# Superconductivity in Ce-based heavy-fermion systems under high pressure

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In this paper, the possibility of a superconducting state mediated by the valence fluctuations in Ce-based heavy-fermion systems under high pressure is investigated for the extended periodic Anderson model. In this extended version, an additional local Coulomb repulsion between the localized and conduction electrons is included. In the framework of the projector-based renormalization method, we derive self-consistent equations for the superconducting order parameters. Our numerical evaluation for a two-dimensional case specifies that superconductivity in the heavy-fermion systems has a $d$-wave character and is mediated by valence fluctuations. By use of some additional simplifications, a BCS-like equation is found; an effective pairing interaction then is delivered. The interaction depends strongly on momentum and becomes dominant in the valence transition regime.

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## I. INTRODUCTION

Since the discovery of superconductivity in the heavy-fermion compound $CeCu_2Si_2$ in 1979 [1], the pairing mechanism is still a subject of controversy and has become one of the most attractive problems in condensed matter physics. Measurements in $CeCu_2(Si_{1-x}Ge_x)_2$ show a small superconducting dome at small applied pressures ($\leqslant$1 GPa) close to an antiferromagnetic phase [2]. Due to this closeness, one believes that pairing, in this case, is mediated by spin fluctuations [3–5]. When the pressure is increased, a second superconducting dome with a higher critical temperature opens at a higher pressure and it is believed that the superconducting state in this regime is mediated by charge fluctuations [6–8].

The abrupt change of the valence of the Ce ion under high pressure was qualitatively described by including a large Coulomb repulsion $U_{fc}$ between localized $f$ and conduction electrons [9]. Enhanced charge fluctuations caused by repulsive interactions in a multiband system were also proposed as a possible mechanism of superconductivity in high-$T_c$ cuprates [10]. Motivated by further study of this mechanism [11,12] the relationship between valence fluctuation and superconductivity in heavy-fermion systems was initially put on a theoretical footing by Miyake in 1998 by including an extra term which represents the Coulomb repulsion $U_{fc}$ between the localized $f$ and the conduction $c$ electrons in the periodic Anderson model (PAM) [13]. Solving this extended periodic Anderson model (EPAM) in three dimensions by a slave-boson mean-field approximation, the authors in Ref. [14] found that valence fluctuations were considerably enhanced by a moderate strength of $U_{fc}$ when the Coulomb repulsion between localized electrons on the same site was assumed to be infinitely large. The valence fluctuations occur if the $f$-electron level $\epsilon_f$ is tuned relative to the Fermi level. In a mean-field approximation, this special value of $\epsilon_f$ is on the order of half of the bandwidth. Associated with the rapid valence change, $d$-wave superconductivity was found and the authors pointed out the possibility of superconductivity caused by valence fluctuations. This scenario could explain various properties found in $CeCu_2Si_2$, at least qualitatively [15]. Solving the one-dimensional EPAM by use of the density matrix renormalization group (DMRG), the authors in Ref. [16] also obtained the valence instability. However, it occurred when $U_{fc}$ was larger than the conduction bandwidth and the $f$-electron energy $\epsilon_f$ was deeper than the lower bound of the conduction band. In this case, only singlet pairing superconducting correlation functions were considered by assuming that the investigated system can be described in analogy to the single-band Tomonaga-Luttinger liquid. The obtained results showed that in the sharp valence transition regime, the superconducting correlation functions for singlet pairing become dominant. This once more affirmed that the EPAM can be used as a possible explanation of superconductivity due to the valence fluctuations.

Recently, the EPAM has also been studied in the dynamical mean field theory (DMFT), combined with exact diagonalization for infinite dimensions [17]. The obtained results are in agreement with the ones found by the DMRG method. The work was done by the same group for the EPAM in two dimensions by applying the fluctuation-exchange approximation. It showed that in the weak-coupling region (modest strength of $U_{fc}$), a charge density wave was also unstable which may cause superconductivity as well [18]. Therefore, it is still unclear whether in the weak-coupling or in the strong-coupling regime superconductivity due to the valence fluctuations occurs in the EPAM. This means that other possible theoretical methods should also be used to study this problem.

The influence of $U_{fc}$ on the valence transition was first discussed in the impurity Anderson model [19]. In a mean-

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field approximation, a discontinuous valence transition was obtained for some large values of $U_{fc}$. For the PAM, there exist some studies of the effect of $U_{fc}$ on valence fluctuations within Hartree-Fock-like approximations, slave bosons, and large-$N$ expansions [14,20,21]. In all these approaches, $U_{fc}$ could explain a rapid change of the number of $f$ electrons as the $f$ level, $\epsilon_f$, increases. Without $U_{fc}$, the PAM was successfully solved by a projector-based renormalization method (PRM) in order to investigate the valence transition in the case of fixed chemical potential [22,23]. In the case of small values of $\nu_f$, the $f$ occupation drastically changes which shows a breakdown of a mixed-valence state.

In this paper, we use the PRM [24] to investigate the valence transition and superconductivity of the EPAM. The PRM derives a solvable effective Hamiltonian by deriving and solving renormalization equations using unitary transformations. The method has already been used to study the valence transition in the PAM [22]. Nevertheless, due to the complicated process of deriving the renormalization equations for the strongly correlated systems, various approximations had to be applied and no solution could be obtained for degeneracy $\nu_f = 2$. To overcome these restrictions and simplify the renormalization process we use an extended version of the PRM based on choosing a suitable generator [25–28]. For this generator, we can restrict ourselves to second-order renormalization contributions during the unitary transformations, and instead of difference equations we obtain differential equations which can easily be solved.

One of the greatest advantages of the PRM is the possibility to investigate quantum phase transitions. Already with the simplest version of the PRM with respect to perturbation theory, a BCS-like equation was derived for the coupled electron-phonon system [29]. In contrast to the Fröhlich interaction [30] the deduced effective electron-electron interaction for Cooper pairs did not contain singularities. Recently, the competition of the excitonic and polaritonic condensations in a microcavity, like the BCS Cooper pair superfluid state, was studied by the PRM [28]. In order to describe quantum phase transitions on both sides of the transition, one often includes infinitesimally small symmetry-breaking fields in the Hamiltonian. During the renormalization processes, the symmetry-breaking fields gain weight. Thus, from the fully renormalized Hamiltonian the order parameters can be found. In our work, we present an application of the PRM to possible superconductivity in the two-dimensional EPAM. Self-consistent equations for determining the superconducting order parameters are obtained. By use of some simplifications, a BCS-like equation is found. Our numerical results for the superconducting energy gaps with $d$-wave symmetry in the two-dimensional system then will be discussed.

The paper is organized as follows. In the next section, we briefly describe the EPAM, which is the PAM including the Coulomb repulsion between conduction and localized electrons. Section III introduces the PRM and its application to the EPAM in a superconducting state. The numerical result for $d$-wave superconducting energy gaps in two dimensions is also discussed. Section IV is left to present analytical solutions for the superconducting energy gaps with some simplifications. In Sec. V, we discuss the nature of the superconducting mechanism in the system. Finally, Sec. VI concludes our work.

## II. EXTENDED PERIODIC ANDERSON MODEL

The extended periodic Anderson model (EPAM) reads

$$\begin{aligned}\mathcal{H} &= (\bar{\varepsilon}_f - \mu)\sum_{i,\sigma}\hat{f}^\dagger_{i\sigma}\hat{f}_{i\sigma} + \sum_{\mathbf{k},\sigma}(\bar{\varepsilon}_\mathbf{k} - \mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} \\ &+ V\frac{1}{\sqrt{N}}\sum_{\mathbf{k},i,\sigma}(\hat{f}^\dagger_{i\sigma}c_{\mathbf{k}\sigma}\,e^{i\mathbf{k}\mathbf{R}_i} + \text{H.c.}) \\ &+ U_{fc}\sum_{i,\sigma\sigma'} n^c_{i\sigma}\hat{n}^f_{i\sigma'}, \end{aligned} \tag{1}$$

which describes a coupled system of conduction and localized $f$ electrons. The excitation energies of the $f$ and conduction electrons are denoted by $\bar{\varepsilon}_f$ and $\varepsilon_\mathbf{k}$. $\mu$ is the chemical potential. The hybridization $V_\mathbf{k}$ between localized and delocalized electrons is given by the third term. Finally, the last term represents the local Coulomb repulsion $U_{fc}$ between $f$ and conduction electrons. Note that already an infinitely large Coulomb repulsion between localized $f$ electrons at the same site was assumed. Thus, whereas $c^\dagger_{\mathbf{k}\sigma}$ ($c_{\mathbf{k}\sigma}$) are the usual fermionic creation (annihilation) operators for the conduction electrons, the operators $\hat{f}^\dagger_{i\sigma}$ ($\hat{f}_{i\sigma}$) are the so-called Hubbard operators [25]

$$\hat{f}^\dagger_{i\sigma} = f^\dagger_{i\sigma}\prod_{\tilde{\sigma}(\neq\sigma)}\left(1 - n^f_{i\tilde{\sigma}}\right) =: f^\dagger_{i\sigma}\mathcal{D}_{i\sigma}. \tag{2}$$

Here, $\mathcal{D}_{i\sigma}$ is a local projection operator on $f$ states which guarantees that a local site $i$ is either empty or singly occupied with an $f$ electron with spin index $\sigma$. The Hubbard operators obey unusual anticommutation relations, e.g.,

$$[\hat{f}^\dagger_{i\sigma}, \hat{f}_{i\sigma}]_+ = \mathcal{D}_{i\sigma}. \tag{3}$$

The spin index of the electrons, $\sigma$, is assumed to be equal for $f$ and $c$ electrons for simplicity.

To simplify the further calculation, we include the mean-field parts of the $U_{fc}$ term in the one-particle energies. With

$$n^c_{i\sigma}\hat{n}^f_{i\sigma'} = n^c_{i\sigma}\langle\hat{n}^f_{i\sigma'}\rangle + \hat{n}^f_{i\sigma'}\langle n^c_{i\sigma}\rangle + \delta\left(n^c_{i\sigma}\right)\delta\left(\hat{n}^f_{i\sigma'}\right),$$

we can rewrite the Hamiltonian (1) as

$$\begin{aligned}\mathcal{H} &= \varepsilon_f\sum_{i,\sigma}\hat{f}^\dagger_{i\sigma}\hat{f}_{i\sigma} + \sum_{\mathbf{k},\sigma}\varepsilon_\mathbf{k}\,c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} \\ &+ V\frac{1}{\sqrt{N}}\sum_{\mathbf{k},i,\sigma}(\hat{f}^\dagger_{i\sigma}c_{\mathbf{k}\sigma}\,e^{i\mathbf{k}\mathbf{R}_i} + \text{H.c.}) \\ &+ U_{fc}\sum_{i,\sigma\sigma'}\delta\left(n^c_{i\sigma}\right)\delta\left(\hat{n}^f_{i\sigma'}\right) - U_{fc}N\langle n^c\rangle\langle\hat{n}^f\rangle, \end{aligned} \tag{4}$$

where $\delta(n^c_{i\sigma}) = n^c_{i\sigma} - \langle n^c_{i\sigma}\rangle$, etc., and

$$\varepsilon_f = \bar{\varepsilon}_f + U_{fc}\langle n^c\rangle - \mu,$$
$$\varepsilon_\mathbf{k} = \bar{\varepsilon}_\mathbf{k} + U_{fc}\langle\hat{n}^f\rangle - \mu.$$

## III. APPLICATION OF THE PRM

### A. Renormalization equations in the superconducting phase

In our work on valence transition in the EPAM, the theoretical PRM was already discussed in some detail [25]. The starting point is the separation of the Hamiltonian into an unperturbed part $\mathcal{H}_0$ and a perturbation $\mathcal{H}_1$. Thereby, the perturbation $\mathcal{H}_1$ is responsible for transitions between the eigenstates of the unperturbed Hamiltonian $\mathcal{H}_0$. The main idea of the PRM is to eliminate all transitions induced by $\mathcal{H}_1$. This is done by starting from transitions with the largest transition energies and successively proceed to the transitions with the lowest energies. Thereby, a diagonal or at least a quasidiagonal Hamiltonian is obtained. Formally, the transformation to a renormalized Hamiltonian $\mathcal{H}_\lambda$, from which all transitions with energies larger than some cutoff $\lambda$ have been eliminated, is done by use of a unitary transformation

$$\mathcal{H}_\lambda = e^{X_\lambda}\mathcal{H}\, e^{-X_\lambda}, \tag{5}$$

where $X_\lambda$ is the generator for the transformation.

Next, the PRM will be applied to the extended periodic Anderson model (4) in order to discuss the possibility of a superconducting phase close to the valence transition. The EPAM is gauge symmetry invariant. Therefore, one has to include infinitesimally small gauge-symmetry-breaking fields. An ansatz for the renormalized Hamiltonian $\mathcal{H}_\lambda$ at cutoff $\lambda$ reads $\mathcal{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda}$, where

$$\mathcal{H}_{0,\lambda} = \varepsilon_{f,\lambda}\sum_{\mathbf{k},\sigma}\hat{f}^\dagger_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma}\gamma_{\mathbf{k},\lambda}(\hat{f}^\dagger_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma})_{\mathrm{NL}} + \sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k},\lambda}\, c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \mathcal{H}^{SC}_{0,\lambda} + E_\lambda \tag{6}$$

and

$$\mathcal{H}_{1,\lambda} = \mathbf{P}_\lambda\mathcal{H}_1 = \mathbf{P}_\lambda\sum_{\mathbf{k},\sigma}V_{\mathbf{k},\lambda}\,(\hat{f}^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \mathrm{H.c.}) + \mathbf{P}_\lambda\sum_{\mathbf{kq},\sigma}U_{\mathbf{k},\mathbf{k+q},\lambda}a_{\mathbf{k},\mathbf{k+q},\sigma}. \tag{7}$$

Note that all parameters of $\mathcal{H}_\lambda$ may now depend on $\lambda$ as a consequence of the elimination of all excitations with energies larger than $\lambda$. Moreover, in the unperturbed renormalized part $\mathcal{H}_{0,\lambda}$ an energy shift $E_\lambda$ and an additional hopping term $\gamma_{\mathbf{k},\lambda}$ between different $f$ sites was generated [second term in Eq. (6)], where

$$(\hat{f}^\dagger_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma})_{\mathrm{NL}} = \frac{1}{N}\sum_{i,j(\neq i)}\hat{f}^\dagger_{i\sigma}\hat{f}_{j\sigma}e^{i\mathbf{k}(\mathbf{R}_i-\mathbf{R}_j)} \tag{8}$$

describes the nonlocal (NL) $f$ particle-hole excitations. The fourth part $\mathcal{H}^{SC}_{0,\lambda}$ in $\mathcal{H}_{0,\lambda}$ breaks the gauge symmetry. It has the following form:

$$\mathcal{H}^{SC}_{0,\lambda} = -\sum_{\alpha\beta,\mathbf{k}}\left(\Delta^{\alpha\beta}_{\mathbf{k},\lambda}\alpha^\dagger_{\mathbf{k}\uparrow}\beta^\dagger_{-\mathbf{k}\downarrow} + \mathrm{H.c.}\right).$$

Here, all possible two-particle and two-hole excitations of conduction and localized electrons have to be included as a consequence of the hybridization term in $\mathcal{H}^{SC}_{0,\lambda}$. The four fields $\Delta^{\alpha\beta}_{\mathbf{k},\lambda}$ ($\alpha,\beta = c$ or $f$) will play the role of the superconducting energy gaps and depend on $\lambda$.

Finally, the perturbation $\mathcal{H}_{1,\lambda}$ consists of two contributions. Aside from the hybridization, a new density-like term of conduction and $f$ electrons is generated in the renormalization procedure where

$$a_{\mathbf{k},\mathbf{k+q},\sigma} = \frac{1}{N}\delta(c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k+q},\sigma})\sum_{i,\sigma}\delta(\hat{f}^\dagger_{i\sigma'}\hat{f}_{i\sigma'})e^{-i\mathbf{q}\mathbf{R}_i}. \tag{9}$$

$\mathbf{P}_\lambda$ is a general projection operator in the Liouville space, which eliminates all high-energy transitions larger than $\lambda$. As already mentioned, the elimination procedure starts from the original model $\mathcal{H}$, which will henceforth be denoted by $\mathcal{H} = \mathcal{H}_{\lambda=\Lambda}$ and proceeds to the fully renormalized model at $\lambda = 0$. For $\lambda = 0$, the perturbation $\mathcal{H}_{1,\lambda}$ will completely be used up for the renormalization of the parameters of $\mathcal{H}_{0,\lambda=0}$. The initial values of the $\lambda$-dependent parameters are fixed by the initial model. Thus, at cutoff $\Lambda$ we have

$$\varepsilon_{f,\Lambda} = \varepsilon_f,\quad \gamma_{\mathbf{k},\Lambda} = 0,\quad \varepsilon_{\mathbf{k},\Lambda} = \varepsilon_{\mathbf{k}},\quad V_{\mathbf{k},\Lambda} = V,$$
$$U_{\mathbf{k},\mathbf{k+q},\Lambda} = U_{fc},\quad E_\Lambda = -NU_{fc}\langle n^c\rangle\langle\hat{n}^f\rangle, \tag{10}$$

and for the gauge-symmetry-breaking fields

$$\Delta^{\alpha\beta}_{\mathbf{k},\Lambda} \to 0^+. \tag{11}$$

In order to derive the renormalization equations for the $\lambda$-dependent parameters, let us consider a renormalization step from $\lambda$ to a somewhat smaller cutoff $\lambda - \Delta\lambda$. The unitary transformation reads according to Eq. (5) $\mathcal{H}_{\lambda-\Delta\lambda} = e^{X_{\lambda,\Delta\lambda}}\mathcal{H}\, e^{-X_{\lambda,\Delta\lambda}}$, where $X_{\lambda,\Delta\lambda}$ is the corresponding generator of the transformation. For the following, we restrict ourselves to a weak-coupling theory. Thereby, the influence of $\mathcal{H}^{SC}_{0,\lambda}$ on $X_{\lambda,\Delta\lambda}$ will be neglected. Thus, $X_{\lambda,\Delta\lambda}$ agrees with the corresponding expression from Ref. [25],

$$X_{\lambda,\Delta\lambda} = \sum_{\mathbf{k},\sigma}\alpha_{\mathbf{k}}(\lambda,\Delta\lambda)(\hat{f}^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} - \mathrm{H.c.}) + \sum_{\mathbf{kq},\sigma}\beta_{\mathbf{k},\mathbf{k+q}}(\lambda,\Delta\lambda)a_{\mathbf{k},\mathbf{k+q},\sigma}, \tag{12}$$

where

$$\alpha_{\mathbf{k}}(\lambda,\Delta\lambda) = \frac{A_{\mathbf{k},\lambda}\theta(\lambda - |A_{\mathbf{k},\lambda}|)}{\kappa(\lambda - |A_{\mathbf{k},\lambda}|)^2}V_{\mathbf{k},\lambda}\Delta\lambda,$$
$$\beta_{\mathbf{k},\mathbf{k+q}}(\lambda,\Delta\lambda) = \frac{B_{\mathbf{k},\mathbf{k+q},\lambda}\theta(\lambda - |B_{\mathbf{k},\mathbf{k+q},\lambda}|)}{\kappa(\lambda - |B_{\mathbf{k},\mathbf{k+q},\lambda}|)^2}U_{\mathbf{k},\mathbf{k+q},\lambda}\Delta\lambda, \tag{13}$$

with

$$A_{\mathbf{k},\lambda} = \varepsilon_{f,\lambda} + D(\gamma_{\mathbf{k},\lambda} - \bar{\gamma}_\lambda) - \varepsilon_{\mathbf{k},\lambda},$$
$$B_{\mathbf{k},\mathbf{k+q},\lambda} = \varepsilon_{\mathbf{k},\lambda} - \varepsilon_{\mathbf{k+q},\lambda}, \tag{14}$$

where $\bar{\gamma}_\lambda = (1/N)\sum_{\mathbf{k}}\gamma_{\mathbf{k},\lambda}$. The constant $\kappa$ in (13) denotes an energy constant to ensure that $\alpha_{\mathbf{k}}(\lambda,\Delta\lambda)$ and $\beta_{\mathbf{k},\mathbf{k+q}}(\lambda,\Delta\lambda)$ are dimensionless. Both coefficients $\alpha_{\mathbf{k}}(\lambda,\Delta\lambda)$ and $\beta_{\mathbf{k},\mathbf{k+q}}(\lambda,\Delta\lambda)$ in $X_{\lambda,\Delta\lambda}$ are proportional to the energy shell $\Delta\lambda$. In a recent review article [31] it was shown that such a choice of $X_{\lambda,\Delta\lambda}$ leads to a declining decay of the coupling parameters, in our case of $V_{\mathbf{k},\lambda}$ and $U_{\mathbf{k},\mathbf{q},\lambda}$, when $\lambda$ decreases.

In the limit $\Delta\lambda \to 0$ only the linear terms in $X_{\lambda,\Delta\lambda}$ contribute to the right-hand side of $\mathcal{H}_{\lambda-\Delta\lambda}$. Defining $X_\lambda = X_{\lambda,\Delta\lambda}/\Delta\lambda$ one finds

$$\frac{d\mathcal{H}_\lambda}{d\lambda} = [X_\lambda, \mathcal{H}_\lambda]. \tag{15}$$

Next, one has to evaluate the commutator on the right-hand side. Here, not only operator expressions occur which are already present in $\mathcal{H}_\lambda$ but also higher-order terms. In order to trace them back to the operator terms of $\mathcal{H}_\lambda$ an additional factorization approximation has to be employed. In particular, also factorizations have to be included which lead back to the superconducting pairing functions, i.e., $\langle \alpha^\dagger_{\mathbf{k}\uparrow}\beta^\dagger_{-\mathbf{k}\downarrow}\rangle \neq 0$ ($\alpha, \beta = c$ or $f$). Finally, comparing the generic differential of the left-hand side with the results from the evaluation of the right-hand side, one arrives at the renormalization equations. Defining $\tilde{\alpha}_{\mathbf{k},\lambda} = \alpha_{\mathbf{k}}(\lambda, \Delta\lambda)/\Delta\lambda$ and $\tilde{\beta}_{\mathbf{k},\mathbf{k+q},\lambda} = \beta_{\mathbf{k},\mathbf{k+q}}(\lambda, \Delta\lambda)/\Delta\lambda$ they read

$$\frac{d\varepsilon_{\mathbf{k},\lambda}}{d\lambda} = 2DV_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda} + \frac{2}{N}\sum_{\mathbf{q}} C^{ff}_\rho(\mathbf{q})\, U_{\mathbf{k},\mathbf{k+q},\lambda}\tilde{\beta}_{\mathbf{k+q},\mathbf{k},\lambda}, \quad (16)$$

$$\begin{aligned}\frac{d\varepsilon_{f,\lambda}}{d\lambda} &= -\frac{1}{N}\sum_{\mathbf{k}}(\gamma_{\mathbf{k},\lambda} - \bar{\gamma}_\lambda)\tilde{\alpha}_{\mathbf{k},\lambda}\langle \hat{f}^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \text{H.c.}\rangle \\ &\quad - \frac{2}{N}\sum_{\mathbf{k}} V_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}[1 + \langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle] \\ &\quad - \frac{2(1-2\langle n^f\rangle)}{N^2}\sum_{\mathbf{qk},\sigma'} U_{\mathbf{k},\mathbf{k+q},\lambda}\tilde{\beta}_{\mathbf{k+q},\mathbf{k},\lambda} \\ &\quad \times \langle c^\dagger_{\mathbf{k+q},\sigma'}c_{\mathbf{k+q},\sigma'}\rangle, \end{aligned} \quad (17)$$

$$\frac{d\gamma_{\mathbf{k},\lambda}}{d\lambda} = -2V_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}, \quad (18)$$

$$\frac{dV_{\mathbf{k},\lambda}}{d\lambda} = A_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}, \quad (19)$$

$$\frac{dU_{\mathbf{k},\mathbf{k+q},\lambda}}{d\lambda} = B_{\mathbf{k},\mathbf{k+q},\lambda}\tilde{\beta}_{\mathbf{k},\mathbf{k+q},\lambda}, \quad (20)$$

$$\begin{aligned}\frac{d\Delta^{cc}_{\mathbf{k},\lambda}}{d\lambda} &= D\big(\Delta^{fc}_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda} + \Delta^{cf}_{\mathbf{k},\lambda}\tilde{\alpha}_{-\mathbf{k},\lambda}\big) \\ &\quad - \frac{1}{N}\sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{k+q},\lambda}(\tilde{\alpha}_{-\mathbf{k},\lambda}\langle \hat{f}_{-(\mathbf{k+q}),\downarrow}c_{\mathbf{k+q},\uparrow}\rangle \\ &\quad + \tilde{\alpha}_{\mathbf{k},\lambda}\langle c_{-(\mathbf{k+q}),\downarrow}\hat{f}_{\mathbf{k+q},\uparrow}\rangle), \end{aligned} \quad (21)$$

$$\begin{aligned}\frac{d\Delta^{ff}_{\mathbf{k},\lambda}}{d\lambda} &= -\big(\Delta^{fc}_{\mathbf{k},\lambda}\tilde{\alpha}_{-\mathbf{k},\lambda} + \Delta^{cf}_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}\big) \\ &\quad + \frac{1}{N}\sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{k+q},\lambda}(\tilde{\alpha}_{\mathbf{k},\lambda}\langle \hat{f}_{-(\mathbf{k+q}),\downarrow}c_{\mathbf{k+q},\uparrow}\rangle \\ &\quad + \tilde{\alpha}_{-\mathbf{k},\lambda}\langle c_{-(\mathbf{k+q}),\downarrow}\hat{f}_{\mathbf{k+q},\uparrow}\rangle), \end{aligned} \quad (22)$$

$$\begin{aligned}\frac{d\Delta^{fc}_{\mathbf{k},\lambda}}{d\lambda} &= -\Delta^{cc}_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda} + D\Delta^{ff}_{\mathbf{k},\lambda}\tilde{\alpha}_{-\mathbf{k},\lambda} \\ &\quad + \frac{1}{N}\sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{k+q},\lambda}(\tilde{\alpha}_{\mathbf{k+q},\lambda}\langle \hat{f}_{-(\mathbf{k+q}),\downarrow}\hat{f}_{\mathbf{k+q},\uparrow}\rangle \\ &\quad - \tilde{\alpha}_{\mathbf{k+q},\lambda}\langle c_{-(\mathbf{k+q}),\downarrow}c_{\mathbf{k+q},\uparrow}\rangle). \end{aligned} \quad (23)$$

In Eq. (16), the function $C^{ff}_\rho(\mathbf{q})$ is a wave-vector-dependent density-density correlation function for the $f$ electrons

$$C^{ff}_\rho(\mathbf{q}) = \frac{1}{N}\sum_{ij,\sigma\sigma'}\langle \delta\hat{n}^f_{i\sigma}\delta\hat{n}^f_{j\sigma'}\rangle e^{i\mathbf{q}(\mathbf{R}_i - \mathbf{R}_j)}. \quad (24)$$

Moreover, in deriving the above equations, the local projector $\mathcal{D}_{i\sigma}$ on the right-hand side of the anticommutator relation (3) was approximated by its expectation value $\langle \mathcal{D}_{i\sigma}\rangle =: D$.

Suppose the expectation values in (16) are known. Then, using the initial values (10) the set of differential equations (16) can be solved. This gives the fully renormalized parameter. Using that $\mathcal{H}_{1,\lambda}$ vanishes for $\lambda \to 0$, the fully renormalized Hamiltonian reads $\mathcal{H}_{\lambda\to 0} = \mathcal{H}_{0,\lambda\to 0} =: \tilde{\mathcal{H}}$ with

$$\begin{aligned}\tilde{\mathcal{H}} &= \tilde{\varepsilon}_f \sum_{\mathbf{k},\sigma}\hat{f}^\dagger_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma}\tilde{\gamma}_{\mathbf{k}}(\hat{f}^\dagger_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma})_{\text{NL}} \\ &\quad + \sum_{\mathbf{k},\sigma}\tilde{\varepsilon}_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \tilde{\mathcal{H}}^{SC}_0 + \tilde{E} \end{aligned} \quad (25)$$

and

$$\tilde{\mathcal{H}}^{SC}_0 = -\sum_{\alpha\beta,\mathbf{k}}\big(\tilde{\Delta}^{\alpha\beta}_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}\uparrow}\beta^\dagger_{-\mathbf{k}\downarrow} + \text{H.c.}\big),$$

where the tilde symbols again denote the fully renormalized quantities at $\lambda \to 0$.

### B. Expectation values

Note that the expectation values in the renormalization equations are in principle defined with the Hamiltonian $\mathcal{H}_\lambda$ since the factorization approximation was done at cutoff $\lambda$. However, it has turned out that they are best evaluated with the full Hamiltonian $\mathcal{H}$ (for details see Ref. [31]). Here, we employ the invariance of traces toward unitary transformations. Thus, for operator variables $\mathcal{A}$ follows

$$\langle \mathcal{A}\rangle = \frac{\text{Tr}(\mathcal{A}e^{-\beta\mathcal{H}})}{\text{Tr}e^{-\beta\mathcal{H}}} = \frac{\text{Tr}(\tilde{\mathcal{A}}e^{-\beta\tilde{\mathcal{H}}})}{\text{Tr}e^{-\beta\tilde{\mathcal{H}}}}, \quad (26)$$

where we have defined $\tilde{\mathcal{A}} = \lim_{\lambda\to 0}\mathcal{A}(\lambda)$ with $\mathcal{A}(\lambda) = e^{X_\lambda}\mathcal{A}\,e^{-X_\lambda}$. Thus, additional renormalization equations for $\mathcal{A}(\lambda)$ have to be derived using the same unitary transformation as before. For the one-particle operators in the expectation values, we make the following ansatz [25],

$$\begin{aligned} c^\dagger_{\mathbf{k}\sigma}(\lambda) &= x_{\mathbf{k},\lambda}c^\dagger_{\mathbf{k}\sigma} + y_{\mathbf{k},\lambda}\hat{f}^\dagger_{\mathbf{k}\sigma}, \\ \hat{f}^\dagger_{\mathbf{k}\sigma}(\lambda) &= -Dy_{\mathbf{k},\lambda}c^\dagger_{\mathbf{k}\sigma} + x_{\mathbf{k},\lambda}\hat{f}^\dagger_{\mathbf{k}\sigma}, \end{aligned} \quad (27)$$

where the $\lambda$ dependence of $c^\dagger_{\mathbf{k}\sigma}(\lambda)$ and $\hat{f}^\dagger_{\mathbf{k}\sigma}(\lambda)$ was shifted to the coefficients $x_{\mathbf{k},\lambda}$ and $y_{\mathbf{k},\lambda}$. Note that the $\lambda$-dependent operators fulfill the correct anticommution relations, provided

$$|x_{\mathbf{k},\lambda}|^2 + D|y_{\mathbf{k},\lambda}|^2 = 1 \quad (28)$$

is fulfilled for any $\mathbf{k}$ and $\lambda$, and the anticommutator (3), $[\hat{f}^\dagger_{i\sigma}, \hat{f}_{i\sigma}]_+ = \mathcal{D}_{i\sigma}$, is again approximated by $D = \langle D_{i\sigma}\rangle$. The operator structure of $c^\dagger_{\mathbf{k}\sigma}(\lambda)$ and $\hat{f}^\dagger_{\mathbf{k}\sigma}(\lambda)$ was taken over from the lowest-order expressions in $\mathcal{H}_{1,\lambda}$, and the values of $x_{\mathbf{k},\lambda}$ and $y_{\mathbf{k},\lambda}$ for the initial model ($\lambda = \Lambda$) are given by

$$x_{\mathbf{k},\Lambda} = 1, \;\; y_{\mathbf{k},\Lambda} = 0. \quad (29)$$

The renormalization equations for $x_{\mathbf{k},\lambda}$ and $y_{\mathbf{k},\lambda}$ are again derived from the transformation step between cutoff $\lambda$ and $\lambda - \Delta\lambda$. We obtain the following differential equations:

$$\frac{dx_{\mathbf{k},\lambda}}{d\lambda} = Dy_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}, \quad \frac{dy_{\mathbf{k},\lambda}}{d\lambda} = -x_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}. \quad (30)$$

Their solutions for $\lambda \to 0$ with the initial conditions (28) lead to the fully renormalized quantities $\tilde{x}_{\mathbf{k}}$ and $\tilde{y}_{\mathbf{k}}$. Using Eqs. (27), we can evaluate the expectation values

$$\begin{aligned}\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle &= |\tilde{x}_{\mathbf{k}}|^2 \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}} + |\tilde{y}_{\mathbf{k}}|^2 \langle \hat{f}^\dagger_{\mathbf{k}\sigma} \hat{f}_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}},\\ \langle \hat{f}^\dagger_{\mathbf{k}\sigma} \hat{f}_{\mathbf{k}\sigma}\rangle &= D|\tilde{y}_{\mathbf{k}}|^2 \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}} + |\tilde{x}_{\mathbf{k}}|^2 \langle \hat{f}^\dagger_{\mathbf{k}\sigma} \hat{f}_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}},\\ \langle \hat{f}^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \text{H.c.}\rangle &= -2D\tilde{x}_{\mathbf{k}}\tilde{y}_{\mathbf{k}}\big[\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}} - D^{-1}\langle \hat{f}^\dagger_{\mathbf{k}\sigma} \hat{f}_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}}\big].\end{aligned} \tag{31}$$

The superconducting pairing functions are given by

$$\begin{aligned}\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle &= \tilde{x}^2_{\mathbf{k}}\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} + \tilde{y}^2_{\mathbf{k}}\langle \hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}\\ &\quad + 2\tilde{x}_{\mathbf{k}}\tilde{y}_{\mathbf{k}}\langle \hat{f}_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}},\\ \langle \hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle &= D^2\tilde{y}^2_{\mathbf{k}}\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} + \tilde{x}^2_{\mathbf{k}}\langle \hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}\\ &\quad - 2D\tilde{x}_{\mathbf{k}}\tilde{y}_{\mathbf{k}}\langle \hat{f}_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}},\\ \langle \hat{f}_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle &= \big(\tilde{x}^2_{\mathbf{k}} - D\tilde{y}^2_{\mathbf{k}}\big)\langle \hat{f}_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}\\ &\quad - \tilde{x}_{\mathbf{k}}\tilde{y}_{\mathbf{k}}(D\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} - \langle \hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}).\end{aligned} \tag{32}$$

What remains is to evaluate the expectation values formed with $\tilde{\mathcal{H}}$. Obviously, $\tilde{\mathcal{H}}$ is not diagonal due to the superconducting part $\tilde{\mathcal{H}}^{SC}$ in expression (25). Therefore, we employ a Bogoliubov transformation using again the approximation $[\hat{f}_{i,\sigma}, \hat{f}^\dagger_{i\sigma}]_+ \approx D$. Thus, $\tilde{\mathcal{H}}$ can be rewritten as

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k},\pm} \mathcal{E}^\pm_{\mathbf{k}}(\zeta^{\pm\dagger}_{\mathbf{k}}\zeta^\pm_{\mathbf{k}} + \eta^{\pm\dagger}_{\mathbf{k}}\eta^\pm_{\mathbf{k}}) + \text{const.}, \tag{33}$$

where $\zeta^{\pm(\dagger)}_{\mathbf{k}}$ and $\eta^{\pm(\dagger)}_{\mathbf{k}}$ are new fermionic annihilation (creation) operators of the quasiparticles. Their eigenenergies are

$$\mathcal{E}^\pm_{\mathbf{k}} = [(u_{\mathbf{k}} \pm \sqrt{\Phi_{\mathbf{k}}})/2]^{1/2} \quad \text{with} \quad \Phi_{\mathbf{k}} = u^2_{\mathbf{k}} - 4v_{\mathbf{k}}, \tag{34}$$

where

$$u_{\mathbf{k}} = \tilde{\varepsilon}^2_{\mathbf{k}} + \tilde{\omega}^2_{\mathbf{k}} + \big|D\tilde{\Delta}^{ff}_{\mathbf{k}}\big|^2 + \big|\tilde{\Delta}^{cc}_{\mathbf{k}}\big|^2 + D\big(\big|\tilde{\Delta}^{fc}_{\mathbf{k}}\big|^2 + \big|\tilde{\Delta}^{cf}_{\mathbf{k}}\big|^2\big)$$

and

$$\begin{aligned}v_{\mathbf{k}} &= \big(\tilde{\varepsilon}^2_{\mathbf{k}} + \big|\tilde{\Delta}^{cc}_{\mathbf{k}}\big|^2\big)\big(\tilde{\omega}^2_{\mathbf{k}} + \big|D\tilde{\Delta}^{ff}_{\mathbf{k}}\big|^2\big)\\ &\quad + D\tilde{\varepsilon}_{\mathbf{k}}\tilde{\omega}_{\mathbf{k}}\big(\big|\tilde{\Delta}^{fc}_{\mathbf{k}}\big|^2 + \big|\tilde{\Delta}^{cf}_{\mathbf{k}}\big|^2\big) + \big|D\tilde{\Delta}^{cf}_{\mathbf{k}}\big|^2|D\tilde{\Delta}^{fc}_{\mathbf{k}}|^2\\ &\quad - D^2\big(\tilde{\Delta}^{cc}_{\mathbf{k}}\tilde{\Delta}^{cf,*}_{\mathbf{k}}\tilde{\Delta}^{fc,*}_{\mathbf{k}}\tilde{\Delta}^{ff}_{\mathbf{k}} + \tilde{\Delta}^{cc,*}_{\mathbf{k}}\tilde{\Delta}^{cf}_{\mathbf{k}}\tilde{\Delta}^{fc}_{\mathbf{k}}\tilde{\Delta}^{ff,*}_{\mathbf{k}}\big).\end{aligned}$$

From the diagonal Hamiltonian (33), one evaluates the free energy in a simple form,

$$\begin{aligned}F &= -\frac{1}{\beta}\ln \operatorname{Tr} e^{-\beta H} = -\frac{1}{\beta}\ln \operatorname{Tr} e^{-\beta\tilde{\mathcal{H}}}\\ &= -\frac{2}{\beta}\sum_{\mathbf{k},\pm}\ln[1 + e^{-\beta\mathcal{E}^\pm_{\mathbf{k}}}] + \text{const.},\end{aligned} \tag{35}$$

from which the superconducting pairing functions can be found. For example,

$$\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} = -\frac{\partial F}{\partial\tilde{\Delta}^{cc,*}_{\mathbf{k}}} = \sum_{\mathbf{k}',\pm}[1 - 2f(\mathcal{E}^\pm_{\mathbf{k}'})]\frac{\partial\mathcal{E}^\pm_{\mathbf{k}'}}{\partial\tilde{\Delta}^{cc,*}_{\mathbf{k}}}.$$

Here, $f(\mathcal{E}_{\mathbf{k}})$ denotes the Fermi function for the energy $\mathcal{E}_{\mathbf{k}}$. With the explicit expression of $\mathcal{E}^\pm_{\mathbf{k}}$ in Eq. (34) one finds

$$\begin{aligned}&\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}\\ &= \sum_{\pm}\frac{1 - 2f(\mathcal{E}^\pm_{\mathbf{k}})}{4\mathcal{E}^\pm_{\mathbf{k}}}\Bigg\{\Bigg(1 \pm \frac{u_{\mathbf{k}}}{\sqrt{\Phi_{\mathbf{k}}}}\Bigg)\tilde{\Delta}^{cc}_{\mathbf{k}}\\ &\quad \mp \frac{2}{\sqrt{\Phi_{\mathbf{k}}}}\big[\big(\tilde{\omega}^2_{\mathbf{k}} + \big|D\tilde{\Delta}^f_{\mathbf{k}}\big|^2\big)\tilde{\Delta}^{cc}_{\mathbf{k}} - D^2\tilde{\Delta}^{cf}_{\mathbf{k}}\tilde{\Delta}^{fc}_{\mathbf{k}}\tilde{\Delta}^{ff,*}_{\mathbf{k}}\big]\Bigg\}.\end{aligned}$$

The remaining pairing functions in (32) can be found as well. As before, the tilde symbols in Eq. (36) denote the renormalized parameters in the limit $\lambda \to 0$, and

$$\tilde{\omega}_{\mathbf{k}} = \tilde{\varepsilon}_f + D(\tilde{\gamma}_{\mathbf{k}} - \bar{\tilde{\gamma}}) \tag{36}$$

is the **k**-dependent excitation energies of the $f$ electrons ($\bar{\tilde{\gamma}} = 1/N\sum_{\mathbf{k}}\tilde{\gamma}_{\mathbf{k}}$).

The normal expectation values in (31) can be easily found as well. By neglecting all superconducting terms, one finds

$$\begin{aligned}\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}} &= \frac{1}{e^{\beta\tilde{\varepsilon}_{\mathbf{k}}} + 1} = f(\tilde{\varepsilon}_{\mathbf{k}}),\\ \langle \hat{f}^\dagger_{\mathbf{k}\sigma} \hat{f}_{\mathbf{k}\sigma}\rangle_{\tilde{\mathcal{H}}} &= \frac{f(\tilde{\omega}_{\mathbf{k}})}{1 + \frac{1}{N}\sum_{\mathbf{p}} f(\tilde{\omega}_{\mathbf{p}})}.\end{aligned} \tag{37}$$

Note that the denominator in the second relation follows from the exclusion of doubly occupied $f$ sites [22,25].

Expressions (31) and (32) together with (36) and (37) allow us to evaluate all expectation values formed with $\mathcal{H}$, as long as the fully renormalized parameters of $\tilde{\mathcal{H}}$ are known. On the other hand, to find the renormalized parameters of $\tilde{\mathcal{H}}$ by solving the renormalization equations (24) the expectation values are needed. Thus, the total composed set of equations for the expectation values and for the renormalization of $\mathcal{H}_\lambda$ has to be solved simultaneously. Starting by given expectation values, one first can evaluate the renormalized parameters of $\tilde{\mathcal{H}}$. With $\tilde{\mathcal{H}}$, one then is able to evaluate a better approximation for the expectation values, and so on. Having arrived at a self-consistent solution, the obtained final Hamiltonian $\tilde{\mathcal{H}}$ allows us to describe all superconducting properties.

### C. Numerical results

In this section, the self-consistent solutions for the superconducting phase for a system with $N = 16 \times 16$ lattice sites are discussed. As discussed before, we start from some guess for the normal expectation values $\langle\hat{n}^f\rangle$, $\langle c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m}\rangle$, and $\langle\hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \text{H.c.}\rangle$ and for the superconducting pairing functions $\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle$, $\langle c_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle$, and $\langle\hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle$. Solving the differential equations (16)–(24) with the initial conditions (10) and (11), the renormalized Hamiltonian (25) in the superconducting state will be obtained. Next, we recalculate all expectation values including the superconducting pairing functions by use of the Bogoliubov diagonalization (33). The entire renormalization procedure has to be repeated until a self-consistent solution is gained. The symmetry for the order parameters has to be put in by hand by choosing an appropriate **k** dependence of the initial pairing functions. For example, to find a solution with $d_{x^2-y^2}$-wave symmetry we choose $\langle\alpha_{-\mathbf{k}\downarrow}\beta_{\mathbf{k}\uparrow}\rangle = A^0_{\alpha\beta}(\cos k_x - \cos k_y)$, where $\alpha$, $\beta$ denote the $c$- or $f$-electron operators. For the choice $\langle\alpha_{-\mathbf{k}\downarrow}\beta_{\mathbf{k}\uparrow}\rangle = A^0_{\alpha\beta}(\cos k_x + \cos k_y)$,

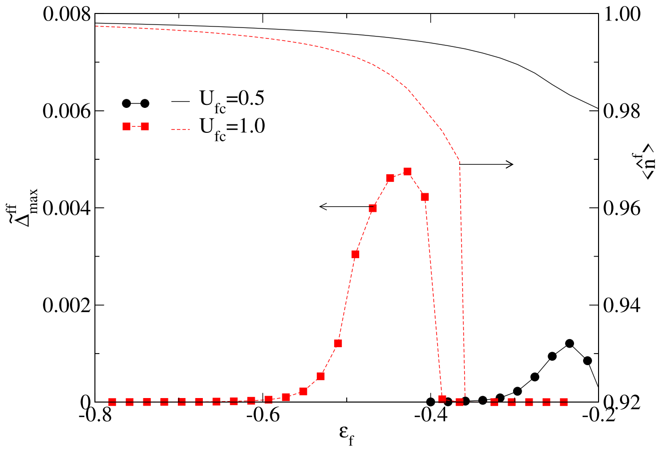


FIG. 1. Maximum value of superconducting order parameter $\tilde{\Delta}^{ff}_{\mathbf{k}}$ and of the $f$ occupation number $\langle \hat{n}^f \rangle$ as functions of the bare $f$ energy $\epsilon_f$ for two values of $U_{fc}$. The other parameters are $T = 10^{-3}$ and $V = 0.1$. Note that only $\langle \hat{n}^f \rangle$ values are shown between 0.92 and 1.

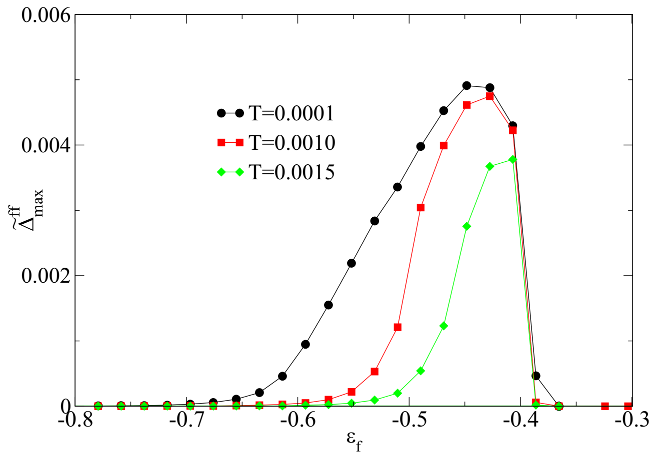


FIG. 2. Maximum value of $\tilde{\Delta}^{ff}_{\mathbf{k}}$ as a function of the bare $f$ energy $\epsilon_f$ for several values of temperature $T$ at $U_{fc} = 1, V = 0.1$.

we would imply $s$-wave symmetry. Note that only solutions with $d$-wave symmetry are found which will be discussed in the following.

Due to the rather small number of **k** points for the lattice viewed in the calculations, only the maximum values of **k**-dependent quantities will be discussed. In Fig. 1, the maximum value of the superconducting gap $\tilde{\Delta}^{ff}_{\max}$ and the density $\langle \hat{n}^f \rangle$ of the $f$ electrons are shown as a function of the bare $f$ energy $\epsilon_f$ for two values of $U_{fc}$. As one can see, in both cases a superconducting phase close to the valence transition regime is found. In particular, note that the superconducting phase already occurs in a region, where the $f$ valence $\langle \hat{n}^f \rangle$ deviates only slightly from the integer valence $\langle \hat{n}^f \rangle = 1$. As is known, in this case the renormalized $f$ energy $\tilde{\varepsilon}_f$ is located still slightly below the Fermi level. For values of $\langle \hat{n}^f \rangle$ lower than $\langle \hat{n}^f \rangle = 0.9$ the superconducting phase disappears again. This result is in agreement with a slave-boson mean-field treatment in Ref. [14] where the superconducting transition temperature with $d$-wave symmetry has a peak at a value $\epsilon_f^*$, which is slightly smaller than the value for $\epsilon_f$ with the steepest slope of $\langle \hat{n}^f \rangle$. For $\epsilon_f > \epsilon_f^*$, the transition temperature drops rapidly down. Moreover, as in the one-dimensional lattice [25], also for the two-dimensional lattice the phase transition becomes sharper for larger values of $U_{fc}$. Also, the superconducting phase becomes enhanced for larger values of $U_{fc}$. Thus, our results confirm that superconductivity becomes more stable by stronger density correlations $\sim U_{fc}$ between localized and conduction electrons. Increasing $U_{fc}$ in the EPAM is crucial for finding a sharp valence transition and $d$-wave superconductivity close to the valence transition regime. This behavior can be explained in Sec. IV below. Finally, note that the valence transition regime and thus the superconducting phase shift to smaller values of $\varepsilon_f$, when $U_{fc}$ is increased. This is not found in the slave-boson mean-field treatment mentioned above.

In Fig. 2, the energy gap $\tilde{\Delta}^{ff}_{\max}$ is shown as a function of $\varepsilon_f$ for different temperatures. Similarly to the one-dimension case, also in two dimensions a sharper valence transition is found when the temperature decreases [25]. Thus, as expected, a more pronounced valence transition for lower temperature also leads to an enhanced superconducting regime.

The pressure dependence in real systems might be simulated by changing either the bare $f$ energy $\varepsilon_f$ or the hybridization $V$ between localized and conduction electrons. Therefore, in Fig. 3, the maximum value of $\tilde{\Delta}^{ff}_{\mathbf{k}}$ is also plotted as a function of the hybridization $V$. Similarly to Figs. 1 and 2, where a superconducting dome is found as a function of $\varepsilon_f$, in Fig. 3 a superconducting phase also appears in a restricted range of $V$. This behavior can easily be understood due to the influence of valence fluctuations. By increasing the hybridization, the renormalized $f$ level approaches the Fermi level from below and leads to quasiparticles which have both a strong localized and conduction electron character. The chance of forming Cooper pairs between $f$ holes is thus enhanced [9].

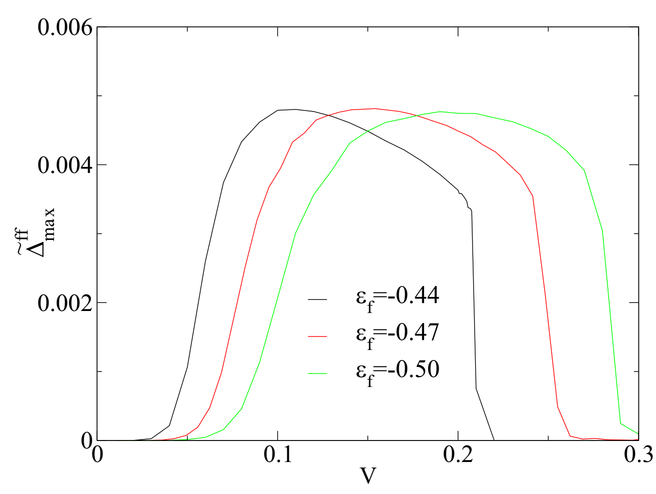


FIG. 3. Maximum value of $\tilde{\Delta}^{ff}_{\mathbf{k}}$ as a function of the hybridization $V$ for several values of the bare $f$ energy $\epsilon_f$. The other parameter are $U_{fc} = 1, T = 10^{-3}$.

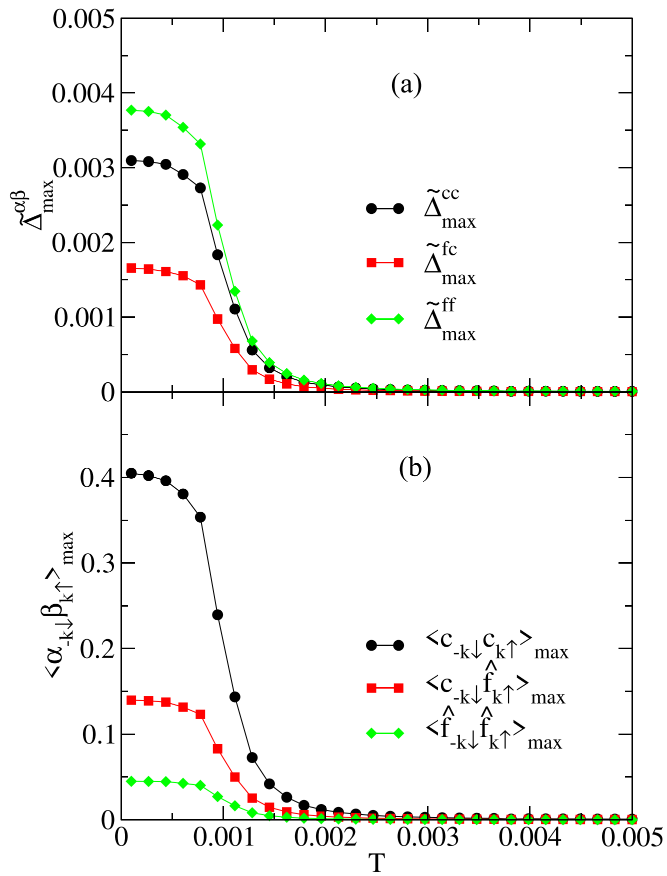


FIG. 4. Maximum values of (a) the superconducting energy gaps and (b) the pairing functions as a function of $T$ ($U_{fc} = 1$, $V = 0.1$, and $\epsilon_f = -0.5$).

If $V$ is large enough, a large number of holes in the $f$ levels suppress the attractive pairing interaction of isolated pairs of $4f^0$ "holes" [9]. Furthermore, the "window" in which superconductivity becomes stable is shifted to smaller $V$ values as $\varepsilon_f$ is increased. Thus, when $\varepsilon_f$ is located far below the Fermi level, the hybridization has to become larger so that $f$ electrons can interact with conduction electrons in order to form Cooper pairs.

In Fig. 4, the $T$ dependence of the superconducting gap and the pairing functions, $\Delta^{\alpha\beta}_{\max}$ and $\langle\alpha_{-\mathbf{k}\downarrow}\beta_{\mathbf{k}\uparrow}\rangle_{\max}$, is shown for all possible combinations of Cooper pairs, i.e., $\alpha, \beta = c, f$. As expected, the overall temperature dependence of all quantities is equivalent. The physical picture which arises is the following. Superconductivity only exists for $f$ occupation $\langle\hat{n}^f\rangle$ between $\langle\hat{n}^f\rangle = 0.9$ and 1. Thus, the density of $f$ holes is still small, which leads to quite small pairing functions $\langle\hat{f}_{-\mathbf{k}\downarrow}\hat{f}_{\mathbf{k}\uparrow}\rangle$ for Cooper pairs created by $f$ holes [green symbols in Fig. 4(b)]. For $\langle\hat{n}^f\rangle > 0.9$, the $f$-hole density is small, which means that it is difficult to find enough $f$ holes, which can interact to form Cooper pairs. This is in contrast to the situation for conduction electrons which are delocalized. Therefore, the probability for the pairing of conduction electrons is dominant as shown by the black symbols in Fig. 4(b). For the superconducting gap functions in Fig. 4(a) the situation is reversed. In order to break the Cooper pairs between the $f$ holes, more energy has to be supplied than for pairs formed by conduction electrons.

## IV. ANALYTICAL SOLUTION

### A. Normal-state parameters

For the two-dimensional lattice under consideration, self-consistent superconducting solutions for the set of renormalization equations can be found only for rather small systems. In order to make sure that a $N = 16 \times 16$ system is large enough to mimic the thermodynamic limit, we want to consider a simplified solution of the renormalization equations. The results can be applied to larger systems.

To simplify the calculations, let us assume from the beginning that the superconducting phase is closely connected to the valence transition regime. According to Sec. III, such a phase is found for $f$ occupations $\langle\hat{n}^f_i\rangle$ between 0.9 and 1; i.e., the $f$ occupation is slightly below integer filling. Thus, the $f$-electron density-density correlation function

$$C^{ff}_\rho(\mathbf{q}) = \frac{1}{N}\sum_{ij,\sigma\sigma'}\langle\delta\hat{n}^f_{i\sigma}\delta\hat{n}^f_{j\sigma'}\rangle e^{i\mathbf{q}(\mathbf{R}_i-\mathbf{R}_j)}$$

almost vanishes since the local density fluctuations are small. Thus, we neglect the second term in Eq. (16) from the beginning and Eqs. (16), (18), and (19) reduce to

$$\frac{d\varepsilon_{\mathbf{k},\lambda}}{d\lambda} = 2DV_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}, \qquad \frac{d\gamma_{\mathbf{k},\lambda}}{d\lambda} = -2V_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda},$$
$$\frac{dV_{\mathbf{k},\lambda}}{d\lambda} = A_{\mathbf{k},\lambda}\tilde{\alpha}_{\mathbf{k},\lambda}. \tag{38}$$

Note that these renormalization equations are the same as in the normal state. Thus, for an analytical solution, we shall proceed as in Ref. [32]. There, as a first approximation the $\lambda$ dependence of the renormalized $f$ level was neglected from the beginning. Note that the spirit of this approximation is similar to that used in the slave-boson mean-field theory. Thus, we approximate $\lambda$

$$\varepsilon_{f,\lambda} - D\bar{\gamma}_\lambda \approx \tilde{\varepsilon}_f - D\tilde{\bar{\gamma}} \approx \tilde{\varepsilon}_f, \tag{39}$$

where the average $f$ dispersion $\tilde{\bar{\gamma}}$ will also be neglected.

To solve the renormalization equations (38), we first combine the first two equations to

$$\frac{d\gamma_{\mathbf{k},\lambda}}{d\lambda} = -\frac{1}{D}\frac{d\varepsilon_{\mathbf{k},\lambda}}{d\lambda}.$$

This differential equations has the solution

$$\gamma_{\mathbf{k},\lambda} = \frac{\varepsilon_{\mathbf{k},\Lambda} - \varepsilon_{\mathbf{k},\lambda}}{D}, \tag{40}$$

where we have used the initial condition (10). With (40), can rewrite the last equation of (38) as

$$\tilde{\alpha}_{\mathbf{k},\lambda} = \frac{1}{\tilde{\varepsilon}^f + \varepsilon_{\mathbf{k},\Lambda} - 2\varepsilon_{\mathbf{k},\lambda}}\frac{dV_{\mathbf{k},\lambda}}{d\lambda}, \tag{41}$$

where the quantity $A_{\mathbf{k},\lambda}$ was replaced by $A_{\mathbf{k},\lambda} = \tilde{\varepsilon}_f + D\gamma_{\mathbf{k},\lambda} - \varepsilon_{\mathbf{k},\lambda}$ due to approximation (39). Finally, inserting (41) into the first equation of (38), one arrives at

$$\frac{d}{d\lambda}\{\varepsilon^2_{\mathbf{k},\lambda} - (\tilde{\epsilon}^f + \varepsilon_{\mathbf{k},\Lambda})\varepsilon_{\mathbf{k},\lambda} + DV^2_{\mathbf{k},\lambda}\} = 0.$$

The integration leads to a quadratic equation for $\varepsilon_{\mathbf{k},\lambda}$. Using the initial conditions (10) for $\lambda = \Lambda$, the solution reads

$$\varepsilon_{\mathbf{k},\lambda}^2 - (\tilde{\epsilon}^f + \varepsilon_{\mathbf{k}})\varepsilon_{\mathbf{k},\lambda} + DV_{\mathbf{k},\lambda}^2 = \varepsilon_{\mathbf{k}}^2 - (\tilde{\epsilon}^f + \varepsilon_{\mathbf{k}})\varepsilon_{\mathbf{k}} + DV_{\mathbf{k}}^2. \tag{42}$$

For $\lambda \to 0$, the quasiparticles of the fully renormalized Hamiltonian $\tilde{\mathcal{H}}$ do not change its ($c$ or $f$) character as a function of the wave vector $\mathbf{k}$. Therefore, $\tilde{\varepsilon}_{\mathbf{k}}$ jumps between the two solutions of the quadratic equation (42) in order to minimize its deviations from the original $\varepsilon_{\mathbf{k}}$,

$$\tilde{\epsilon}_{\mathbf{k}} = \frac{\tilde{\varepsilon}_f + \varepsilon_{\mathbf{k},\Lambda}}{2} - \frac{\mathrm{sgn}(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k},\Lambda})}{2} W_{\mathbf{k}},$$
$$W_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k},\Lambda} - \tilde{\varepsilon}_f)^2 + 4DV^2}. \tag{43}$$

The second quasiparticle band is given by

$$\tilde{\omega}_{\mathbf{k}} := \tilde{\varepsilon}_f + D\tilde{\gamma}_{\mathbf{k}} = \frac{\tilde{\varepsilon}_f + \varepsilon_{\mathbf{k},\Lambda}}{2} + \frac{\mathrm{sgn}(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k},\Lambda})}{2} W_{\mathbf{k}}. \tag{44}$$

Thus, for the normal-state properties, we have obtained a renormalized Hamiltonian which reads

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k},\sigma} \tilde{\varepsilon}_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma} \tilde{\omega}_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{f}_{\mathbf{k}\sigma} + \tilde{E}, \tag{45}$$

where the expression for $\tilde{E}$ is given in Ref. [32]. Note that in approximation (45), the renormalized Hamiltonian $\tilde{\mathcal{H}}$ describes a system of uncoupled quasiparticles where the $f$-like quasiparticle excitations are no longer correlated.

The expectation values $\langle \hat{n}^f \rangle$ and $\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle$ are formed with the full Hamiltonian $\mathcal{H}$. Note that $\mathcal{H}$ and $\tilde{\mathcal{H}}$ are connected by a unitary transformation. Therefore, the expectation values can also be evaluated from the free energy formed with $\tilde{\mathcal{H}}$. In particular, the relation

$$F = -\frac{1}{\beta} \ln \mathrm{Tr}\, e^{-\beta\mathcal{H}} = -\frac{1}{\beta} \ln \mathrm{Tr}\, e^{-\beta\tilde{\mathcal{H}}} =: \tilde{F}$$
$$= -\frac{2}{\beta} \sum_{\mathbf{k}} [\ln(1 + e^{-\beta\tilde{\varepsilon}_{\mathbf{k}}}) + \ln(1 + e^{-\beta\tilde{\omega}_{\mathbf{k}}})] + \tilde{E}$$

holds. Following the analysis of Ref. [31], one finds by functional derivative

$$\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle = \tfrac{1}{2}(1 + \Gamma_{\mathbf{k}}) f(\tilde{\varepsilon}_{\mathbf{k}}) + \tfrac{1}{2}(1 - \Gamma_{\mathbf{k}}) f(\tilde{\omega}_{\mathbf{k}}) \tag{46}$$

and

$$\langle \hat{n}_\sigma^f \rangle = \frac{1}{2N} \sum_{\mathbf{k}} (1 - \Gamma_{\mathbf{k}}) f(\tilde{\varepsilon}_{\mathbf{k}}) + \frac{1}{2N} \sum_{\mathbf{k}} (1 + \Gamma_{\mathbf{k}}) f(\tilde{\omega}_{\mathbf{k}}), \tag{47}$$

where $\Gamma_{\mathbf{k}} = \mathrm{sgn}(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k},\Lambda})(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k},\Lambda})/W_{\mathbf{k}}$. In addition, a self-consistent equation for the yet unknown renormalized $f$ level $\tilde{\varepsilon_f}$ can be found,

$$\tilde{\varepsilon}_f - \varepsilon_f = \frac{1}{N} \sum_{\mathbf{k}} \mathrm{sgn}(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}) \frac{|V_{\mathbf{k}}|^2 [f(\tilde{\varepsilon}_{\mathbf{k}}) + f(\tilde{\omega}_{\mathbf{k}})]}{W_{\mathbf{k}}}.$$

For later use, we need the decomposition of the renormalized one-particle operators $c_{\mathbf{k}\sigma}^\dagger(\lambda \to 0)$ and $\hat{f}_{\mathbf{k}\sigma}^\dagger(\lambda \to 0)$ into $c_{\mathbf{k}\sigma}^\dagger$ and $\hat{f}_{\mathbf{k}\sigma}^\dagger$. According to Eq. (27), we have

$$c_{\mathbf{k}\sigma}^\dagger(\lambda \to 0) = \tilde{x}_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger + \tilde{y}_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^\dagger,$$
$$\hat{f}_{\mathbf{k}\sigma}^\dagger(\lambda \to 0) = -D\tilde{y}_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger + \tilde{x}_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^\dagger. \tag{48}$$

Comparing with Eqs. (46) and (47) leads to

$$|\tilde{x}_{\mathbf{k}}|^2 = \frac{1 + \Gamma_{\mathbf{k}}}{2}, \quad |\tilde{y}_{\mathbf{k}}|^2 = \frac{1 - \Gamma_{\mathbf{k}}}{2D}.$$

### B. Superconducting parameters

In order to find analytical solutions for the renormalization equations (21)–(23), let us take advantage of the fact that the main renormalization occurs when both the $f$ band and the $c$ band are located close to the Fermi level. Suppose that for this case the renormalization of the excitation energies is already completed; the quantity $A_{\mathbf{k},\lambda}$, which governs the hybridization part (13) of the unitary transformation (12), may be replaced by $\tilde{A}_{\mathbf{k}} = A_{\mathbf{k},\lambda\to 0} = \tilde{\omega}_{\mathbf{k}} - \tilde{\varepsilon}_{\mathbf{k}}$. With

$$\tilde{\alpha}_{\mathbf{k},\lambda} \approx \frac{\tilde{A}_{\mathbf{k}} \theta(\lambda - |\tilde{A}_{\mathbf{k}}|)}{\kappa(\lambda - |\tilde{A}_{\mathbf{k}}|)^2} V_{\mathbf{k},\lambda}, \tag{49}$$

the differential equation (38) for $V_{\mathbf{k},\lambda}$ then leads to

$$V_{\mathbf{k},\lambda} = V \exp \frac{\tilde{A}_{\mathbf{k}}^2}{\kappa(\Lambda - |\tilde{A}_{\mathbf{k}}|)}.$$

Here, the constant $\kappa$ ensures that the exponent is dimensionless. The quantity $\tilde{\alpha}_{\mathbf{k},\lambda}$, thus, reads

$$\tilde{\alpha}_{\mathbf{k},\lambda} = \frac{V\theta(\lambda - |\tilde{A}_{\mathbf{k}}|)}{\tilde{A}_{\mathbf{k}}} \delta(\lambda - |\tilde{A}_{\mathbf{k}}|). \tag{50}$$

Note that $\tilde{\alpha}_{\mathbf{k},\lambda}$ as a function of $\lambda$ shows a peaklike behavior around $\lambda \approx \tilde{A}_{\mathbf{k}} = \tilde{\omega}_{\mathbf{k}} - \tilde{\varepsilon}_{\mathbf{k}}$. This peaklike structure is mostly pronounced for the lowest possible value of $\tilde{A}_{\mathbf{k}}$, i.e., close to the valence transition regime, when both $\tilde{\omega}_{\mathbf{k}}$ and $\tilde{\varepsilon}_{\mathbf{k}}$ are small. This feature of $\tilde{\alpha}_{\mathbf{k},\lambda}$ can be used for the integration of the renormalization Eqs. (21)–(23). For the superconducting gap functions one finds

$$\tilde{\Delta}_{\mathbf{k}}^{cc} = -\frac{2DV}{\tilde{A}_{\mathbf{k}}} \tilde{\Delta}_{\mathbf{k}}^{fc} + \frac{2V}{\tilde{A}_{\mathbf{k}}} \frac{1}{N} \sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{k}+\mathbf{q}} \langle \hat{f}_{-(\mathbf{k}+\mathbf{q}),\downarrow} c_{\mathbf{k}+\mathbf{q},\uparrow} \rangle, \tag{51}$$

$$\tilde{\Delta}_{\mathbf{k}}^{ff} = \frac{2V}{\tilde{A}_{\mathbf{k}}} \tilde{\Delta}_{\mathbf{k}}^{fc} - \frac{2V}{\tilde{A}_{\mathbf{k}}} \frac{1}{N} \sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{k}+\mathbf{q}} \langle \hat{f}_{-(\mathbf{k}+\mathbf{q}),\downarrow} c_{\mathbf{k}+\mathbf{q},\uparrow} \rangle, \tag{52}$$

$$\tilde{\Delta}_{\mathbf{k}}^{fc} = (\tilde{\Delta}_{\mathbf{k}}^{cc} - D\tilde{\Delta}_{\mathbf{k}}^{ff}) \frac{V}{\tilde{A}_{\mathbf{k}}} - \frac{V}{N} \sum_{\mathbf{q}} \frac{U'_{\mathbf{k},\mathbf{k}+\mathbf{q}}}{\tilde{A}_{\mathbf{k}+\mathbf{q}}} \times (\langle \hat{f}_{-(\mathbf{k}+\mathbf{q}),\downarrow} \hat{f}_{\mathbf{k}+\mathbf{q},\uparrow} \rangle - \langle c_{-(\mathbf{k}+\mathbf{q}),\downarrow} c_{\mathbf{k}+\mathbf{q},\uparrow} \rangle). \tag{53}$$

Here, we have used the relations $\tilde{\Delta}_{\mathbf{k}}^{fc} = \tilde{\Delta}_{\mathbf{k}}^{cf}$ and $\langle \hat{f}_{-(\mathbf{k}+\mathbf{q}),\downarrow} c_{\mathbf{k}+\mathbf{q},\uparrow} \rangle = \langle c_{-(\mathbf{k}+\mathbf{q}),\downarrow} \hat{f}_{\mathbf{k}+\mathbf{q},\uparrow} \rangle$ and the $\lambda$-independent terms reduced from $U_{\mathbf{k},\mathbf{k}+\mathbf{q},\lambda}$,

$$U_{\mathbf{k},\mathbf{k}+\mathbf{q}} \approx U_{fc}\, \theta(|\tilde{A}_{\mathbf{k}}| - |\tilde{B}_{\mathbf{k},\mathbf{k}+\mathbf{q}}|) \times \exp\left(-\frac{|\tilde{B}_{\mathbf{k},\mathbf{k}+\mathbf{q}}|^2}{\kappa(|\tilde{A}_{\mathbf{k}}| - |\tilde{B}_{\mathbf{k},\mathbf{k}+\mathbf{q}}|)}\right),$$
$$U'_{\mathbf{k},\mathbf{k}+\mathbf{q}} \approx U_{fc}\, \theta(|\tilde{A}_{\mathbf{k}+\mathbf{q}}| - |\tilde{B}_{\mathbf{k},\mathbf{k}+\mathbf{q}}|) \times \exp\left(-\frac{|\tilde{B}_{\mathbf{k},\mathbf{k}+\mathbf{q}}|^2}{\kappa(|\tilde{A}_{\mathbf{k}+\mathbf{q}}| - |\tilde{B}_{\mathbf{k},\mathbf{k}+\mathbf{q}}|)}\right). \tag{54}$$

Our aim is to find a closed set of equations for the gap functions $\tilde{\Delta}^{cc}_{\mathbf{k}}$, $\tilde{\Delta}^{ff}_{\mathbf{k}}$, and $\tilde{\Delta}^{fc}_{\mathbf{k}}$. Therefore, on the right-hand side of Eqs. (51)–(53), the superconducting pairing functions have to be expressed by the gap functions. In Eqs. (51)–(53) they are formed with the full Hamiltonian. Thus, using Eqs. (31) together with expressions (48) for $\tilde{x}_{\mathbf{k}}$ and $\tilde{y}_{\mathbf{k}}$, the pairing functions can first be written as linear combinations of pairing functions $\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}$, $\langle \hat{f}_{-\mathbf{k}\downarrow}\hat{f}_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}$, and $\langle \hat{f}_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}$, which are formed with $\tilde{\mathcal{H}}$. Finally, using Eq. (36) and similar expressions for the remaining superconducting pairing functions $\langle \hat{f}_{-\mathbf{k}\downarrow}\hat{f}_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}$ and $\langle \hat{f}_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}}$, one finds that in lowest order the latter pairing functions are directly proportional to the corresponding gap functions,

$$\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} = g_{1,\mathbf{k}}\tilde{\Delta}^{cc}_{\mathbf{k}}, \quad \langle \hat{f}_{-\mathbf{k}\downarrow}\hat{f}_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} = Dg_{2,\mathbf{k}}\tilde{\Delta}^{ff}_{\mathbf{k}},$$
$$\langle \hat{f}_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} = Dg_{3,\mathbf{k}}\tilde{\Delta}^{fc}_{\mathbf{k}}, \quad (55)$$

where

$$g_{i,\mathbf{k}} = \sum_{\pm}\frac{1-2f(\mathcal{E}^{\pm}_{\mathbf{k}})}{4\mathcal{E}^{\pm}_{\mathbf{k}}}(1 \pm \psi_{i,\mathbf{k}}). \quad (56)$$

Here, we have denoted $\psi_{1,\mathbf{k}} = -(u_{\mathbf{k}} - 2\tilde{\omega}^2_{\mathbf{k}})/\sqrt{\phi_{\mathbf{k}}}$, $\psi_{2,\mathbf{k}} = (u_{\mathbf{k}} - 2\tilde{\varepsilon}^2_{\mathbf{k}})/\sqrt{\phi_{\mathbf{k}}}$, and $\psi_{3,\mathbf{k}} = (u_{\mathbf{k}} - 2\tilde{\omega}_{\mathbf{k}}\tilde{\varepsilon})/\sqrt{\phi_{\mathbf{k}}}$. Taking together Eqs. (51)–(55), we have arrived at a closed set of equations for the gap functions $\tilde{\Delta}^{cc}_{\mathbf{k}}$, $\tilde{\Delta}^{ff}_{\mathbf{k}}$, and $\tilde{\Delta}^{fc}_{\mathbf{k}}$ which can numerically be evaluated for larger systems than was done by the original equations of the previous section.

### C. Numerical evaluation

In this subsection, we discuss our numerical results for the superconducting energy gaps for a large system by solving self-consistently Eqs. (51)–(53) with the analytical results of Eqs. (43) and (45) and Eqs. (46) and (47). This problem is done in two steps. In the first step, Eqs. (43) and (45) and Eqs. (46) and (47) are solved self-consistently by arbitrary initial choices for the expectation values $\langle n^c\rangle$ (density of the conduction electrons) and $\langle \hat{n}^f\rangle$ (density of the localized electrons). After a self-consistent solution is found, the obtained results are used to continue to solve Eqs. (51)–(53) self-consistently to obtain the superconducting energy gaps. In order to find $d$-wave superconductivity, we choose $\tilde{\Delta}^{\alpha\beta}_{k_xk_y} = A^{\alpha\beta}_0(\cos k_x - \cos k_y)$ (where $\alpha, \beta$ denote $c$ or $f$) as initial values of the superconducting energy gaps with amplitudes $2A^{\alpha\beta}_0$. The self-consistent procedure is stopped, when convergence is achieved. In the subsection, we keep the total occupation number of electrons $n = \langle n^c\rangle + \langle \hat{n}^f\rangle = 1.75$ and the dispersion relation of noninteracting conduction electrons $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ as used before. We set $2t = 1$ as a unit of energy in order to have the same bandwidth of the conduction electrons as in the one-dimensional case [25]. Therefore, the present results and the one-dimensional results, which have been discussed in the previous section, can be compared. A two-dimensional system with $N = 320 \times 320$ sites is investigated. The temperature is set to be very small, $T = 10^{-3}$. The former typical values, $U_{fc} = 1$, $V = 0.1$, and $n = 1.75$, are still kept.

At first, in Fig. 5 the dispersion relations of the two quasiparticle bands are shown for $\epsilon_f = -0.53$. The red (plus)

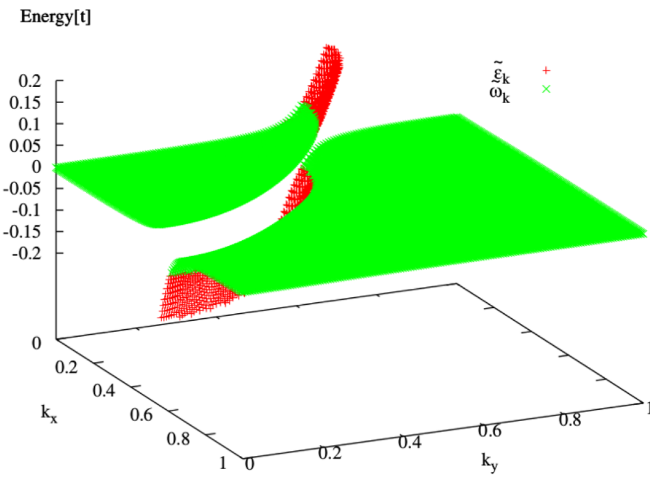


FIG. 5. Renormalized energies of the conduction electrons, $\tilde{\varepsilon}_{\mathbf{k}}$, and of the localized electrons, $\tilde{\omega}_{\mathbf{k}}$, as functions of momentum $\mathbf{k}$ in the first quarter of the Brillouin zone at $\epsilon_f = -0.53$ for $U_{fc} = 1$, $V = 0.1$, and $T = 10^{-3}$.

symbols are for $c$ electrons and the green (cross) symbols are for $f$ electrons. Because of the hybridization, each quasiparticle band has a jump at the crossover between $\tilde{\epsilon}_f$ and the unrenormalized $c$ dispersion $\varepsilon_{\mathbf{k},\Lambda}$. For $\epsilon_f = -0.53$, the jump is located close to the Fermi level in which both conduction and localized electrons contribute to the formation of the Fermi surface. This picture describes the situation at a valence fluctuation regime.

In addition to the result of the dispersion relations in Fig. 5, the result for the superconducting energy gap $\tilde{\Delta}^{ff}_{\mathbf{k}}$ is shown in Fig. 6 as function of momentum $\mathbf{k}$ in the first quarter of the Brillouin zone for the same parameters as in Fig. 5. Note

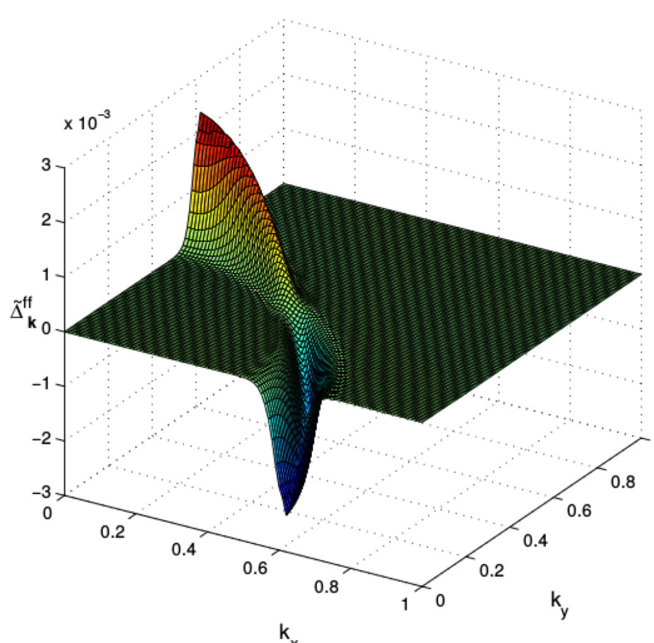


FIG. 6. Superconducting energy gap, $\tilde{\Delta}^{ff}_{\mathbf{k}}$, with $d_{x^2-y^2}$-wave symmetry as a function of momentum $\mathbf{k}$ in the first quarter of the Brillouin zone at $\epsilon_f = -0.53$ for $U_{fc} = 1$, $V = 0.1$, and $T = 10^{-3}$.

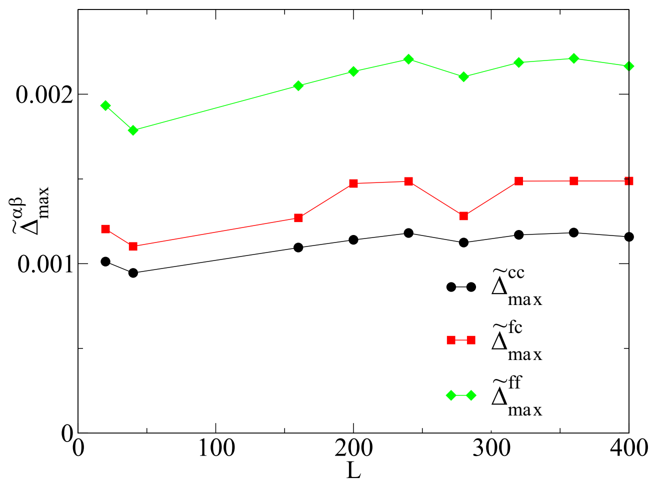


FIG. 7. Maximum value of the superconducting energy gaps as a function of $L$ for a two-dimensional system with $N = L \times L$ lattice sites at $\epsilon_f = -0.53$ for $U_{fc} = 1$, $V = 0.1$, and $T = 10^{-3}$.

that the nodes of $\tilde{\Delta}^{ff}_{\mathbf{k}}$ are right in the diagonal direction of the Brillouin zone and the relation $\tilde{\Delta}^{ff}_{k_x k_y} = -\tilde{\Delta}^{ff}_{k_y k_x}$ if fulfilled. Here the result is shown only for the superconducting energy gap built by the localized electrons. However, $d_{x^2-y^2}$ symmetry is also valid for the other possible superconducting energy gaps $\tilde{\Delta}^{cc}_{\mathbf{k}}$ and $\tilde{\Delta}^{fc}_{\mathbf{k}}$ as well as for the superconducting pairing functions $\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle$, $\langle c_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle$, and $\langle \hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle$. The maximum of the superconducting energy gap is located at the Fermi level which corresponds to the jump in the dispersion relation of the quasiparticle bands. In other words, the superconducting state is dominant in the valence transition regime, in which some $f$ electrons become delocalized. The maximum position of the superconducting energy gap is shifted in correspondence to the shift of the jump position of the quasiparticle bands in momentum space. This means that if the Fermi line is a square with the corners at $(\pm\pi, 0)$ and $(0, \pm\pi)$, the maximum of the superconducting energy gap is located in the vicinity of $(\pm\pi, 0)$ or $(0, \pm\pi)$, which follows from the initial choice of the $d_{x^2-y^2}$ symmetry for the superconducting energy gap in self-consistent iteration. Furthermore, note that the superconducting state is only found in a small region in the momentum space, where the value of the superconducting energy gap is large. Therefore, the assumption we have used in (50) is applicable. The nonmonotonic behavior in Fig. 6 of the superconducting energy gap as function of $\mathbf{k}$ is similar to that of the superconducting energy gap in the high-temperature superconductors, which might be mediated by magnetic fluctuations [33–36]. In the present study, the superconductivity is believed to be mediated by valence fluctuations.

By varying the number of lattice sites we have also examined the size effect of the superconducting energy gaps in our problem. For instance, the maximum values of $\tilde{\Delta}^{\alpha\beta}_{\mathbf{k}}$ ($\alpha$ and $\beta$ denote $c$ or $f$) are shown as functions of $L$ ($N = L \times L$) in Fig. 7 for the same parameters as in Figs. 5 and 6. For small $L$, the maximum of each superconducting energy gap first somewhat decreases and then slowly increases till it reaches a size-independent value as large $L$. Therefore, already a small system is able to mimic the thermodynamic limit.

## V. DISCUSSION OF THE RESULTS

Next, we want to discuss the origin of the superconducting pairing mechanism. First note that according to Fig. 1 the superconducting phase does not occur right at the valence transition regime but somewhat below. That is, superconductivity already sets in when the renormalized $f$ energy $\tilde{\varepsilon}_f$ is still located somewhat below the Fermi surface $\varepsilon_F$ and the $f$ level is still almost filled, $\langle \hat{n}^f\rangle \leqslant 1$. To understand this feature one first has to realize that the excitation spectrum for $\tilde{\varepsilon}_{\mathbf{k}}$ and $\tilde{\omega}_{\mathbf{k}}$ is dominated at the valence transition by a hybridization gap of order $V$. In the valence transition regime, $\tilde{\varepsilon}_f$ lies close to the Fermi energy and both $\tilde{\varepsilon}_f$ and $\varepsilon_F$ lie inside the hybridization gap. On the other hand, the superconducting energies $\mathcal{E}^+_{\mathbf{k}}$, $\mathcal{E}^-_{\mathbf{k}}$ would reduce to $|\tilde{\varepsilon}_{\mathbf{k}}|$ and $|\tilde{\omega}_{\mathbf{k}}|$ in the case of vanishing superconducting gaps $\tilde{\Delta}^{\alpha\beta}_{\mathbf{k}}$. Thus, no superconducting excitations become important for $\mathbf{k}$ values close to the hybridization gap since $\tilde{A}_{\mathbf{k}} = \tilde{\omega}_{\mathbf{k}} - \tilde{\varepsilon}_{\mathbf{k}} \sim O(V)$ would be too large. The situation becomes different when $\tilde{\varepsilon}_f$ lies somewhat below the Fermi surface. In this case, the superconducting excitation energy $\mathcal{E}^-_{\mathbf{k}} \approx \sqrt{\tilde{\omega}^2_{\mathbf{k}} + O(\tilde{\Delta}^{\alpha\beta}_{\mathbf{k}})^2}$ reduces to a gap energy of order $|\tilde{\Delta}^{\alpha\beta}_{\mathbf{k}}|$ for the Fermi wavevector $k_F$ where $\tilde{\omega}_{\mathbf{k}}$ vanishes, which is close to the hybridization gap.

To find a superconducting gap equation for this case, let us approximate the weights in Eq. (48) as follows: $\tilde{x}_{\mathbf{k}} \approx 1$ and $\tilde{y}_{\mathbf{k}} \approx 0$ for $\mathbf{k}$ close to $k_F$. This follows from the fact that valence transitions are yet not dominant in this regime. Thus according to Eqs. (32) the superconducting pairing function formed with the full Hamiltonian $\mathcal{H}$ can be approximated by

$$\begin{aligned}
\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle &= \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}}\uparrow\rangle_{\tilde{\mathcal{H}}} = g_{1,\mathbf{k}} \tilde{\Delta}^{cc}_{\mathbf{k}},\\
\langle \hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle &= \langle \hat{f}_{-\mathbf{k}\downarrow} \hat{f}_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} = D g_{2,\mathbf{k}} \tilde{\Delta}^{ff}_{\mathbf{k}},\\
\langle \hat{f}_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle &= \langle \hat{f}_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}\rangle_{\tilde{\mathcal{H}}} = D g_{3,\mathbf{k}} \tilde{\Delta}^{fc}_{\mathbf{k}}.
\end{aligned} \tag{57}$$

With Eqs. (57) the relations (51)–(53) for the superconducting gap functions reduce to

$$\tilde{\Delta}^{cc}_{\mathbf{k}} = -\frac{2DV}{\tilde{A}_{\mathbf{k}}}\left(\tilde{\Delta}^{fc}_{\mathbf{k}} - \frac{1}{N}\sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{k}+\mathbf{q}} g_{3,\mathbf{k}+\mathbf{q}} \tilde{\Delta}^{fc}_{\mathbf{k}+\mathbf{q}}\right), \tag{58}$$

$$\tilde{\Delta}^{ff}_{\mathbf{k}} = \frac{2V}{\tilde{A}_{\mathbf{k}}}\left(\tilde{\Delta}^{fc}_{\mathbf{k}} - \frac{D}{N}\sum_{\mathbf{q}} U_{\mathbf{k},\mathbf{k}+\mathbf{q}} g_{3,\mathbf{k}+\mathbf{q}} \tilde{\Delta}^{fc}_{\mathbf{k}+\mathbf{q}}\right), \tag{59}$$

$$\begin{aligned}
\tilde{\Delta}^{fc}_{\mathbf{k}} &= \frac{V}{\tilde{A}_{\mathbf{k}}}\left(\tilde{\Delta}^{cc}_{\mathbf{k}} - D\tilde{\Delta}^{ff}_{\mathbf{k}}\right)\\
&\quad - \frac{V}{N}\sum_{\mathbf{q}} \frac{U'_{\mathbf{k},\mathbf{k}+\mathbf{q}}}{\tilde{A}_{\mathbf{k}+\mathbf{q}}}\left(D g_{2,\mathbf{k}+\mathbf{q}} \tilde{\Delta}^{ff}_{\mathbf{k}+\mathbf{q}} - g_{1,\mathbf{k}+\mathbf{q}} \tilde{\Delta}^{cc}_{\mathbf{k}+\mathbf{q}}\right).
\end{aligned} \tag{60}$$

From Eqs. (58) and (59) we can eliminate the prefactor $(\tilde{\Delta}^{cc}_{\mathbf{k}} - D\tilde{\Delta}^{ff}_{\mathbf{k}})$ in Eq. (60) and arrive at

$$\begin{aligned}
\tilde{\Delta}^{fc}_{\mathbf{k}} = \frac{1}{R_{\mathbf{k}} N}\sum_{\mathbf{q}} \Bigg[&\frac{2V^2 D(1+D)}{\tilde{A}^2_{\mathbf{k}}} U_{\mathbf{k},\mathbf{k}+\mathbf{q}} g_{3,\mathbf{k}+\mathbf{q}} \tilde{\Delta}^{fc}_{\mathbf{k}+\mathbf{q}}\\
&- \frac{V}{\tilde{A}_{\mathbf{k}+\mathbf{q}}} U'_{\mathbf{k},\mathbf{k}+\mathbf{q}}\left(D g_{2,\mathbf{k}+\mathbf{q}} \tilde{\Delta}^{ff}_{\mathbf{k}+\mathbf{q}} - g_{1,\mathbf{k}+\mathbf{q}} \tilde{\Delta}^{cc}_{\mathbf{k}+\mathbf{q}}\right)\Bigg],
\end{aligned} \tag{61}$$

where $R_{\mathbf{k}} = 1 + 4DV^2/\tilde{A}^2_{\mathbf{k}}$. Using $\tilde{\varepsilon}^2_{\mathbf{k}} > \tilde{\omega}^2_{\mathbf{k}}$ and $\mathcal{E}^-_{\mathbf{k}} \sim O(|\tilde{\Delta}^{\alpha\beta}_{\mathbf{k}}|)$ for $\mathbf{k} \approx k_F$, one easily finds that the relations $g_{2,\mathbf{k}} \gg$

$g_{1,\mathbf{k}}$ and $g_{2,\mathbf{k}} \gg g_{3,\mathbf{k}}$ are always fulfilled. In this case, we have $g_{2,\mathbf{k}} \approx [1 - 2f(\mathcal{E}_{\mathbf{k}}^{-})]/2\mathcal{E}_{\mathbf{k}}^{-}$. This simplifies Eq. (61); thus

$$\tilde{\Delta}_{\mathbf{k}}^{fc} = -\frac{DV}{R_{\mathbf{k}}N}\sum_{\mathbf{q}}\frac{U'_{\mathbf{k},\mathbf{k+q}}}{\tilde{A}_{\mathbf{k+q}}}g_{2,\mathbf{k+q}}\tilde{\Delta}_{\mathbf{k+q}}^{ff}. \tag{62}$$

We then arrive at

$$\tilde{\Delta}_{\mathbf{k}}^{ff} = -\frac{2DV^2}{\tilde{A}_{\mathbf{k}}R_{\mathbf{k}}N}\sum_{\mathbf{q}}\frac{U'_{\mathbf{k},\mathbf{k+q}}}{\tilde{A}_{\mathbf{k+q}}}g_{2,\mathbf{k+q}}\tilde{\Delta}_{\mathbf{k+q}}^{ff} \tag{63}$$

and

$$\tilde{\Delta}_{\mathbf{k}}^{cc} = \frac{2D^2V}{\tilde{A}_{\mathbf{k}}R_{\mathbf{k}}N}\sum_{\mathbf{q}}\frac{U'_{\mathbf{k},\mathbf{k+q}}}{\tilde{A}_{\mathbf{k+q}}}g_{2,\mathbf{k+q}}\tilde{\Delta}_{\mathbf{k+q}}^{ff}. \tag{64}$$

Note that Eq. (63) is a gap equation for the gap function $\tilde{\Delta}_{\mathbf{k}}^{ff}$ for the $f$ electrons. This makes sense since the effective $f$ dispersion $\tilde{\omega}_{\mathbf{k}}$ is crossing the Fermi surface leading to the superconducting transition. Comparing Eqs. (62)–(64), one finds the following very simple relations:

$$\tilde{\Delta}_{\mathbf{k}}^{fc} = \frac{\tilde{A}_{\mathbf{k}}}{2V}\tilde{\Delta}_{\mathbf{k}}^{ff}, \quad \tilde{\Delta}_{\mathbf{k}}^{cc} = -D\tilde{\Delta}_{\mathbf{k}}^{ff}. \tag{65}$$

With $D = 1 - \langle n^f \rangle/2 \approx 1/2$ and $\tilde{A}_{\mathbf{k}} \sim O(V)$ one immediately sees that the absolute values of $\tilde{\Delta}_{\mathbf{k}}^{fc}$ and $\tilde{\Delta}_{\mathbf{k}}^{cc}$ are approximately half of that of $\tilde{\Delta}_{\mathbf{k}}^{ff}$. This seems to be in nice agreement with the numerical results in Fig. 7.

To discuss the superconducting feature mediated by the valence fluctuations in the study, we rewrite Eq. (63) in the following form,

$$\tilde{\Delta}_{\mathbf{k}}^{ff} = -\frac{1}{N}\sum_{\mathbf{q}}V_{\mathbf{k},\mathbf{k+q}}^{\text{eff}}g_{2,\mathbf{k+q}}\tilde{\Delta}_{\mathbf{k+q}}^{ff}, \tag{66}$$

where

$$V_{\mathbf{k},\mathbf{k+q}}^{\text{eff}} = \frac{2DV^2U'_{\mathbf{k},\mathbf{k+q}}}{\tilde{A}_{\mathbf{k}}\tilde{A}_{\mathbf{k+q}}R_{\mathbf{k}}} \tag{67}$$

plays a role of the effective two-particle pairing interaction. Equation (66) looks similar to the BCS-type self-consistent equation for the superconducting order parameter in momentum space. $V_{\mathbf{k},\mathbf{k+q}}^{\text{eff}}$ becomes dominant if $U'_{\mathbf{k},\mathbf{k+q}}$ is large and $\tilde{A}_{\mathbf{k}}\tilde{A}_{\mathbf{k+q}}R_{\mathbf{k}}$ is small. The former situation happens if the Coulomb interaction between the localized electrons and conduction electrons is large leading to the sharp valence fluctuation, whereas the latter corresponds to the small values of $\tilde{A}_{\mathbf{k}}$, i.e., at the momentum at which both quasiparticle bands are located close to the Fermi level and close to each other, or in the valence fluctuation regime. The superconducting phase, therefore, appears and becomes enhanced due to the strong valence fluctuations. Moreover, $V_{\mathbf{k},\mathbf{k+q}}^{\text{eff}}$ in Eq. (67) is strongly dependent on momentum; a $d$-wave symmetrical solution for the superconducting energy gap in momentum space, thus, is stabilized [37].

## VI. CONCLUSION

To conclude, we have discussed the possibility of superconductivity which is induced by enhanced valence fluctuations in the Ce-based heavy-fermion systems under high pressure. The enhancement of the valence fluctuations is modeled by including a Coulomb repulsion term between the conduction and the localized electrons in the periodic Anderson model (PAM). This two-dimensional extended PAM (EPAM) is investigated by a recently developed projector-based renormalization method (PRM). In order to apply the PRM to the superconducting state, small gauge-symmetry-breaking fields are included in the EPAM. The renormalized Hamiltonian of the EPAM in the superconducting state is found. After being diagonalized by the use of the Bogoliubov method, this Hamiltonian allows determining the superconducting pairing functions of all possible Cooper pairs. By the use of some additional simplifications, a BCS-like equation is found. The resulting effective pairing interaction depends strongly on momentum and becomes dominant in the valence transition regime. Our numerical evaluation verifies that superconductivity in the heavy-fermion systems has a $d$-wave character and is mediated by valence fluctuations.


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