigma} + \sum_i H_{loc}[i] - \mu \sum_i \hat{n}_i, \quad (74)$$

where t_{ij}^{ab} are the intersite hopping amplitudes (including possible interband hybridization terms) and μ is the chemical potential controlling the average electron density. We should note, however, that interband hybridization can actually be avoided whenever the hopping terms are restricted to nearest neighbors only, $t_{ij}^{ab} = t^{ab}\delta_{\langle ij \rangle}$; in such case, indeed, we can exploit the $O(3)$ orbital symmetry of H_{loc} in order to diagonalize t^{ab}, so that we can set, without loss of generality, $t_{ij}^{ab} = t^a \delta_{ab}\delta_{\langle ij \rangle}$. Throughout our analysis we will use the latter expression for the hopping-matrix elements, focusing in particular on the orbitally degenerate case $t^a = -t$ (we will consider the possibility of a crystal-field splitting of the three bands and of different bandwidths in a future study).

B. Slave-boson representation of the model

As pointed out in previous studies,[13,14,27,30] the zero-temperature phase diagram of the model Eq. (74) as a function of the ratios J/W and U/W (W being the noninteracting bandwidth) displays several interesting features, the most striking one being undoubtedly the presence of a strongly enhanced superconducting phase in the proximity of the metal-to-insulator Mott transition. The model represents therefore a valuable test for the rotationally invariant slave-boson method, at the same time providing an analytical tool to treat strongly correlated superconductors.

1. Slave-boson amplitudes

From the rotationally invariant slave-boson representation of physical states defined by Eq. (11), it should be clear that there are, in principle, 2^{2M-1} (with $M=6$ in our model) slave-boson fields ϕ_{An} describing the system. However, we must note that when the partition function is approximated at saddle-point level, i.e., when the slave-boson fields are replaced by their mean-field expectation values ($\phi_{An} \to \langle \phi_{An} \rangle \equiv \varphi_{An}$), the number of independent slave-boson amplitudes entering the saddle-point equations becomes much smaller, as we will show in the following, its specific value depending on which symmetries of the model Hamiltonian remain unbroken.

As discussed at end of Sec. III A, we choose the hopping matrix to be diagonal and degenerate in both spin and orbital indices so that the atomic $SU(2) \otimes O(3)$ symmetry characterizing H_{loc} can be promoted to a global symmetry for the full

lattice Hamiltonian H_{latt}. If we impose this symmetry to be preserved at saddle-point level, i.e., we do not allow for any spin and orbital ordering, we must then set to zero all the possible order parameters which are not invariant under $SU(2) \otimes O(3)$, and this will strongly limit the possibility of independent slave-boson amplitudes. Indeed, considering the normal-state solution of the saddle-point equations, i.e., do not allowing for a superconducting order parameter, it is quite straightforward to prove, using Wigner-Eckart's theorem, that the nonzero slave-boson amplitudes must be of the form

$$\varphi_{\Gamma n} = \langle n | \Gamma \rangle \Phi(E_\Gamma), \quad (75)$$

where we have taken as the basis set for the local physical states the eigenstates $\{|\Gamma\rangle\}$ of H_{loc} with eigenvalues E_Γ. Note that in this case the quasiparticle Fock states $|n\rangle$ have exactly the same number of particles of the physical state $|\Gamma\rangle$ to which they are linked, assuring the solution to represent a normal state; indeed, as long as the latter condition is satisfied, no superconducting order parameter can be ever developed, as can be easily seen taking the expectation values of Eq. (70)

$$\langle d_\alpha^\dagger d_\beta^\dagger \rangle = \sum_{\Gamma\Gamma'} \langle \Gamma | d_\alpha^\dagger d_\beta^\dagger | \Gamma' \rangle \sum_n \varphi_{\Gamma n}^* \varphi_{\Gamma' n}. \quad (76)$$

On the other hand, if we do allow for a superconducting symmetry breaking, we must add to the normal amplitudes defined in Eq. (75) also those amplitudes connecting physical states to QP states with a different number of particles so that particle number would no longer be conserved; however, if we still want to preserve the $SU(2) \otimes O(3)$ symmetry as in the normal case, we should consider only those amplitudes which correspond to an invariant, with respect to spin and orbital rotations, superconducting order parameter. Assuming pairing to be purely local, corresponding to an s-wave order parameter, the only invariant pairing amplitude is then given by the spin and orbital singlet channel

$$\psi_{sc}^0 \equiv \left\langle \sum_a d_{i,a\uparrow}^\dagger d_{i,a\downarrow}^\dagger \right\rangle. \quad (77)$$

At this point, it is worthwhile to observe that Eq. (77) represents the most favorable pairing channel even if we do not explicitly impose the $SU(2) \otimes O(3)$ symmetry since the local pairing attraction is driven by the reversed Hund's term, which favors the formation of two-particle states locked in the $L = S = 0$ spin-orbital configuration. Our assumption of preserving the $SU(2) \otimes O(3)$ symmetry is then fully justified whenever the system turns out to be superconducting since any rotational symmetry-breaking pairing would be ruled out by the singlet channel; on the other hand, in our study we will only compare the superconducting solution with a rotationally invariant normal state and therefore we cannot exclude the possibility that some other ordered phase would win the competition for the lowest-energy phase.

We can now turn to the problem of establishing the independent slave-boson amplitudes required by our model in order to describe a superconducting solution characterized by the $L = S = 0$ order parameter defined in Eq. (77). Using the Wigner-Eckart theorem as for the normal-state solution, in

this case we find the following expression for the nonzero amplitudes:

$$\varphi_{\Gamma n} = \langle n|\Gamma\rangle\Phi(E_\Gamma) + \sum_{q=1}^{3}\left[\frac{\langle n|\hat{\psi}^q|\Gamma\rangle}{\sqrt{\langle\Gamma|(\hat{\psi}^\dagger)^q\hat{\psi}^q|\Gamma\rangle}}\Psi(E_\Gamma,2q)\right.$$

$$\left. + \frac{\langle n|(\hat{\psi}^\dagger)^q|\Gamma\rangle}{\sqrt{\langle\Gamma|\hat{\psi}^q(\hat{\psi}^\dagger)^q|\Gamma\rangle}}\Psi(E_\Gamma,-2q)\right], \quad (78)$$

$$\hat{\psi} = \sum_a d_{a\uparrow}^\dagger d_{a\downarrow}^\dagger.$$

We have denoted with $\Phi(E_\Gamma)$ the "normal" slave-boson amplitudes, which relate physical and quasiparticle states characterized by the same number of particles and with $\Psi(E_\Gamma,\Delta N)$ the "anomalous" ones, in which the number of particles characterizing the QP state $|n\rangle$ differs by ΔN from that of the physical state $|\Gamma\rangle$. We remark, however, that the presence of nonvanishing anomalous amplitudes is not sufficient, by itself, to assure a superconducting solution, the latter requiring the superconducting order parameter ψ_{sc}^0, which is a specific quadratic form in the slave-boson amplitudes, to be finite. The normalization factors for the anomalous amplitudes, in Eq. (78), are chosen in order to simplify the expression for the probability associated with the physical configuration $|\Gamma\rangle$

$$P(\Gamma) = \sum_n |\varphi_{\Gamma n}|^2 = |\Phi(E_\Gamma)|^2 + \sum_{\Delta N}|\Psi(E_\Gamma,\Delta N)|^2. \quad (79)$$

Using Eq. (78), which relates all the slave-boson amplitudes $\varphi_{\Gamma n}$ to the independent variables $\Phi(E_\Gamma)$ and $\Psi(E_\Gamma,\Delta N)$, we are almost ready to write the free-energy functional Eq. (53) in terms of only Φ's and Ψ's, obtaining therefore a much smaller number of saddle-point equations to be solved. The last step needed to achieve this goal, in fact, is to evaluate the matrix elements $\langle n|\hat{\mathcal{O}}_d|\Gamma\rangle$ between the eigenstates of H_{loc} and the Fock states $|n\rangle_d$ expressed in terms of the physical electron operators $d_{a\sigma}^\dagger$.

As discussed in Sec. III A, the effective local Hamiltonian for the electron dynamics of the C_{60}^{n-} ion is given, in the antiadiabatic limit, by

$$H_{\text{loc}} = \frac{U}{2}(\hat{n}-3)^2 - \mu\hat{n} + J\left[2\mathbf{S}\cdot\mathbf{S} + \frac{1}{2}\mathbf{L}\cdot\mathbf{L} + \frac{5}{6}(\hat{n}-3)^2\right], \quad (80)$$

where we have included also the chemical-potential term, as required by the general formalism described in Sec. II, and we have dropped, for simplicity, the redundant lattice site index. In comparison to Eq. (71), the Coulomb interaction is here written in a particle-hole symmetric form by properly redefining the chemical potential.

We can then readily identify the eigenstates of H_{loc} among the atomic multiplets $|\Gamma\rangle$ which are simultaneous eigenstates of the density operator $\hat{n}$ and of the orbital and spin angular-momentum operators $\mathbf{L}^2$ and $\mathbf{S}^2$, with eigenvalues

$$E_\Gamma = E(n,\ell,s) = \frac{U}{2}(n-3)^2$$

$$- \mu n + J\left[2s(s+1) + \frac{1}{2}\ell(\ell+1) + \frac{5}{6}(n-3)^2\right]. \quad (81)$$

The degeneracy associated to each eigenvalue is given by

$$g_{[n,\ell,s]} = (2\ell+1)(2s+1) \quad (82)$$

and it is therefore natural to choose as a basis set for the corresponding degenerate subspace the simultaneous eigenstates of both one of the components of $\mathbf{L}$ and $\mathbf{S}$, say L_z (Ref. 31) and S_z, so that we can finally set

$$|\Gamma\rangle \equiv |n,(\ell,\ell_z),(s,s_z)\rangle. \quad (83)$$

These states must then be expressed in terms of the Fock states $|n\rangle_d$, in order to evaluate the matrix elements which characterize Eq. (78). We note, however, that

$$|n\rangle_d \equiv \prod_{a=1}^{3}\prod_{\sigma=\uparrow,\downarrow}(d_{a\sigma}^\dagger)^{n_{a\sigma}}|\text{vac}\rangle \quad [n_{a\sigma}=0,1] \quad (84)$$

are not eigenstates of any of the orbital angular-momentum operators L_a, making the representation of the atomic multiplets Eq. (83) in terms of such states a bit involved: it is more convenient, instead, using the rotational invariance of H_{loc}, to choose an orbital basis for the physical electron operators in which L_z is diagonal

$$c_{m\sigma}^\dagger = \sum_a U_{ma}d_{a\sigma}^\dagger, \quad (85)$$

$$L_z = \sum_{m,\sigma} m c_{m\sigma}^\dagger c_{m\sigma}, \quad [m=1,0,-1] \quad (86)$$

so that the corresponding Fock states

$$|n\rangle_c \equiv \prod_{m,\sigma}(c_{m\sigma}^\dagger)^{n_{m\sigma}}|\text{vac}\rangle = \mathcal{U}(U)_{nn'}|n'\rangle_d \quad (87)$$

are eigenstates of both L_z and S_z. Since we are assuming the three bands to be degenerate, the rotation of the orbital basis Eq. (85) does not change the form of the kinetic term in H_{latt} while the expression for the singlet pair-creation operator $\hat{\psi} \equiv \sum_a d_{a\uparrow}^\dagger d_{a\downarrow}^\dagger$ reads, in the new basis

$$\hat{\psi} = c_{1\uparrow}^\dagger c_{-1\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{-1\uparrow}^\dagger - c_{0\uparrow}^\dagger c_{0\downarrow}^\dagger. \quad (88)$$

The representation of the atomic eigenstates $|\Gamma\rangle$ in terms of the Fock states $|n\rangle_c$ is listed in Table I, where they are classified according to the quantum numbers (n,ℓ,s) which determine, through Eq. (81), the corresponding eigenvalues; note, however, that for a given value of the particle number n, the Pauli-principle prevents the orbital and spin angular momenta ℓ and s to take independent values, so that each degenerate multiplet can actually be identified specifying only two quantum numbers, n and ℓ. For each multiplet, we have written out explicitly only the component characterized

TABLE I. Electronic eigenstates of the C_{60}^{n-} molecular ion and the corresponding slave-boson amplitudes: the latter are selected in order to preserve, at the saddle-point level, the rotational invariance of the local Hamiltonian.

$\lvert\Gamma\rangle$	$n\ (\ell,\ell_z)\ (s,s_z)$	$\varphi_{\Gamma n}$
$\lvert 0,0,0\rangle$	$0\ (0,0)\ (0,0)$	$\Phi(0,0)$ $\Psi(0,0;2)$ $\Psi(0,0;4)$ $\Psi(0,0;6)$
$\lvert\uparrow,0,0\rangle$	$1\ (1,1)\ (\tfrac{1}{2},\tfrac{1}{2})$	$\Phi(1,1)$ $\Psi(1,1;2)$ $\Psi(1,1;4)$
$\lvert\uparrow\downarrow,0,0\rangle$	$2\ (2,2)\ (0,0)$	$\Phi(2,2)$ $\Psi(2,2;2)$
$\lvert\uparrow,\uparrow,0\rangle$	$2\ (1,1)\ (1,1)$	$\Phi(2,1)$ $\Psi(2,1;2)$
$\frac{1}{\sqrt{3}}[\lvert\uparrow,0,\downarrow\rangle-\lvert\downarrow,0,\uparrow\rangle-\lvert0,\uparrow\downarrow,0\rangle]$	$2\ (0,0)\ (0,0)$	$\Phi(2,0)$ $\Psi(2,0;-2)$ $\Psi(2,0;2)$ $\Psi(2,0;4)$
$\lvert\uparrow\downarrow,\uparrow,0\rangle$	$3\ (2,2)\ (\tfrac{1}{2},\tfrac{1}{2})$	$\Phi(3,2)$
$\frac{1}{\sqrt{2}}[\lvert\uparrow,\uparrow\downarrow,0\rangle+\lvert\uparrow\downarrow,0,\uparrow\rangle]$	$3\ (1,1)\ (\tfrac{1}{2},\tfrac{1}{2})$	$\Phi(3,1)$ $\Psi(3,1;-2)$ $\Psi(3,1;2)$
$\lvert\uparrow,\uparrow,\uparrow\rangle$	$3\ (0,0)\ (\tfrac{3}{2},\tfrac{3}{2})$	$\Phi(3,0)$
$\lvert\uparrow\downarrow,\uparrow\downarrow,0\rangle$	$4\ (2,2)\ (0,0)$	$\Phi(4,2)$ $\Psi(4,2;-2)$
$\lvert\uparrow\downarrow,\uparrow,\uparrow\rangle$	$4\ (1,1)\ (1,1)$	$\Phi(4,1)$ $\Psi(4,1;-2)$
$\frac{1}{\sqrt{3}}[\lvert\downarrow,\uparrow\downarrow,\uparrow\rangle-\lvert\uparrow,\uparrow\downarrow,\downarrow\rangle-\lvert\uparrow\downarrow,0,\uparrow\downarrow\rangle]$	$4\ (0,0)\ (0,0)$	$\Phi(4,0)$ $\Psi(4,0;-4)$ $\Psi(4,0;-2)$ $\Psi(4,0;2)$
$\lvert\uparrow\downarrow,\uparrow\downarrow,\uparrow\rangle$	$5\ (1,1)\ (\tfrac{1}{2},\tfrac{1}{2})$	$\Phi(5,1)$ $\Psi(5,1;-4)$ $\Psi(5,1;-2)$
$\lvert\uparrow\downarrow,\uparrow\downarrow,\uparrow\downarrow\rangle$	$6\ (0,0)\ (0,0)$	$\Phi(6,0)$ $\Psi(6,0;-6)$ $\Psi(6,0;-4)$ $\Psi(6,0;-2)$

by the maximum value of ℓ_z and s_z, all the other components being easily obtainable from the former by repeatedly acting on it with the lowering operators

$$L_- = \sqrt{2}\sum_\sigma (c_{0\sigma}^\dagger c_{1\sigma} + c_{-1\sigma}^\dagger c_{0\sigma}), \tag{89}$$

$$S_- = \sum_m c_{m\downarrow}^\dagger c_{m\uparrow}. \tag{90}$$

The last column of the Table contains the independent slave-boson amplitudes $\Phi(n,\ell)$ and $\Psi(n,\ell;\Delta N)$ associated, according to Eq. (78), to all the components of a given degenerate multiplet: the total number of amplitudes required by our model is therefore 35, if we consider the full rotationally invariant solution, while it reduces to 13 if we force the system into the normal state, setting $\Psi(n,\ell;\Delta N)\equiv 0$.

2. Lagrange multipliers

The Lagrange multipliers $\mathcal{A}^0$, $\Lambda_{\alpha\beta}$, and $\Pi_{\alpha\beta}$, introduced in Secs. II D and II E to enforce the constraints Eqs. (12)–(14), form, together with the slave-boson amplitudes, the set of variables on which the free-energy functional Eq. (53) is defined. However, similarly to what we established in the case of the slave-boson amplitudes, we must note that the symmetries of our problem greatly reduce the number of independent Lagrange multipliers required for the solution of the model and in the following we will identify the form of such variables.

Denoting with $\alpha\equiv(m,\sigma)$ both the orbital and spin indices, the constraints Eqs. (12)–(14) read, at the saddle-point level

$$\sum_\Gamma P(\Gamma) = 1, \tag{91}$$

$$\mathcal{Q}_{\alpha\beta}^N = \langle f_\alpha^\dagger f_\beta\rangle = \sum_{\mathbf{k}} G_f(\mathbf{k},0^-)_{\beta\alpha}, \tag{92}$$

$$\mathcal{Q}_{\alpha\beta}^A = \langle f_\alpha^\dagger f_\beta^\dagger\rangle = \sum_{\mathbf{k}} F_f(\mathbf{k},0^-)_{\beta\alpha}, \tag{93}$$

where $P(\Gamma)$ is the probability distribution defined in Eq. (79), $\mathbf{G}_f(\mathbf{k},\tau)$ and $\mathbf{F}_f(\mathbf{k},\tau)$ are the normal and anomalous quasiparticle Green's functions, and

$$\mathcal{Q}_{\alpha\beta}^N \equiv \sum_{\Gamma nn'} \varphi_{\Gamma n}^* \varphi_{\Gamma n'}\langle n'\lvert f_\alpha^\dagger f_\beta\rvert n\rangle, \tag{94}$$

$$\mathcal{Q}_{\alpha\beta}^A \equiv \sum_{\Gamma nn'} \varphi_{\Gamma n}^* \varphi_{\Gamma n'}\langle n'\lvert f_\alpha^\dagger f_\beta^\dagger\rvert n\rangle \tag{95}$$

are defined as the normal and anomalous quasiparticle density matrices. As for $P(\Gamma)$, we can then make use of Eq. (78) in order to rewrite the left-hand side of Eqs. (92) and (93) directly in terms of the independent slave-boson amplitudes, obtaining the following expressions:

$$\mathcal{Q}_{\alpha\beta}^N = \mathcal{Q}^N[\Phi,\Psi]\delta_{\alpha\beta}, \tag{96}$$

$$\mathcal{Q}_{\alpha\beta}^A = \mathcal{Q}^A[\Phi,\Psi]\delta_{\alpha,\bar{\beta}}(-1)^{\eta_\alpha},$$

$$\eta_\alpha = m + \sigma + \frac{1}{2}, \quad \left[\sigma = \pm\frac{1}{2}\right] \tag{97}$$

where the spin and orbital indices of $\bar{\alpha}$ are opposite to those of α. The specific choice we have made for the independent

slave-boson amplitudes thus reflects in a very simplified form of the quasiparticle density matrices and it is not hard to recognize in this structure the symmetry properties which characterize our model, i.e., the band degeneracy and the $SU(2) \otimes O(3)$ rotational invariance. The quasiparticle energy matrix $\mathbf{h}(\mathbf{k})$ (Ref. 32) must then be rotationally invariant as well, in order to yield quasiparticle expectation values with the same structure of the QP density matrices

$$\langle f_\alpha^\dagger f_\beta \rangle \propto \delta_{\alpha\beta}, \quad \langle f_\alpha^\dagger f_\beta^\dagger \rangle \propto \delta_{\alpha,\bar{\beta}}(-1)^{\eta_\alpha}.$$

The kinetic part of $\mathbf{h}(\mathbf{k})$, namely, $\mathbf{R}^\dagger \widetilde{\boldsymbol{\epsilon}}(\mathbf{k})\mathbf{R}$, is guaranteed to be $SU(2) \otimes O(3)$ invariant, since it depends only on the degenerate band dispersion $\epsilon_{\alpha\beta}(\mathbf{k}) = \epsilon(\mathbf{k})\delta_{\alpha\beta}$ and on the slave-boson amplitudes $\varphi_{\Gamma n}[\Phi, \Psi]$ (through the R matrices) which have been properly selected in order to yield rotationally invariant solutions. On the other hand, the Lagrange multipliers matrices $\boldsymbol{\Lambda}$ and $\boldsymbol{\Pi}$ are, in principle, two generic Hermitian and antisymmetric matrices, respectively, and we must therefore set

$$\Lambda_{\alpha\beta} = \Lambda \delta_{\alpha\beta}, \quad \Pi_{\alpha\beta} = \Pi \delta_{\alpha,\bar{\beta}}(-1)^{\eta_\alpha}, \quad (98)$$

in order to guarantee the rotational invariance of the quasiparticle Hamiltonian.

In the end, we are left with just three Lagrange multipliers, $\mathcal{A}^0$, Λ, and Π, to which we can eventually add the chemical potential μ if we decide to solve the model keeping the physical electron density fixed: in the latter case, in fact, the chemical potential plays the role of a Lagrange multiplier for the number equation

$$n_{\text{phys}} \equiv \sum_{m,\sigma} \langle c_{m\sigma}^\dagger c_{m\sigma} \rangle = \sum_\Gamma n(\Gamma)P(\Gamma) \quad (99)$$

rather than being an external parameter as in the grand-canonical ensemble.

3. Spectral weight and low-energy excitations

As shown in Sec. II F, the expression for the quasiparticle spectral weight matrix $\mathbf{Z}$, defined as

$$\mathbf{Z} = \left[\mathbf{1} - \frac{\partial \boldsymbol{\Sigma}}{\partial \omega} \right]_{\omega=0}^{-1} \quad (100)$$

is given, in terms of the slave-boson amplitudes, by

$$\mathbf{Z} = \mathbf{R}\mathbf{R}^\dagger, \quad (101)$$

$\mathbf{R}[\{\varphi\}]$ being the matrix which relates the physical electron operators to the quasiparticle ones [see Eqs. (18) and (30) for its definition]. In our model, this relation reads

$$c_{m\sigma}^\dagger = r_p[\Phi, \Psi]^* f_{m\sigma}^\dagger + (-1)^{m+\sigma+1/2} r_h[\Phi, \Psi] f_{-m\bar{\sigma}} \quad (102)$$

and it can be easily recognized, as in the case of the quasiparticle density matrices, the specific structure of the normal (r_p) and anomalous (r_h) terms, dictated by the symmetries of the problem. Inserting this relation in the definition of the quasiparticle weight matrix, we finally obtain

$$\mathbf{Z} = (|r_p|^2 + |r_h|^2)\mathbf{1}, \quad (103)$$

which states that, for rotationally invariant solutions to this model, all the electronic degrees of freedom are renormalized by the same factor and do not mix each other due to the interaction terms.

Besides the quasiparticle spectral weight, we can actually extract, from the saddle-point values of the slave-boson fields and Lagrange multipliers, the entire low-energy spectrum of the system, i.e., its coherent single-particle excitations. They are defined as the frequency poles of the physical electron propagator

$$\mathbf{D}_c(\mathbf{k}, \omega) = \mathbf{R}\mathbf{D}_f(\mathbf{k}, \omega)\mathbf{R}^\dagger = \mathbf{R}[\omega - \mathbf{h}(\mathbf{k})]^{-1}\mathbf{R}^\dagger \quad (104)$$

and, in terms of the saddle-point variables, they are given by the sixfold degenerate branches

$$E_{1p}(\mathbf{k}) = \pm \sqrt{[\epsilon_{\mathbf{k}}(|r_p|^2 + |r_h|^2) + \lambda]^2 + |\widetilde{\Delta}|^2},$$

$$\lambda = \frac{\Lambda(|r_p|^2 - |r_h|^2) + r_p r_h \Pi + (r_p r_h \Pi)^*}{|r_p|^2 + |r_h|^2},$$

$$\widetilde{\Delta} = \frac{r_p^2 \Pi - (r_h^2 \Pi)^* - 2\Lambda r_p r_h^*}{|r_p|^2 + |r_h|^2}. \quad (105)$$

From Eq. (105) we can then readily establish the expression for the low-energy spectral gap

$$\Delta = \sqrt{|\widetilde{\Delta}|^2 + R_2\left[|\lambda| - \frac{W}{2}(|r_p|^2 + |r_h|^2)\right]},$$

$$R_2(x) \equiv x^2 \theta(x), \quad (106)$$

where we have assumed, for the free-electron dispersion, $\epsilon_{\mathbf{k}} \in [-\frac{W}{2}, \frac{W}{2}]$, W being the uncorrelated bandwidth. It is important, however, to keep in mind that the onset of superconductivity in the system is signaled by the presence of a nonzero order parameter ψ_{sc}^0 rather than by the opening of a gap in the spectrum: these two quantities, in fact, are directly proportional to each other only in the weak-coupling regime ($J/W \ll 1$ and $U \lesssim J$), where we find the solution to be BCS like, becoming instead disentangled for stronger values of either the electron correlation U or the pairing attraction J.

IV. ILLUSTRATION OF RESULTS

As mentioned previously, the major strength of slave-boson approaches relies in the possibility of obtaining, with a relatively low computational effort, approximate analytical solutions which describe quite well, on a qualitative footing, the effects of electronic interactions on the low-energy part of the spectrum. With such methods we can thus investigate the behavior of a given model over the entire range of variability of the parameters on which the model is defined.

Using the slave-boson representation introduced in the previous section for the description of superconducting fullerides, we will here illustrate the behavior of the saddle-point solutions across the zero-temperature "phase diagram," where the external parameters of the model are represented by the electron density n_{phys} and the two ratios U/W and J/W, which measure, respectively, the strength of the Coulomb and Jahn-Teller interactions with respect to the kinetic
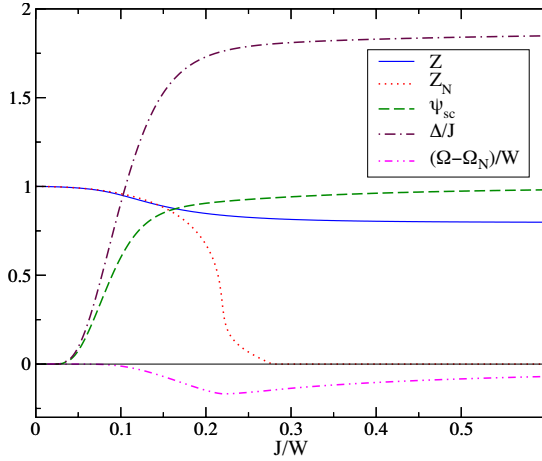
FIG. 1. (Color online) Normal and superconducting solutions at half filling and $U=0$: Z_N and Z are the corresponding quasiparticle weights, Δ and ψ_{sc} are the superconducting gap and order parameter, and $(\Omega - \Omega_N)$ represents the free-energy difference between the normal and the superconducting state.
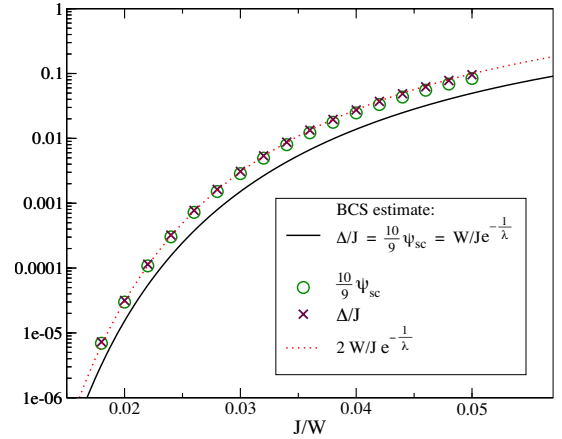

FIG. 2. (Color online) Superconductivity in the weak-coupling regime: slave-boson solution (circles and crosses) vs BCS estimate. For $J/W \ll 1$ and $U=0$ the superconducting parameters satisfy the BCS relation $\Delta/J = \frac{10}{9}\psi_{sc}^0$ and, apart from a constant prefactor, they follow the BCS functional form $\Delta(J)_{BCS} = We^{-1/\lambda}$ [$\lambda = \frac{10}{3}(J/W)$ is the dimensionless superconducting coupling constant].

bandwidth $W \propto t$. We will primarily focus on the half-filled case, where it can be found the most interesting experimental feature of these systems, namely the relatively high superconducting critical temperature in comparison to the strength of the pairing coupling and then we will briefly analyze how the superconducting behavior extends to finite values of doping. The solutions are obtained using, for simplicity, a flat density of states $D(\epsilon) = \frac{1}{W}$ since the qualitative behavior of the system does not depend much on the specific form of $D(\epsilon)$.

A. Half-filling ($n_{phys} = 3$)

We begin the analysis of the half-filled model illustrating, in Fig. 1, the normal and superconducting solutions obtained, at $U=0$, for increasing values of the Jahn-Teller coupling J/W. Since we are turning off the Coulomb repulsion, this is a purely attractive model, with the Jahn-Teller coupling playing the role of an attractive local interaction acting on spin and orbital degrees of freedom; the physics of this system is therefore characterized by the competition between singlet formation and kinetic delocalization, and we find the results of this competition to be remarkably different whether we are considering a purely normal-state solution or we are allowing for a superconducting order parameter. As expected for a purely attractive interaction, the superconducting solution is always energetically favored at finite J.

As soon as the pairing interaction J is turned on, the behavior of the normal-state solution is initially characterized by a slow decrease in the quasiparticle weight Z_N from the noninteracting value $Z_N(0) = Z(0) = 1$, which is then followed by a steep descent toward zero for $J/W \gtrsim 0.2$; finally, when the coupling is further increased, the metallic state turns into an insulating one, where all the electrons are locked in local singlets formed by two or four electrons,[33] the binding energy of the singlet configuration being much more favorable than the kinetic-energy gain associated to the electron hop-

ping. This state is analogous to the paired insulator found, at strong coupling, in the normal solution of the attractive Hubbard model within dynamical mean-field theory (DMFT).[34] On the other hand, if we do allow for superconducting ordering, we find the static singlet-formation mechanism characterizing the normal solution to be replaced by the more favorable Cooper-pair formation, in which the singlet pairs can still gain some kinetic energy through their propagation: the solution, in this case, is therefore characterized by a finite quasiparticle weight Z over the entire range of the pairing interaction. We must however notice that the difference in the behavior of the normal solution between the weak- and strong-coupling regimes (metallic vs insulating) can still be traced in the behavior of the superconducting solution. In fact, for increasing values of J/W, we observe a crossover between a weak-coupling BCS-like superconductivity, where the gap Δ/J and the superconducting order parameter ψ_{sc}^0 are proportional to each other and exponentially small in the pairing coupling (Fig. 2)

$$\Delta/J = \frac{10}{9}\psi_{sc}^0 \sim \frac{1}{\lambda}e^{-1/\lambda}, \quad \lambda = \frac{10}{3}(J/W) \qquad (107)$$

and a strong-coupling superconductivity associated to Bose-Einstein condensation (BEC) of preformed pairs, where both the gap and the superconducting order parameter are saturated.[35] While in the former regime the formation of Cooper pairs subtracts some kinetic energy from the normal state in order to gain the binding energy associated to the superconducting singlets, as evidenced by the lower spectral weight $Z < Z_N$, which corresponds to more localized particles, in the large J/W regime, where the local singlets are already formed, the energy gain of the superconducting state is due to the finite kinetic energy of the Cooper pairs in comparison to the static singlets characterizing the insulating normal state.[36]

The most interesting aspect of the half-filling solutions, however, is represented by the behavior of the quasiparticle
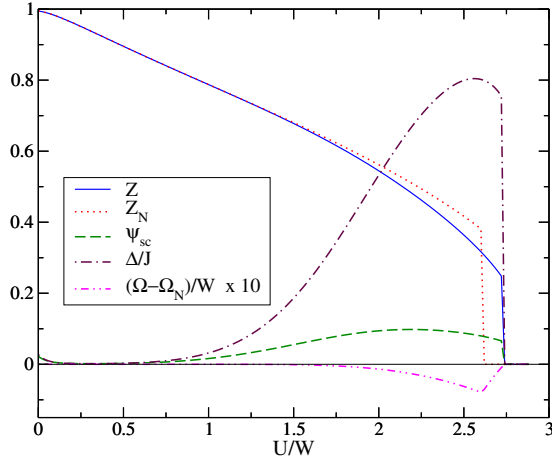
FIG. 3. (Color online) U dependence of the half-filling solutions at $J/W=0.04$. The condensation energy $(\Omega-\Omega_N)/W$ is multiplied by a factor of 10 for visibility reasons.

weight and of the superconducting observables (spectral gap and order parameter) as functions of the electron correlation U, at different values of the Jahn-Teller coupling J. In Fig. 3 we plot the U dependence of the normal quasiparticle weight Z_N and of the observables characterizing the complete solution (Z, Δ, and ψ_{sc}^0) at $J/W=0.04$, corresponding to a coupling strength located in the upper end of the weak-coupling regime, or, in other words, just before the $U=0$ crossover region. The relevant feature to be noticed in this figure is the nonmonotonic behavior of the superconducting parameters for increasing values of the electron correlation: while at small U the net effect of the Coulomb repulsion is to rapidly destroy the superconducting order, as expected in a weak-coupling BCS superconductor (notice the small value of the superconducting order parameter at $U=0$ and its sudden disappearance as soon as U is turned on), at larger U values the system turns back superconducting, with an enhancement in the values of Δ and ψ_{sc}^0 in comparison to $U=0$, until it undergoes a first-order Mott transition at $U=U_c$, just above the corresponding Mott transition of the normal state. It is evident of the huge enhancement of the superconducting amplitude ψ_{sc}^0 with respect to the noncorrelated regime. From a physical point of view, the reemergence of superconductivity at large U has been explained in terms of the strongly correlated superconductivity scenario put forward using DMFT to solve the same model[13,14] and a related simplified model.[37,38] The key mechanism is the different effect of the correlation on the various interaction terms: when strong repulsion freezes charge fluctuations, the resulting strongly correlated quasiparticles experience a strongly reduced repulsion, while the attraction is essentially unscreened. As a result, the net effect is that $J/W \rightarrow J/(ZW)$:[13] when the electrons become more localized, the relative strength of the Jahn-Teller interaction grows in comparison to the renormalized hopping. The precise nature of the interaction, involving orbital and spin degrees of freedom, is crucial in this effect, and proves the ability of our rotationally invariant slave bosons to properly treat every kind of interaction. The superconducting behavior in this region is clearly non-BCS-like, as evidenced by the nonproportionality between the gap and the order pa-
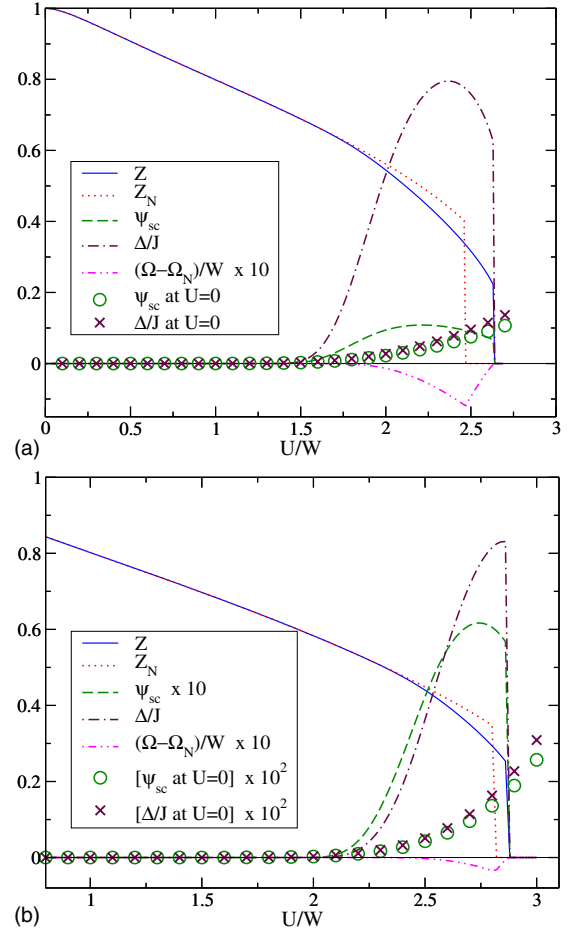

FIG. 4. (Color online) U dependence of the half-filling solutions for fixed ratios $J/U=0.02$ (top) and 0.01 (bottom). Circles and crosses represent the superconducting parameters evaluated at $U=0$ for the same values of J.

rameter: Δ/J is indeed much larger (up to ten times) than ψ_{sc}^0 and its maximum is located much closer to the Mott transition than the order parameter's one. On the other hand, the pairing mechanism cannot be explained within a purely strong-coupling BEC-like picture since in this case the pairing singlets are not already "preformed" in the normal phase (which is either a correlated metal or an $S=1/2$ Mott insulator) and their fraction is much smaller than in standard BEC superconductivity. We are rather in the presence of a strongly correlated superconductor, in which a small local pairing coupling turns out to be enhanced, rather than suppressed, by the effects of a strong on-site repulsion.

The correlation-driven enhancement of superconductivity in the proximity of the Mott transition is even more evident in Fig. 4, where the solutions are evaluated at a fixed ratio J/U for increasing values of the correlation; together with the normal and complete solutions, we have plotted for comparison the (BCS-like) superconducting parameters Δ/J and ψ_{sc}^0 obtained, at $U=0$, for the same values of J. Besides the different relation between Δ/J and ψ_{sc}^0 in the correlated case compared to the $U=0$ solutions, these plots emphasize how the enhancement of the superconducting gap becomes stronger (up to 3 orders of magnitude in the lower panel) at
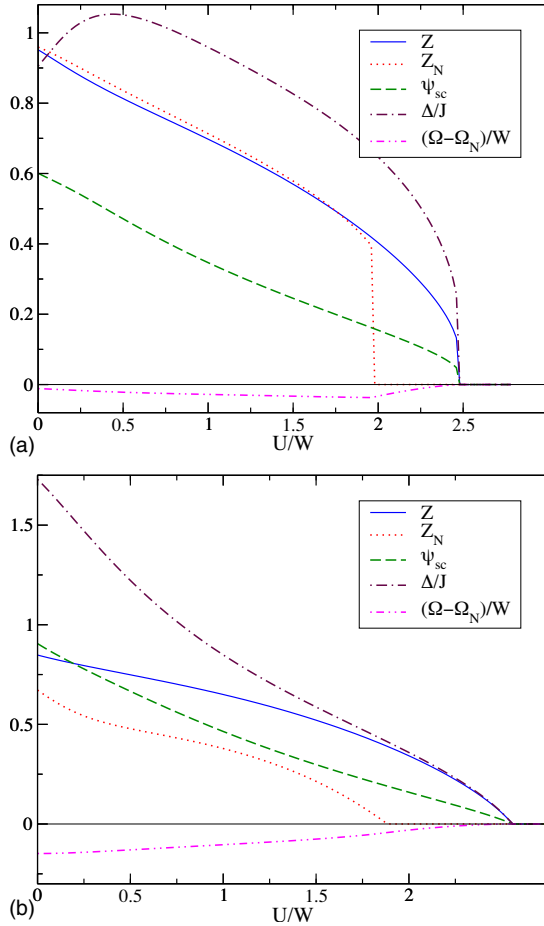
FIG. 5. (Color online) U dependence of the half-filling solutions at intermediate-to-strong pairing couplings $J/W=0.1$ (a) and 0.2 (b).
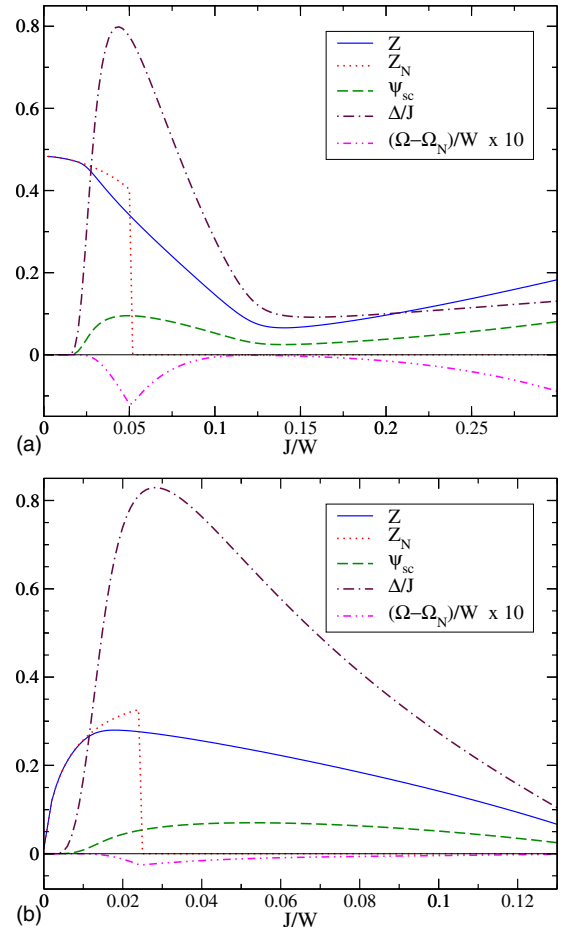

FIG. 6. (Color online) J dependence of the half-filling solutions in the strongly correlated regime: the top panel corresponds to a fixed value of the correlation, $U/W=2.45$ while in the bottom panel the solution follows the Mott-transition line $U_c(J)$.

smaller values of the pairing coupling: for $J/W \ll 1$, indeed, the value of Δ/J in the proximity of the Mott transition turns out to be $\mathcal{O}(1)$ while it is exponentially small in J/W in the BCS regime (see Fig. 2).

As already found in DMFT in a two-orbital model,[37] a completely different scenario is instead observed for larger values of the Jahn-Teller coupling, corresponding to the strong-coupling regime of the $U=0$ attractive model (shown in Fig. 5). In these cases, in fact, the superconducting order parameter decreases monotonically with U from the large $U=0$ value, until a weakly first-order Mott transition (which becomes second order when J/W is increased) turns the system into an insulator; a similar behavior characterizes the superconducting gap, except for an initial rise at small values of U/W in the case $J/W=0.1$. At strong-coupling values of the pairing attraction the superconducting solution is therefore always energetically favorable compared to the metallic one and the electronic correlation has only the effect of reducing throughout the noninsulating phase the superconducting ordering.

We conclude the analysis of the half-filling solutions showing, in Fig. 6, the nonmonotonic behaviors of the superconducting parameters Δ/J and ψ_{sc}^0, as functions of J, in the strongly correlated region of the phase diagram: in the top panel the value of U/W is held fixed while in the bottom one

it follows the Mott-transition line from below, $U(J)=U_c(J)-\delta U$. Combining these results with the ones discussed previously, we can then infer the existence of a second region in the $J-U$ plane, beside the strong-coupling BEC-like region at $J \gg U$, in which superconductivity is found to be optimal: almost surprisingly, it is located at very small values of the pairing attraction J and at correspondingly large values of the on-site electron repulsion U, just before the Mott-localization transition line.

The results presented in this section confirm that the rotationally invariant slave-boson approach is able to accurately treat interactions of different kinds and, particularly, it is not limited to charge interactions. Indeed we have found that the present approach is able to reproduce the relevant physics of a three-orbital Hubbard model for the fullerenes, and, in particular, the huge enhancement of phonon-mediated superconductivity in the proximity of the Mott transition. The only qualitative aspect of the DMFT solution which is not found in the present study is the second-order (or very weakly first-order) character of the superconductor-insulator transition.
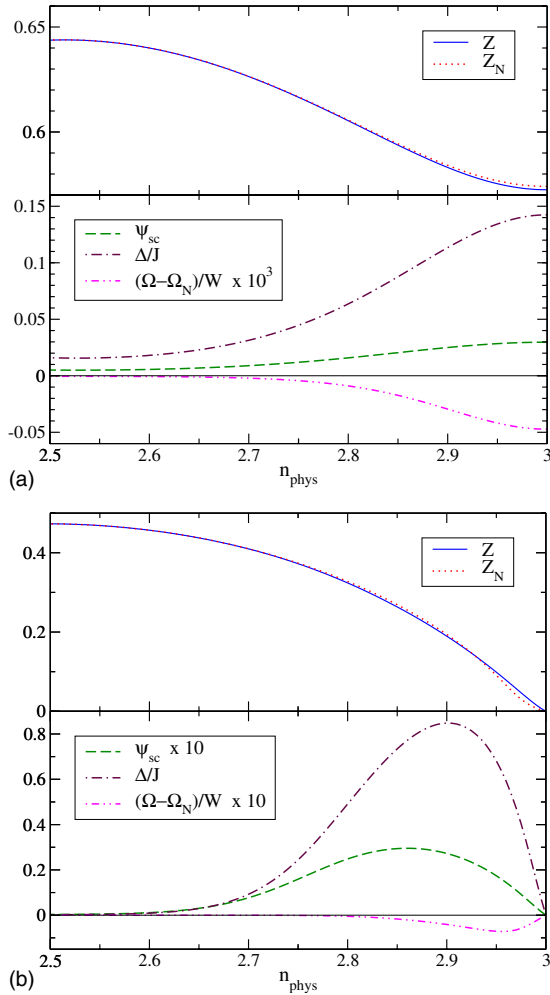
FIG. 7. (Color online) Doping dependence of the solutions for correlation strengths respectively below (top panel, $U/W=2$, and $J/W=0.03$) and above (bottom panel, $U/W=5$, and $J/W=0.02$) the $n_{\text{phys}}=3$ Mott transition.

B. Finite doping ($n_{\text{phys}}=3-\delta$)

In this section we consider the effect of doping the half-filled three-band model. While this situation cannot be experimentally realized, at the moment, in fullerides, the effect of doping is clearly suggestive for analogies with the physics of cuprates.

The behavior as a function of doping, in the neighborhood of $n_{\text{phys}}=3$, is shown in Fig. 7 for correlation strengths, respectively, below and above the critical Mott-transition value $U_c(J)$; in both cases, however, we have $U \gg J$, so that they both belong to the strongly correlated region of the phase diagram, where the presence of a finite superconducting order parameter is due to the localization-driven enhancement of the effective pairing coupling.

We find that for $U<U_c$ the superconducting parameters decrease monotonically upon doping (eventually vanishing at larger doping values) while the normal and superconducting quasiparticle weights increase from their finite half-filling values; as long as the superconducting order is present, we have $Z<Z_N$. On the other hand, for $U>U_c$ we observe a dome-shaped behavior in the superconducting pa-

rameters, the gap reaching its maximum at a very small doping value $\delta_{\text{opt}} \approx 0.1$, while the order parameter being maximum at a slightly larger optimal doping $\delta_{\text{opt}}^{(\psi)} \approx 0.15$. In this case, both the normal and superconducting quasiparticle weights grow linearly with the doping δ but while in the overdoped region $\delta>\delta_{\text{opt}}$ we find the standard weak-coupling behavior $Z<Z_N$, at lower dopings we have $Z>Z_N$.

The behaviors of both the normal and superconducting solutions in the two correlation regions $U \gtrless U_c$ are therefore remarkably different from each other; however, at a closer sight, we find that they can be actually explained through the same physical mechanism, namely, the competition between Mott localization, which can eventually enhance the superconducting pairing as we have seen in the discussion of the half-filling solutions, and the delocalization tendency introduced by doping. In fact, when the correlation strength at half filling is not large enough to completely destroy the quasiparticle coherence (in other words, when the quasiparticle degrees of freedom are nor completely frozen), we find the superconducting parameters to be maximum at zero doping, where the electrons are more localized and the enhancement of the effective pairing coupling is stronger. When the system is in the Mott-insulating phase, on the contrary, there are no available quasiparticles at half filling in order to develop a superconducting order parameter: the reintroduction of quasiparticle coherence due to a finite level of doping becomes then essential in order to recover a superconducting solution. At small dopings, therefore, the superconducting ordering increases, due to the regained coherence of quasiparticles and a still strong enhancement of pairing due to Mott localization; for larger values of doping, instead, the loosening of the localization-induced pairing enhancement disfavors the superconducting ordering, which turns to decrease as in the $U<U_c$ scenario. It is interesting to note that in the underdoped region we have $Z>Z_N$, which means that the formation of superconducting pairs is energetically more favorable also from the kinetic point of view, compared to the normal state.

V. CONCLUSIONS

We have generalized to superconducting solutions (allowing for the spontaneous breaking of charge symmetry) the rotationally invariant slave-boson approach introduced by Lechermann *et al.*[4] on the basis of the work by Li and Wölfle.[7] The crucial ingredient of the rotationally invariant version of slave-boson methods is that the boson fields cannot be simply seen as probability amplitudes for the different quasiparticle states but they are expressed as a nondiagonal density matrix that connects the different quasiparticle states to the whole set of physical states. This is easily generalized to include matrix elements between states with different number of particles which allow to describe superconducting ordering.

After a thorough description of the formalism, we apply the method to solve a three-band model which has been proposed and studied to understand the properties of alkali-doped fullerides.[14,30,37] This model has been previously solved using DMFT (Ref. 15) for integer fillings, providing a

striking realization of strongly correlated superconductivity, i.e., of a situation in which strong electron-electron correlations favor superconductivity. A crucial element of the model is that the pairing attraction, which can be modelized as an inverted Hund's rule term, only involves spin and orbital degrees of freedom, which are not heavily affected when the charge degrees of freedom are frozen by the proximity to the Mott transition. This interorbital nature of the pairing interaction is crucial to give rise to the correlation-driven enhancement of pairing. In this light, this model represents an ideal test field for our approach, which is tailored to properly treat interorbital interactions that cannot be expressed in a density-density form. Indeed the method provides good results for this model and it is actually the first mean-field-like approach able to reproduce the enhancement of superconductivity observed in DMFT.

The good performance of the method is very encouraging in view of other applications. The most challenging direction is obviously the study of the two-dimensional Hubbard model, which is believed to be the basic model to understand high-temperature superconductivity in the cuprates. While the full solution of the model on a lattice appears too cumbersome, a viable direction is the use of cluster extensions of DMFT, such as the cellular-DMFT (CDMFT) (Ref. 39) or the dynamical cluster approximation (DCA),[40] where the rotationally invariant slave-boson method can be used as an approximate analytical impurity solver for the cluster Hamiltonian. This approach has been used, for example, in Refs. 4 and 41 for normal solutions without superconducting ordering. To investigate the superconducting properties of the Hubbard model, on the other hand, our formalism can be applied either to the 2×2 plaquette, where it can be used to better understand the outcomes of fully numerical solutions,[42] or to slightly larger clusters, such as small rectangles in CDMFT or the five-site "cross" in DCA, which have been proposed as ideal compromises between reasonable cluster size and adequate accuracy.[43]

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