Solution for the U-negative Hubbard superconductor including second-order correlation effects

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We analyze the effects of fluctuations on the gap and critical temperature of a superconductor. The model Hamiltonian chosen is one of the simplest: the U-negative Hubbard model. A diagrammatic self-consistent approach is used, and a second-order self-energy is calculated in order to take into account local fluctuations. Our results show a decrease of the superconductor gap and critical temperature with respect to the mean-field solution. The ratio $2\Delta/k_B T_c$ is not modified, however, by the local fluctuations if the self-energy matrix in a site representation extends only to the lattice nearest neighbors. In this approximation, the superconductor gap is found to be constant along the Fermi surface. Further nearest-neighbor interactions introduce a superconductor gap that changes along this surface.

I. INTRODUCTION

The appearance of high-T_c superconductors[1,2] has renewed the general interest in superconductivity. The mechanism leading to the Cooper pair formation[3-5] (electron-phonon or electron-electron interactions), and the role played by magnetism in these compounds are not yet clear. In a phenomenological approach, different model Hamiltonians have been proposed.[6,7] The aim of this work is to explore one of the simplest of these phenomenological Hamiltonians (the U-negative Hubbard model), analyzing the electronic properties beyond the mean-field approximation. The interest of this analysis is suggested by the strong electron-electron (e-e) coupling shown by these high-T_c superconductors. In particular, the coherence length is rather small in these materials, $\xi \sim 10-20$ Å, and comparable to the e-e distance. One may expect that in these conditions, corrections to the mean-field solution could be non-negligible, and that quantum fluctuations may play a role in the superconducting properties of the materials.

We have chosen to analyze the U-negative Hubbard Hamiltonian, but a more general case could be discussed following the same ideas developed below. In particular, we argue that our results have a more general validity and can be extended to other, more complex, Hamiltonians.

In Sec. II, we begin by reviewing the mean-field solution of this Hamiltonian, introducing, subsequently, correlation effects through the inclusion of the second-order self-energy, calculated using a self-consistent perturbative approach. In Sec. III we analyze the effects of fluctuations on the gap and critical temperature, using a local approximation for the proper self-energy. The rather cumbersome calculation of the second-order self-energy has been included in Appendix A.

Finally, we have checked the correctness of our self-consistent perturbative approach, by evaluating the total energy of the superconductor up to $O(U^2)$, as given by our calculation. It is shown in Appendix B that this expression coincides exactly with the second-order expansion of the energy calculated in Ref. 15.

II. SECOND-ORDER PERTURBATIVE SOLUTION OF THE U-NEGATIVE HUBBARD SUPERCONDUCTOR

We start from the U-negative Hubbard Hamiltonian:

$$\hat{H}=\sum_{i,\sigma}(\epsilon_0-\mu)\hat{n}_{i\sigma}+\sum_{i\neq j,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}+U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\ , \tag{1}$$

where indices i and j run over all atomic positions of the system. The hopping parameters are $t_{ij}=t$ for nearest neighbor and zero otherwise, and we take $U=-|U|$. As we will be interested in working with a variable number of particles, the usual term depending on the chemical potential, μ, is included. A very complete and up to date review on the problematic of this Hamiltonian can be found in Ref. 8.

The superconducting solution of Hamiltonian (1) has been obtained using a mean-field approximation.[8] Our purpose in this paper is to go beyond, including correlation effects up to second order in a self-consistent perturbation theory. We will concentrate in studying the trends of the superconductor gap Δ and the critical temperature T_c, as the effects of fluctuations are included. Moreover, we will only consider the situation in which Δ is much less than the bandwidth. Therefore, our results will not be valid, in principle, in the strong-coupling regime.

It is convenient to make a change in Hamiltonian (1), from a localized basis to a Bloch one (the one which diagonalizes the one-electron part of the Hamiltonian):

$$\hat{H}=\sum_{\mathbf{k},\sigma}(\epsilon_{\mathbf{k}}-\mu)\hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}-\frac{|U|}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q},\uparrow}\hat{c}_{\mathbf{k},\uparrow}\hat{c}^{\dagger}_{\mathbf{k}'-\mathbf{q},\downarrow}\hat{c}_{\mathbf{k}',\downarrow}\ . \tag{2}$$

As is well known, the mean-field solution of Hamiltonian (2) can be obtained from first-order self-consistent perturbation theory.[10,11] In order to introduce the formalism that will be used throughout the paper, we review, briefly, this mean-field solution. Using the Nambu formalism,[11-13] we introduce the following 2×2 Matsubara matrix propagator:

$$\hat{G}(\mathbf{k},\tau)=\begin{bmatrix} G(\mathbf{k},\tau) & F(\mathbf{k},\tau) \\ F^{\dagger}(\mathbf{k},\tau) & G'(\mathbf{k},\tau) \end{bmatrix} , \tag{3}$$

where

$$G(\mathbf{k},\tau)=G_{11}(\mathbf{k},\tau)=-\langle \hat{T}_{\tau}[\hat{c}_{\mathbf{k}\uparrow}(\tau)\hat{c}^{\dagger}_{\mathbf{k}\uparrow}(0)]\rangle , \tag{4}$$

$$F(\mathbf{k},\tau)=G_{12}(\mathbf{k},\tau)=-\langle \hat{T}_{\tau}[\hat{c}_{\mathbf{k}\uparrow}(\tau)\hat{c}_{-\mathbf{k}\downarrow}(0)]\rangle , \tag{5}$$

$$F^{\dagger}(\mathbf{k},\tau)=G_{21}(\mathbf{k},\tau)=-\langle \hat{T}_{\tau}[\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}(\tau)\hat{c}^{\dagger}_{\mathbf{k}\uparrow}(0)]\rangle , \tag{6}$$

$$G'(\mathbf{k},\tau)=G_{22}(\mathbf{k},\tau)=-\langle \hat{T}_{\tau}[\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}(\tau)\hat{c}_{-\mathbf{k}\downarrow}(0)]\rangle , \tag{7}$$

which correspond, respectively, to propagation of electrons, annihilation and creation of electron pairs, and propagation of holes.

In Fig. 1 is shown the graphical convention used to represent the Matsubara frequency-dependent propagators, corresponding to the ones defined in Eqs. (4)–(7). These four propagators are not wholly independent; $F(\mathbf{k},\omega_n)=F^{\dagger}(\mathbf{k},\omega_n)$, and $G'(\mathbf{k},\omega_n)=-G(-\mathbf{k},-\omega_n)$.

In self-consistent perturbation theory one solves the matrix Dyson equation to any desired order of the perturbation

$$\hat{G}=\hat{G}^{(0)}+\hat{G}^{(0)}\hat{\Sigma}\hat{G} , \tag{8}$$

where the proper self-energy matrix $\hat{\Sigma}$, is calculated using the full matrix propagator $\hat{G}$, which is then determined in a self-consistent way.[10–12]. $\hat{G}^{(0)}$ represents the unperturbed propagators and has therefore the off-diagonal elements equal to zero.

To first order in the interaction we have two coupled equations for $G(\mathbf{k},\omega_n)$ and $F^{\dagger}(\mathbf{k},\omega_n)$ [see Figs. 2(a) and 2(b)]. These equations can be written in the following algebraic form:

$$(i\omega_n-\epsilon_{\mathbf{k}}+\mu)G(\mathbf{k},\omega_n)=1+\Sigma_{11}G(\mathbf{k},\omega_n)+\Sigma_{12}F^{\dagger}(\mathbf{k},\omega_n) , \tag{9}$$

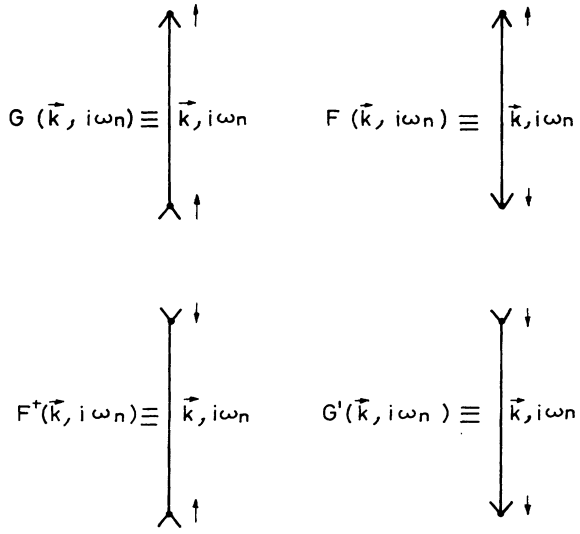

FIG. 1. Graphical convention used to represent the propagators $G(\mathbf{k},\omega_n)$, $F(\mathbf{k},\omega_n)$, $F^{\dagger}(\mathbf{k},\omega_n)$, and $G'(\mathbf{k},\omega_n)$.

$$(i\omega_n+\epsilon_{\mathbf{k}}-\mu)F^{\dagger}(\mathbf{k},\omega_n)=\Sigma_{21}G(\mathbf{k},\omega_n)+\Sigma_{22}F^{\dagger}(\mathbf{k},\omega_n) . \tag{10}$$

The diagonal self-energy [see Fig. 2(c)], can be dealt with as a simple renormalization of the diagonal level:

$$\epsilon_{\mathbf{k}}+\text{Hartree term}-\mu\equiv\tilde{\epsilon}_{\mathbf{k}} . \tag{11}$$

The off-diagonal self-energy Σ_{12} will provide the gap equation and can be calculated from the diagram represented in Fig. 2(d):

$$\Sigma_{12}=-\frac{|U|}{N\beta}\sum_{\nu_n,\mathbf{q}}F^{\dagger}(\mathbf{k}-\mathbf{q},\omega_n-\nu_n) . \tag{12}$$

Equations (9), (10), and (12) have the self-consistent solution:

$$\Sigma_{12}=\Sigma_{21}=-\Delta=\text{const} \tag{13}$$

and

$$G(\mathbf{k},\omega_n)=\frac{u_{\mathbf{k}}^2}{i\omega_n-E_{\mathbf{k}}}+\frac{v_{\mathbf{k}}^2}{i\omega_n+E_{\mathbf{k}}} , \tag{14}$$

$$F^{\dagger}(\mathbf{k},\omega_n)=-u_{\mathbf{k}}v_{\mathbf{k}}\left[\frac{1}{i\omega_n-E_{\mathbf{k}}}-\frac{1}{i\omega_n+E_{\mathbf{k}}}\right] , \tag{15}$$

where

$$E_{\mathbf{k}}=\sqrt{\tilde{\epsilon}_{\mathbf{k}}^2+\Delta^2} , \tag{16}$$

$$u_{\mathbf{k}}^2=1-v_{\mathbf{k}}^2=\frac{1}{2}\left[1+\frac{\tilde{\epsilon}_{\mathbf{k}}}{E_{\mathbf{k}}}\right] , \tag{17}$$

$$u_{\mathbf{k}}v_{\mathbf{k}}=\frac{\Delta}{2E_{\mathbf{k}}} . \tag{18}$$

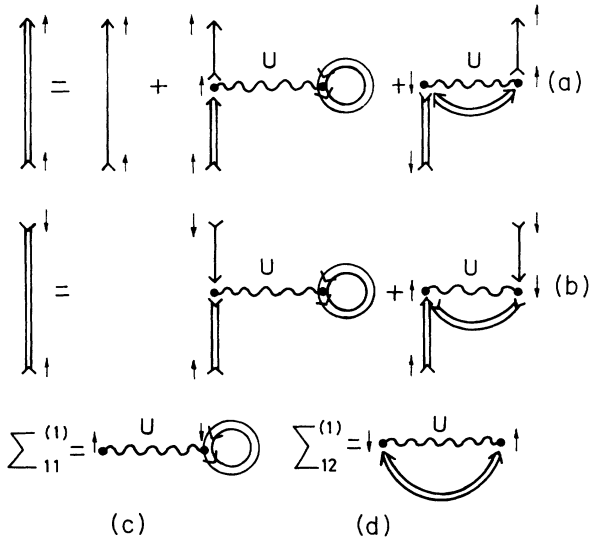

FIG. 2. Diagrams contributing to the first-order proper self-energy. Double and single lines represent, respectively, dressed and undressed propagators. (a) Dyson equation for the propagator $G(\mathbf{k},\omega_n)$. (b) Dyson equation for $F^{\dagger}(\mathbf{k}\omega_n)$. (c) First-order diagonal self-energy. (d) First-order nondiagonal self-energy.

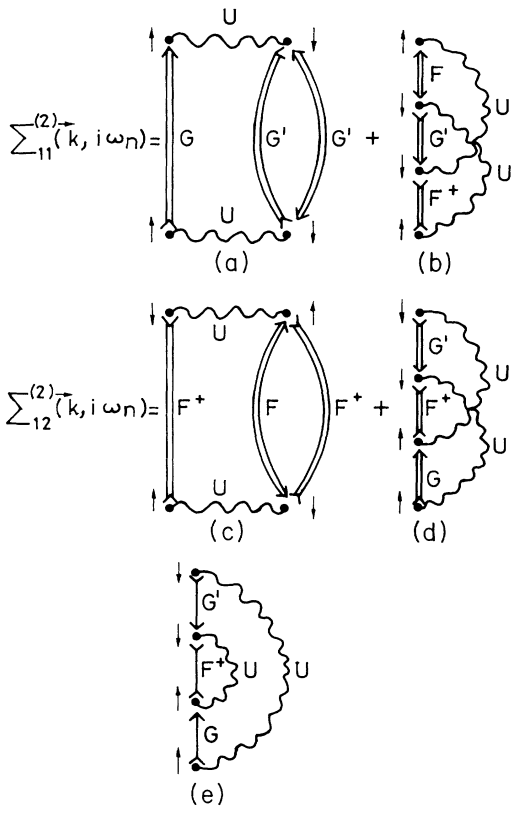

FIG. 3. Different contributions to the second-order proper self-energy (see the text).

We will discuss further the gap equation [that can be obtained straightforwardly from Eqs. (12) and (13)], and its solution in Sec. III.

Let us explore now the possibility of going beyond this mean-field solution, by calculating higher-order terms in the diagrammatic expansion of the proper self-energy. In this paper we will consider the effect of second-order corrections.

In Fig. 3 these second-order diagrams of the proper self-energy are drawn. Diagrams in Figs. 3(a) and 3(b) are the ones contributing to the diagonal self-energy $\Sigma_{11}^{(2)}(\mathbf{k},\omega_n)$ and in Figs. 3(c) and 3(d) to the nondiagonal self-energy $\Sigma_{12}^{(2)}(\mathbf{k},\omega_n)$. Other second-order diagrams, like the one represented in Fig. 3(e), can be ruled out because they are taken into account when using dressed propagators.

The exact expressions of these four diagrams are given in Appendix A. We are interested, however, in a situation where $\Delta \ll B$ (B being the bandwidth), and the following approximations can be made in this limit.

First, we neglect dynamical corrections in the evaluation of the gap and critical temperature, taking the limit $\omega_n \to 0$ in the calculation of the self-energy diagrams. Obviously, this would not be correct in the strong-coupling regime where dynamical corrections should be included.

Within this approximation, the diagram in Fig. 3(a), which is the only one that survives in the normal phase, tends to a constant value (zero in the half-filled band case), and plays a negligible role in the gap and critical temperature, simply renormalizing the level $\epsilon_{\mathbf{k}}$. On the other hand, the remaining three diagrams tend to a nonzero constant value. We can see, however, that the diagram of Fig. 3(b), which contains two anomalous propagators (anomalous in the sense of being absent in the normal phase), F and $F^{\dagger}$, must be of order $\sim\Delta^2$. For the same reason the diagram in Fig. 3(c) is of order $\sim\Delta^3$. It is clear, therefore, that the leading correction in the limit of the small gap parameter, Δ, is given by the diagram represented in Fig. 3(d), contributing to the nondiagonal self-energy, and which is obviously of order $\sim\Delta$. It must be remembered that this neglect of terms of order greater than the leading one is the usual procedure for obtaining, for instance, the gap equation in the mean-field approximation.

We are left, then, with the diagram in Fig. 3(d). Therefore, we approximate the full off-diagonal self-energy $\Sigma_{12}^{(2)}(\mathbf{k},\omega_n)$ by this diagram. Details of the evaluation of the temperature-dependent $\Sigma_{12}^{(2)}$ are given in the Appendix.

Let us comment that a self-consistent second-order solution to the Dyson equation (8) can be obtained using as an ansatz, expressions for the dressed propagators G and $F^{\dagger}$ formally identical to the BCS ones, Eqs. (14) and (15), the only difference being the appearance of a $\mathbf{k}$ dependence on the gap due, obviously, to the $\mathbf{k}$ dependence of $\Sigma_{12}^{(2)}(\mathbf{k},\omega_n)$. Therefore, we will use Eqs. (14)–(18) for the evaluation of the diagram with the substitution of Δ for $\Delta(\mathbf{k})$. It is important to stress that this procedure does not imply our "forcing" the self-consistent solution for the propagators G and $F^{\dagger}$ to be BCS-like. As a matter of fact, the inclusion of a self-energy will always give a self-consistent expression for G and $F^{\dagger}$ formally similar to the one given by Eqs. (14)–(18) [with the above substitution of Δ by $\Delta(\mathbf{k})$], provided we can neglect the frequency dependence of $\Sigma^{(2)}(\mathbf{k},\omega_n)$. As commented above, approximating $\Sigma^{(2)}(\mathbf{k},\omega_n)$ by its value at $\omega_n=0$ is reasonable, as we are only interested in evaluating the gap parameters and the critical temperature, and we are in a regime where $\Delta, T_c \ll B$.

Equation (A17) in the Appendix gives our final results for $\Sigma_{12}^{(2)}(\mathbf{R},\omega_n=0)$ (the second-order self-energy matrix elements in a site representation, $\mathbf{R}$ being any vector of the direct lattice), as a function of $\Delta(\mathbf{k})$, the superconducting gap, a quantity depending itself on $\Sigma_{12}^{(2)}$.

We will use the following shorthand notation:

$$\Sigma_{12}^{(2)}(\mathbf{R},\omega_n=0)=\Sigma_{12}^{(2)}(\mathbf{R}) , \tag{19}$$

$$\Sigma_{12}^{(2)}(\mathbf{k},\omega_n=0)=\Sigma_{12}^{(2)}(\mathbf{k}) . \tag{20}$$

Both expressions are related by

$$\Sigma_{12}^{(2)}(\mathbf{k})=\sum_{\mathbf{R}}\Sigma_{12}^{(2)}(\mathbf{R})e^{i\mathbf{k}\cdot\mathbf{R}} . \tag{21}$$

We can write, now, the self-consistent equation for $\Delta(\mathbf{k})$ as

$$\Delta(\mathbf{k})=-\Sigma_{12}(\mathbf{k}) , \tag{22}$$

where $\Sigma_{12}(\mathbf{k})$ represents the sum of the first- and second-order contributions:

$$\Sigma_{12}(\mathbf{k})=\Sigma_{12}^{(1)}(\mathbf{k})+\Sigma_{12}^{(2)}(\mathbf{k}) . \tag{23}$$

For our purposes it is more convenient to express the self-consistent condition, Eq. (22), using the site representation. Then writing $\Delta(\mathbf{k})$ as

$$\Delta(\mathbf{k})=\Delta_0+\sum_{\mathbf{R}\neq 0}\Delta(\mathbf{R})e^{i\mathbf{k}\cdot\mathbf{R}} , \tag{24}$$

we have the following self-consistent equations:

$$-\Delta_0=\Sigma_{12}^{(1)}+\Sigma_{12}^{(2)}(\mathbf{R}=0) , \tag{25}$$

$$-\Delta(\mathbf{R})=\Sigma_{12}^{(2)}(\mathbf{R}\neq 0) . \tag{26}$$

Equations (25) and (26) provide a system with an infinite number of equations which must be trunctated in some way. For instance, retaining only Eq. (25) is equivalent to taking a local approximation for the self-energy, giving a gap with no $\mathbf{k}$ dependence. A better approximation and, probably, a very reasonable one in most situations, will involve using nearest neighbors in Eq. (26). For instance, for the two-dimensional (2D) square lattice, we will have

$$\Sigma_{12}=\Sigma_{12}^{(1)}+\Sigma_{12}^{(2)}(\mathbf{R}=0) +2\Sigma_{12}^{(2)}(\mathbf{R}_1)[\cos(k_x a)+\cos(k_y a)] . \tag{27}$$

were $\mathbf{R}_1$=nearest-neighbor vector, and a is the lattice constant. Accordingly, we introduce the following $\Delta(\mathbf{k})$ function:

$$\Delta(\mathbf{k})=\Delta_0+2\Delta_1[\cos(k_x a)+\cos(k_y a)] \tag{28}$$

and write down the following equations of consistency:

$$-\Delta_0=\Sigma_{12}^{(1)}+\Sigma_{12}^{(2)}(\mathbf{R}=0) , \tag{29}$$

$$-\Delta_1=\Sigma_{12}^{(2)}(\mathbf{R}_1) . \tag{30}$$

III. THE SUPERCONDUCTOR GAP AND THE CRITICAL TEMPERATURE

We will discuss now the main results of our calculation. Let us consider first the mean-field solution, introduced in Sec. II.

The self-consistent Eq. (13) leads us to the well-known gap equation:

$$1=\frac{|U|}{2}\int_{-\infty}^{\infty}\frac{\tanh(\sqrt{\omega^2+\Delta^2}/2k_BT)\rho(\omega)}{\sqrt{\omega^2+\Delta^2}}d\omega , \tag{31}$$

where $\rho(\omega)$ is the unperturbed electronic density of states. The superconductor gap at $T=0$ is then easily obtained from

$$1=\frac{|U|}{2}\int_{-\infty}^{\infty}\frac{\rho(\omega)}{\sqrt{\omega^2+\Delta^2}}d\omega , \tag{32}$$

while the critical temperature T_c is given by

$$1=\frac{|U|}{2}\int_{-\infty}^{\infty}\frac{\tanh(|\omega|/2k_BT_c)\rho(\omega)}{|\omega|}d\omega . \tag{33}$$

From Eqs. (32) and (33) one can derive the well-known ratio

$$\frac{2\Delta}{k_BT_c}\simeq 3.53 \tag{34}$$

irrespective of the detailed form of $\rho(\omega)$. (Notice that this is due to the fact that both integrals diverge in the same way if Δ and k_BT_c go to zero, keeping $2\Delta/k_BT_c=3.53$.)

Let us turn now our attention to the effects of fluctuations on the gap and critical temperature, as introduced by our second-order calculation.

First, we will analyze the simplest case, approximating $\Sigma_{12}^{(2)}(\mathbf{k})$ by its local part:

$$\Sigma_{12}^{(2)}(\mathbf{k})\simeq\Sigma_{12}^{(2)}(\mathbf{R}=0) . \tag{35}$$

From Eq. (A17) in Appendix A, we have

$$\Sigma_{12}^{(2)}(\mathbf{R}=0) \simeq\beta\frac{U^2}{2}\Delta\int_{-\infty}^{\infty}\frac{\tanh(\sqrt{\omega^2+\Delta^2}/2k_BT)\rho(\omega)}{\sqrt{\omega^2+\Delta^2}}d\omega , \tag{36}$$

where β is defined as

$$\beta\equiv 2\int_{-\infty}^{\mu}d\epsilon_2\int_{\mu}^{\infty}d\epsilon_3\frac{\rho(\epsilon_2)\rho(\epsilon_3)}{|\epsilon_2|+|\epsilon_3|} . \tag{37}$$

Then, the self-consistent Eq. (25) gives the following gap equation:

$$1=\frac{|U'|}{2}\int_{-\infty}^{\infty}\frac{\tanh(\sqrt{\omega^2+\Delta^2}/2k_BT)\rho(\omega)}{\sqrt{\omega^2+\Delta^2}}d\omega , \tag{38}$$

where $U'=U+\beta U^2$.

The term $\Sigma_{12}^{(2)}(\mathbf{R}=0)$ in Eq. (25) has the opposite sign to the first-order term, $\Sigma_{12}^{(1)}$. As a result, Δ is smaller than the mean-field gap. Thus, we conclude that the second-order correction tends to decrease the superconductor gap. This effect is analogous to the decrease of the correlation gap in the U-positive Hubbard model when fluctuations are included, as should be expected, due to the mapping between the $U>0$ and $U<0$ models at half filling.[14]

The same can be said of T_c, which decreases too. The ratio $2\Delta/k_BT_c$ is not changed, however. This is understood by realizing that, whatever the form of $\rho(\omega)$ and $g(\omega)$, the integrals appearing in Eq. (38) give the same value for the case $T=0$ as for the case $T=T_c$, $\Delta=0$, if we take in both cases $2\Delta/k_BT_c=3.53$.

Let us comment now briefly on the effect of a nondiagonal nearest-neighbor self-energy in the self-consistent equations [see Eqs. (29) and (30)]. Let us consider, for the sake of simplicity, the case of the 2D square lattice discussed in Sec. II. Then, the energy dispersion for the electron band, with nearest-neighbor interactions, yields

$$\epsilon(\mathbf{k})=\epsilon_0+2t[\cos(k_x a)+\cos(k_y a)] . \quad (39)$$

This equation shows that $[\cos(k_x a)+\cos(k_y a)]$ is a constant at the Fermi surface. Then, we conclude that in the approximation we are considering [see Eq. (28)]

$$\Delta(\mathbf{k})=\Delta_0+\Delta_1\frac{\epsilon_F-\epsilon_0}{t} \quad (40)$$

ϵ_F being the Fermi energy.

As a result of this, with the inclusion of nearest-neighbor terms in the self-energy, the superconductor gap is still a constant and independent of $\mathbf{k}$. Moreover, following the argument given for the on-site approximation, it is easy to show that also in this case $2\Delta/k_B T_c \simeq 3.53$, although Δ and $k_B T_c$ are reduced somehow by the local-field effects associated with the nearest-neighbor self-energy. The inclusion of further terms in the site expansion of $\Sigma_{12}^{(2)}(\mathbf{k})$, beyond nearest neighbor will introduce some $\mathbf{k}$ dependence on the gap. One hopes these corrections to be negligible for a 3D system, but maybe they ought to be considered for a detailed calculation in the 2D case.

In order to analyze more specifically the previous results for the gap and the critical temperature, we present here some analytical and numerical results for a very simple case. To this end, we consider the most simple dependence for the unperturbed density of states:

$$\rho(\omega)=\begin{cases}1/B & \text{if } |\omega|<B/2\\ 0 & \text{otherwise} ,\end{cases} \quad (41)$$

where B is the bandwidth. We place the Fermi level at $\omega=0$, and approximate the second-order self-energy by its local part.

Then, Eq. (38) can be easily solved for the cases $T=0$, $\Delta\neq 0$, and $T=T_c$, $\Delta=0$. For $T=0$, we find

$$1=\frac{|U|}{B}\ln\left[\frac{B}{\Delta}\right]-2\ln(2)\left[\frac{U}{B}\right]^2\ln\left[\frac{B}{\Delta}\right] . \quad (42)$$

A comment should be made on the parameters of the model, B and U. Though it has no physical meaning to attempt any direct comparison between our results for Δ and T_c, and those of the actual systems, some fitting can be made for B and U, in order to get values of Δ and T_c not too far from the ones found in experiments for the high-T_c materials.

From Eq. (42), we have

$$\Delta\simeq Be^{-B/|U'|} \quad (43)$$

with

$$|U'|=|U|[1-2\ln(2)|U|/B] , \quad (44)$$

whereas the mean-field value is

$$\Delta\simeq Be^{-B/|U|} . \quad (45)$$

Obviously, as $|U'|<|U|$, there is a decrease in the gap. For $T=T_c$ and $\Delta=0$, we have

$$1=\frac{|U|}{B}\ln\left[\frac{Be^{\gamma}}{k_B T_c\pi}\right]-2\ln(2)\left[\frac{U}{B}\right]^2\ln\left[\frac{Be^{\gamma}}{k_B T_c\pi}\right] , \quad (46)$$

where γ is the Euler constant. This equation yields

$$k_B T_c\simeq\frac{e^{\gamma}}{\pi}Be^{-B/|U'|} . \quad (47)$$

So, the critical temperature enhancement with respect to its mean-field value:

$$k_B T_c\simeq\frac{e^{\gamma}}{\pi}Be^{-B/|U|} \quad (48)$$

is exactly the same as for the gap. Therefore, within this approximation, the ratio

$$\frac{2\Delta}{k_B T_c}=\frac{2\pi}{e^{\gamma}}\simeq 3.53 \quad (49)$$

is not changed with respect to its mean-field value, as it was discussed above.

For an estimation of the order of magnitude of this decrease, let us take $B=2$ eV and $U=0.40$ eV. We find from Eqs. (43) and (45)

$$2\Delta_{\mathrm{MF}}\simeq 0.0267 \text{ eV} , \quad (50)$$

$$2\Delta_{\mathrm{corr}}\simeq 0.0040 \text{ eV} , \quad (51)$$

where $2\Delta_{\mathrm{corr}}$ and $2\Delta_{\mathrm{MF}}$ represents, respectively, the gap calculated with correlation effects included, and in the mean-field approximation. Due to Eq. (47), there is an equivalent decrease T_c.

IV. CONCLUSIONS

These results show the important effect that local fluctuations introduce in the superconductor gap and critical temperature, although the ratio $2\Delta/k_B T_c$ is not changed with the self-energy matrix elements extending only up to nearest neighbors. It should be mentioned, however, that we cannot exclude that further interactions, with $\Sigma_{12}^{(2)}(\mathbf{R})$ extending up to second or third neighbors [or what could be even more important, the inclusion of electron-electron interactions in Hamiltonian (1) between different sites[9]], might introduce a gap variation along the Fermi surface. Work along these lines is in progress in our laboratory.

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APPENDIX A: CALCULATION OF THE SECOND-ORDER SELF-ENERGY

The most compact way of evaluating self-energy corrections in the superconducting phase is using the full matrix notation of Nambu [see Eqs. (3)–(7)]. To this end,

is convenient to write down the Hamiltonian (2) as a function of the Nambu matrix propagators. (A similar procedure can be found in Ref. 11 for the case of the superconductor phase of the electron gas.)

Defining the matrix field operator:

$$\hat{\psi}_{\mathbf{k}} \equiv \begin{bmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \end{bmatrix} \tag{A1}$$

we can write the Hamiltonian as

$$\hat{H} = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu)[\hat{\psi}^{\dagger}_{\mathbf{k}} \tfrac{1}{2}(\hat{\tau}_3 + \hat{\tau}_0)\hat{\psi}_{\mathbf{k}}] + \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu)[\hat{\psi}^{\dagger}_{\mathbf{k}} \tfrac{1}{2}(\hat{\tau}_3 - \hat{\tau}_0)\hat{\psi}_{\mathbf{k}}] - \frac{|U|}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} [\hat{\psi}^{\dagger}_{\mathbf{k}+\mathbf{q}} \tfrac{1}{2}(\hat{\tau}_3 + \hat{\tau}_0)\hat{\psi}_{\mathbf{k}}][\hat{\psi}^{\dagger}_{\mathbf{k}'-\mathbf{q}} \tfrac{1}{2}(\hat{\tau}_3 - \hat{\tau}_0)\hat{\psi}_{\mathbf{k}'}] , \tag{A2}$$

where the matrix $\hat{\tau}_3$ is

$$\hat{\tau}_3 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{A3}$$

and $\hat{\tau}_0$ is simply the identity matrix.

It is worth noticing the difference between vertex with spin $\uparrow$, characterized by a matrix factor $\frac{1}{2}(\hat{\tau}_3 + \hat{\tau}_0)$, and the ones with spin $\downarrow$, for which the factor is $\frac{1}{2}(\hat{\tau}_3 - \hat{\tau}_0)$.

Written in this form, we can apply the Feynman-Dyson perturbation theory on the interaction term $\hat{H}_{\text{int}}$ to calculate the matrix propagator:

$$\hat{G}(\mathbf{k},\tau) = -\langle \hat{T}_{\tau}[\hat{\psi}_{\mathbf{k}}(\tau)\hat{\psi}^{\dagger}_{\mathbf{k}}(0)] \rangle . \tag{A4}$$

The only change in the usual Feynman rules is that each vertex coupling an electron line to an interaction line includes a factor $\frac{1}{2}(\hat{\tau}_3 + \hat{\tau}_0)$ for spin up and $\frac{1}{2}(\hat{\tau}_3 - \hat{\tau}_0)$ for spin down, as mentioned above.

Using these rules we can evaluate $\hat{\Sigma}^{(2)}(\mathbf{k},\omega_n)$, the second-order matrix self-energy. In Figs. 3(a) and 3(b) are represented the diagrams contributing to the diagonal matrix element, $\Sigma^{(2)}_{11}(\mathbf{k},\omega_n)$, and in Figs. 3(c) and 3(d) the ones contributing to $\Sigma^{(2)}_{12}(\mathbf{k},\omega_n)$. The other two matrix elements, $\Sigma^{(2)}_{21}(\mathbf{k},\omega_n)$ and $\Sigma^{(2)}_{22}(\mathbf{k},\omega_n)$, are related to $\Sigma^{(2)}_{11}(\mathbf{k},\omega_n)$ and $\Sigma^{(2)}_{12}(\mathbf{k},\omega_n)$ by

$$\begin{aligned} \Sigma^{(2)}_{22}(\mathbf{k},\omega_n) &= -\Sigma^{(2)}_{11}(-\mathbf{k},-\omega_n) , \\ \Sigma^{(2)}_{21}(\mathbf{k},\omega_n) &= \Sigma^{(2)}_{12}(\mathbf{k},\omega_n) . \end{aligned} \tag{A5}$$

As commented in Sec. II, diagrams like the one drawn in Fig. 3(e) do not contribute to the self-energy when using a self-consistent perturbation theory because they are included when using dressed propagators.

Representing by $\Sigma^{(2)}_{11,a}, \Sigma^{(2)}_{11,b}, \Sigma^{(2)}_{12,a}$, and $\Sigma^{(2)}_{12,b}$, respectively, the four diagrams of Figs. 3(a), 3(b), 3(b), and 3(d) we have the following expressions:

$$\Sigma^{(2)}_{11,a}(\mathbf{k},\omega_n) = -\left[\frac{U}{N\beta}\right]^2 \sum_{\mathbf{q},\mathbf{k}'} \sum_{\nu_n,\omega'_n} G(\mathbf{k}-\mathbf{q},\omega_n-\nu_n)G(\mathbf{k}'+\mathbf{q},\omega'_n+\nu_n)G'(\mathbf{k}',\omega'_n) , \tag{A6}$$

$$\Sigma^{(2)}_{11,b}(\mathbf{k},\omega_n) = \left[\frac{U}{N\beta}\right]^2 \sum_{\mathbf{q},\mathbf{q}'} \sum_{\nu_n,\nu'_n} F^{\dagger}(\mathbf{k}-\mathbf{q},\omega_n-\nu_n)G'(\mathbf{k}-\mathbf{q}-\mathbf{q}',\omega_n-\nu_n-\nu'_n)F(\mathbf{k}-\mathbf{q}',\omega_n-\nu'_n) , \tag{A7}$$

$$\Sigma^{(2)}_{12,a}(\mathbf{k},\omega_n) = -\left[\frac{U}{N\beta}\right]^2 \sum_{\mathbf{q},\mathbf{k}'} \sum_{\nu_n,\omega'_n} F^{\dagger}(\mathbf{k}-\mathbf{q},\omega_n-\nu_n)F(\mathbf{k}'+\mathbf{q},\omega'_n+\nu_n)F^{\dagger}(\mathbf{k}',\omega'_n) , \tag{A8}$$

$$\Sigma^{(2)}_{12,b}(\mathbf{k},\omega_n) = \left[\frac{U}{N\beta}\right]^2 \sum_{\mathbf{q},\mathbf{q}'} \sum_{\nu_n,\nu'_n} G(\mathbf{k}-\mathbf{q},\omega_n-\nu_n)F^{\dagger}(\mathbf{k}-\mathbf{q}-\mathbf{q}',\omega_n-\nu_n-\nu'_n)G'(\mathbf{k}-\mathbf{q}',\omega_n-\nu'_n) , \tag{A9}$$

where ω_n and ω'_n represents fermionic discrete frequencies whereas ν_n and ν'_n are bosonic ones. The Green functions G, F, $F^{\dagger}$, and G' are defined in Eqs. (4)–(7).

In Sec. II it is argued that the nondiagonal self-energy $\Sigma^{(2)}_{12,b}(\mathbf{k},\omega_n)$ gives the leading term ($\sim\Delta$) for the obtainment of the gap and critical temperature. We proceed, then, to obtain the explicit expression of the full temperature-dependent $\Sigma^{(2)}_{12,b}(\mathbf{k},\omega_n)$. We have

$$\begin{aligned} \Sigma^{(2)}_{12}(\mathbf{k},i\omega_n) = \frac{1}{2}\left[\frac{U}{N}\right]^2 \sum_{\mathbf{q},\mathbf{q}'} \frac{\Delta(\mathbf{k}-\mathbf{q}-\mathbf{k}')}{E_{\mathbf{k}-\mathbf{q}-\mathbf{q}'}} [u^2_{\mathbf{k}-\mathbf{q}} v^2_{\mathbf{k}-\mathbf{q}'} A(i\omega_n, E_{\mathbf{k}-\mathbf{q}-\mathbf{q}'}, E_{\mathbf{k}-\mathbf{q}}, E_{\mathbf{k}-\mathbf{q}'}) \\ + (u^2_{\mathbf{k}-\mathbf{q}} u^2_{\mathbf{k}-\mathbf{q}'} + v^2_{\mathbf{k}-\mathbf{q}} v^2_{\mathbf{k}-\mathbf{q}'}) B(i\omega_n, E_{\mathbf{k}-\mathbf{q}-\mathbf{q}'}, E_{\mathbf{k}-\mathbf{q}}, E_{\mathbf{k}-\mathbf{q}'})] , \end{aligned} \tag{A10}$$

where we have made the following abbreviations:

$$A(i\omega_n, E_1, E_2, E_3) \equiv \frac{f(E_1,E_2,E_3)}{i\omega_n + E_1 + E_2 + E_3} - \frac{f(-E_1,-E_2,-E_3)}{i\omega_n - E_1 - E_2 - E_3} + \frac{f(E_1,-E_2,-E_3)}{i\omega_n + E_1 - E_2 - E_3} - \frac{f(-E_1,E_2,E_3)}{i\omega_n - E_1 + E_2 + E_3} , \tag{A11}$$

$$B(i\omega_n,E_1,E_2,E_3)\equiv\frac{f(E_1,-E_2,E_3)}{i\omega_n+E_1-E_2+E_3}-\frac{f(-E_1,-E_2,E_3)}{i\omega_n-E_1-E_2+E_3}\ , \tag{A12}$$

and

$$f(E_1,E_2,E_3)\equiv n_F(E_1)n_F(E_2)n_F(E_3)+n_F(-E_1)n_F(-E_2)n_F(-E_3)\ , \tag{A13}$$

where n_F is the Fermi distribution function.

For the discussion made in the paper, it is convenient to calculate this self-energy in a site representation:

$$\Sigma_{12}^{(2)}(\mathbf{R},i\omega_n)=\frac{1}{N}\sum_{\mathbf{k}}\Sigma_{12}^{(2)}(\mathbf{k},i\omega_n)e^{-i\mathbf{k}\mathbf{R}}\ , \tag{A14}$$

where $\mathbf{R}$ is any vector of the direct lattice. Then, from Eqs. (A10), (A11), and (A12), and making use of the translational symmetry of our system, we have

$$\Sigma_{12}^{(2)}(\mathbf{R},i\omega_n)=\frac{1}{2}\frac{U^2}{N^3}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}\frac{\Delta(\mathbf{k}_1)e^{-i(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)\mathbf{R}}}{E_{\mathbf{k}_1}}[u_{\mathbf{k}_1}^2v_{\mathbf{k}_3}^2A(i\omega_n,E_{\mathbf{k}_1},E_{\mathbf{k}_2},E_{\mathbf{k}_3})+(u_{\mathbf{k}_2}^2u_{\mathbf{k}_3}^2+v_{\mathbf{k}_2}^2v_{\mathbf{k}_3}^2)B(i\omega_n,E_{\mathbf{k}_1},E_{\mathbf{k}_2},E_{\mathbf{k}_3})]\ . \tag{A15}$$

Now, this last expression can be simplified a great deal, as we are only interested in the limit of low temperature and small gap (both much smaller than the bandwidth).

First, we note that for very low temperatures, most of the Fermi factors appearing in Eq. (A15) [through Eqs. (A11) and (A12)], can be taken as either 1 or 0. A special caution must be followed when dealing with the term $\Delta(\mathbf{k}_1)/E_{\mathbf{k}_1}$ and its corresponding Fermi factors, because the logarithmic divergence that can arise from this term must be taken into account in a proper way. With this caution, we can take $B=0$ in Eq. (A15), and rewrite the remaining term as

$$\Sigma_{12}^{(2)}(\mathbf{R},\omega_n)\simeq\frac{1}{2}\frac{U^2}{N^3}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}\frac{\Delta(\mathbf{k}_1)\tanh(\beta E_{\mathbf{k}_1}/2)}{E_{\mathbf{k}_1}}e^{-i\mathbf{k}_1\mathbf{R}}u_{\mathbf{k}_2}^2v_{\mathbf{k}_3}^2\left[\frac{1}{i\omega_n+E_{\mathbf{k}_1}+E_{\mathbf{k}_2}+E_{\mathbf{k}_3}}-\frac{1}{i\omega_n-E_{\mathbf{k}_1}-E_{\mathbf{k}_2}-E_{\mathbf{k}_3}}\right]\ , \tag{A16}$$

where $\beta=1/k_BT$.

We can simplify further the above expression, taking inside the parentheses $E_{\mathbf{k}_i}\simeq|\tilde{\epsilon}_{\mathbf{k}_i}|$ (remember that $\Delta\ll$ *bandwidth*). Moreover, as we are interested in the region where $\omega_n\to0$, we will neglect the frequency dependence in Eq. (A8), setting $\omega_n=0$.

Then, converting the summations into integrals:

$$\Sigma_{12}^{(2)}(\mathbf{R},\omega_n=0)=U^2\frac{1}{[(2\pi)^n]^3}\int d\mathbf{k}_1\frac{\Delta(\mathbf{k}_1)\tanh(\beta E_{\mathbf{k}_1}/2)e^{-i\mathbf{k}_1\mathbf{R}}}{\sqrt{\tilde{\epsilon}_{\mathbf{k}_1}^2+\Delta^2(\mathbf{k}_1)}}\int d\mathbf{k}_2u_{\mathbf{k}_2}^2e^{-i\mathbf{k}_2\mathbf{R}}\int d\mathbf{k}_3v_{\mathbf{k}_3}^2e^{-i\mathbf{k}_3\mathbf{R}}\frac{1}{|\tilde{\epsilon}_{\mathbf{k}_1}|+|\tilde{\epsilon}_{\mathbf{k}_2}|+|\tilde{\epsilon}_{\mathbf{k}_3}|}\ , \tag{A17}$$

where n is the dimension of the lattice. This is our final result.

APPENDIX B: CALCULATION OF THE GROUND-STATE ENERGY

In this appendix we calculate the ground-state energy of the superconductor, as given by our self-consistent perturbative method.

It is shown that it coincides, up to $O(U^2)$, with an independent calculation,[15] consisting of a perturbative expansion of the free energy.

Finally, we rederive the gap equation obtained previously in Sec. III, minimizing the ground-state energy with respect to the gap parameter.

We first derive an exact expression for the ground-state energy of the Hubbard superconductor as a function of the one-particle Green functions. As we will work at $T=0$, it will be more convenient to use the Green functions as defined in the $T=0$ formalism, instead of the Matsubara ones. We have

$$G(\mathbf{k},t)=G_{11}(\mathbf{k},t)=-i\langle\hat{T}[\hat{c}_{\mathbf{k}_\uparrow}(t)\hat{c}_{\mathbf{k}_\uparrow}^{\dagger}(0)]\rangle\ , \tag{B1}$$

$$F(\mathbf{k},t=G_{12}(\mathbf{k},t)=-i\langle\hat{T}[\hat{c}_{\mathbf{k}\uparrow}(t)\hat{c}_{-\mathbf{k}\downarrow}(0)]\rangle\ , \tag{B2}$$

$$F^{\dagger}(\mathbf{k},t)=G_{21}(\mathbf{k},t)=-i\langle\hat{T}[\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}(t)\hat{c}_{\mathbf{k}\uparrow}^{\dagger}(0)]\rangle\ , \tag{B3}$$

$$G'(\mathbf{k},t)=G_{22}(\mathbf{k},t)=-i\langle\hat{T}[\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}(t)\hat{c}_{-\mathbf{k}_\downarrow}(0)]\rangle\ . \tag{B4}$$

The obtainment of the $T=0$ Green functions is straightforward from the Matsubara ones. The prescription in this case is trivial: substitute $i\omega_n\to\omega+i\eta$ for the electron part of the spectrum and $i\omega_n\to\omega-i\eta$ for the

hole part.[13]

Now, from the Hubbard Hamiltonian, Eq. (2), the following exact result can be derived (see, for instance, Ref. 16):

$$\langle \hat{H} \rangle = \frac{1}{2\pi i} \sum_{\sigma} \oint d\omega \frac{\omega + \epsilon_{\mathbf{k}}}{2} G_c^{\sigma}(\mathbf{k},\omega) , \tag{B5}$$

where the contour integral must be taken in the upperhalf part of the complex plane.

The subindex c on $G_c^{\sigma}(\mathbf{k},\omega)$ indicates that causal Green functions must be used. It would be more convenient, however, to write down this expression as a function of the Nambu Green functions, Eqs. (B1)–(B4), we are using to describe the superconducting phase, instead of the causal ones. We have

$$G_c^{\uparrow}(\mathbf{k},\omega) = G_{11}(\mathbf{k},\omega) , \tag{B6}$$

$$G_c^{\downarrow}(\mathbf{k},\omega) = -G_{22}(-\mathbf{k},-\omega) . \tag{B7}$$

Then, it is easy to write Eq. (B5) as

$$\langle \hat{H} \rangle = \frac{1}{2\pi i} \oint d\omega \frac{\omega + \epsilon_{\mathbf{k}}}{2} G_{11}(\mathbf{k},\omega) + \frac{1}{2\pi i} \oint d\omega \frac{-\omega + \epsilon_{\mathbf{k}}}{2} G_{22}(\mathbf{k},\omega) , \tag{B8}$$

where the contours of integration of the first and second integrals are to be taken in the upper and lower complex half-planes, respectively.

We can modify this expression, making use of the Dyson equations for G_{11} and G_{22}, and write Eq. (B8) in a more useful form for our purposes:

$$\langle \hat{H} \rangle = \frac{1}{2\pi i} \oint d\omega [\epsilon_{\mathbf{k}} G_{11}(\mathbf{k},\omega) + \tfrac{1}{2}\Sigma_{11}(\mathbf{k},\omega) G_{11}(\mathbf{k},\omega) + \tfrac{1}{2}\Sigma_{12}(\mathbf{k},\omega) G_{21}(\mathbf{k},\omega)] + \frac{1}{2\pi i} \oint d\omega [\epsilon_{\mathbf{k}} G_{22}(\mathbf{k},\omega) - \tfrac{1}{2}\Sigma_{22}(\mathbf{k},\omega) G_{22}(\mathbf{k},\omega) - \tfrac{1}{2}\Sigma_{21}(\mathbf{k},\omega) G_{12}(\mathbf{k},\omega)] . \tag{B9}$$

Again, the contour must be taken in the upper and lower complex half-plane, respectively.

Equation (B9) can be written in a more compact form, making use of the full matrix notation:

$$\langle \hat{H} \rangle = \frac{1}{2\pi i} \oint d\omega \, \mathrm{Tr}[(\epsilon_{\mathbf{k}} \hat{\tau}_0 + \tfrac{1}{2}\hat{\Sigma}\hat{\tau}_3)\hat{G}] , \tag{B10}$$

taking the precaution, on evaluating the trace, of integrating the first element in the upper complex half-plane and second one on the lower. The matrices $\hat{\tau}_3$ and $\hat{\tau}_0$ are defined in Appendix A.

We pass now to evaluate the expression of the energy, up to $O(U^2)$, substituting in Eq. (B9) the second-order self-energies, calculated from Eqs. (A6)–(A9). The explicit form of these self-energies is

$$\Sigma_{11,a}^{(2)}(\mathbf{k},\omega) = \left[\frac{U}{N}\right]^2 \sum_{\mathbf{q},\mathbf{k}'} \left[\frac{u_{\mathbf{k}-\mathbf{q}}^2 v_{\mathbf{k}'+\mathbf{q}}^2 u_{\mathbf{k}'}^2}{\omega - E_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{k}} - E_{\mathbf{k}'+\mathbf{q}} + i\eta} + \frac{v_{\mathbf{k}-\mathbf{q}}^2 u_{\mathbf{k}'+\mathbf{q}}^2 v_{\mathbf{k}'}^2}{\omega + E_{\mathbf{k}-\mathbf{q}} + E_{\mathbf{k}} + E_{\mathbf{k}'+\mathbf{q}} - i\eta} \right] , \tag{B11}$$

$$\Sigma_{11,b}^{(2)}(\mathbf{k},\omega) = -\left[\frac{U}{N}\right] \sum_{\mathbf{q},\mathbf{q}'} \left[\frac{u_{\mathbf{k}-\mathbf{q}} v_{\mathbf{k}-\mathbf{q}} u_{\mathbf{k}-\mathbf{q}-\mathbf{q}'}^2 u_{\mathbf{k}-\mathbf{q}'} v_{\mathbf{k}-\mathbf{q}'}}{\omega - E_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{k}-\mathbf{q}'} - E_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} + i\eta} + \frac{u_{\mathbf{k}-\mathbf{q}} v_{\mathbf{k}-\mathbf{q}} v_{\mathbf{k}-\mathbf{q}-\mathbf{q}'}^2 u_{\mathbf{k}-\mathbf{q}'} v_{\mathbf{k}-\mathbf{q}'}}{\omega + E_{\mathbf{k}-\mathbf{q}} + E_{\mathbf{k}-\mathbf{q}'} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} - i\eta} \right] , \tag{B12}$$

$$\Sigma_{12,a}^{(2)}(\mathbf{k},\omega) = \left[\frac{U}{N}\right]^2 \sum_{\mathbf{q},\mathbf{k}'} \left[\frac{u_{\mathbf{k}-\mathbf{q}} v_{\mathbf{k}-\mathbf{q}} u_{\mathbf{k}'} v_{\mathbf{k}'} u_{\mathbf{k}'+\mathbf{q}} v_{\mathbf{k}'+\mathbf{q}}}{\omega - E_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{k}} - E_{\mathbf{k}'+\mathbf{q}} + i\eta} - \frac{u_{\mathbf{k}-\mathbf{q}} v_{\mathbf{k}-\mathbf{q}} u_{\mathbf{k}'} v_{\mathbf{k}'} u_{\mathbf{k}'+\mathbf{q}} v_{\mathbf{k}'+\mathbf{q}}}{\omega + E_{\mathbf{k}-\mathbf{q}} + E_{\mathbf{k}} + E_{\mathbf{k}'+\mathbf{q}} - i\eta} \right] , \tag{B13}$$

$$\Sigma_{12,b}^{(2)}(\mathbf{k},\omega) = \left[\frac{U}{N}\right]^2 \sum_{\mathbf{q},\mathbf{q}'} \left[-\frac{u_{\mathbf{k}-\mathbf{q}}^2 u_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} v_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} v_{\mathbf{k}-\mathbf{q}'}^2}{\omega - E_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{k}-\mathbf{q}'} - E_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} + i\eta} + \frac{v_{\mathbf{k}-\mathbf{q}}^2 u_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} v_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} u_{\mathbf{k}-\mathbf{q}'}^2}{\omega + E_{\mathbf{k}-\mathbf{q}} + E_{\mathbf{k}-\mathbf{q}'} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}'} - i\eta} \right] . \tag{B14}$$

Now substituting in Eq. (B9) and neglecting terms of order greater than $O(U^2)$, we have

$$\langle \hat{H} \rangle = 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} v_{\mathbf{k}}^2 + \frac{N}{4} \left[n^2 + \left[\frac{1}{N} \sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}} \right]^2 \right] - \left[\frac{U}{N}\right]^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \frac{(v_{\mathbf{k}}^2 u_{\mathbf{k}'-\mathbf{q}}^2 - u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'-\mathbf{q}})(v_{\mathbf{k}'}^2 u_{\mathbf{k}+\mathbf{q}}^2 - u_{\mathbf{k}'} v_{\mathbf{k}'} u_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}+\mathbf{q}})}{E_{\mathbf{k}} + E_{\mathbf{k}'} + E_{\mathbf{k}+\mathbf{q}} + E_{\mathbf{k}'-\mathbf{q}}} , \tag{B15}$$

where n is the number of electrons per site. This is the same expression found in Ref. 15 for the expansion of the energy up to $O(U^2)$.

The second-order term of Eq. (B15) presents some features of interest related to the discussion of Secs. II and III. It can be decomposed into four different contributions coming from the four terms of the numerator. The one containing the term $v_{\mathbf{k}}^2 u_{\mathbf{k}'-\mathbf{q}}^2 v_{\mathbf{k}'}^2 u_{\mathbf{k}+\mathbf{q}}^2$ comes from the contribution of the diagram in Fig. 3(a) ($\Sigma_{11,a}^{(2)}$). The term containing $u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'-\mathbf{q}} u_{\mathbf{k}'} v_{\mathbf{k}'} u_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}+\mathbf{q}}$ is produced by the diagram in Fig. 3(b) ($\Sigma_{12,a}^{(2)}$). Obviously, these two terms will not contribute to the gap equation in the limit of small gap parameter. The remaining two terms, containing the factor $-u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'}^2 u_{\mathbf{k}+\mathbf{q}}^2$, are equal and come from the diagrams in Fig. 3(b) ($\Sigma_{11,b}^{(2)}$), and 3(d) ($\Sigma_{12,b}^{(2)}$). Both

terms contribute in $O(\Delta^2)$ to the energy and give the leading second-order correction when deriving the gap equation.

It may seem surprising that the self-energy diagram, $\Sigma^{(2)}_{11,b}(\mathbf{k},\omega)$ [see Fig. 3(b)] that we have neglected when deriving the gap equation in Secs. II and III, because it was of order $\sim\Delta^2$, must be included in order to obtain the correct energy and, hence, the correct gap equation when obtained from the energy.

There is no contradiction in this. In Sec. II, the gap equation was obtained from the self-consistent condition

$$\Delta(\mathbf{k})=\Sigma_{12}(\mathbf{k},\omega=0)=\Sigma^{(1)}_{12}+\Sigma^{(2)}_{12}(\mathbf{k},\omega=0)\ . \tag{B16}$$

In this expression all terms of order greater than the leading one ($\sim\Delta$) must be neglected in the limit of small Δ.

However, when calculating the gap equation from the energy, the diagonal self-energy $\Sigma^{(2)}_{11,b}\sim\Delta^2$ must be included in order to obtain an expression for the energy correct in order Δ^2.

To illustrate this point, we will derive the gap equation from the expression of the energy, using the same approximations as those in Sec. III. First, we approximate the four self-energies, $\Sigma^{(2)}_{11,a}$, $\Sigma^{(2)}_{11,b}$, $\Sigma^{(2)}_{12,a}$, and $\Sigma^{(2)}_{12,b}$, by their local value:

$$\Sigma^{(2)}_{ij,\alpha}\rightarrow\frac{1}{N}\sum_{\mathbf{k}}\Sigma^{(2)}_{ij,\alpha}(\mathbf{k},\omega),\quad i,j=1,2,\ \alpha=a,b\ . \tag{B17}$$

When doing this, the expression of the energy is not exactly that of Eq. (B15). Instead we have

$$\langle\hat{H}\rangle=2\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}v^2_{\mathbf{k}}+\frac{\mathrm{N}}{4}\left[n^2+\left[\frac{1}{N}\sum_{\mathbf{k}}\frac{\Delta}{2E_{\mathbf{k}}}\right]\right]-\frac{U^2}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'}\frac{(v^2_{\mathbf{k}}u^2_{\mathbf{q}}-u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{q}}v_{\mathbf{q}})(v^2_{\mathbf{k}'}u^2_{\mathbf{q}'}-u_{\mathbf{k}'}v_{\mathbf{k}'}u_{\mathbf{q}'}v_{\mathbf{q}'})}{E_{\mathbf{k}}+E_{\mathbf{k}'}+E_{\mathbf{q}}+E_{\mathbf{q}'}}\ . \tag{B18}$$

We are interested in retaining only the terms that will contribute to the gap equation in the limit $\Delta\rightarrow0$. Then, we approximate the second-order term of the above equation by

$$2\frac{U^2}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'}\frac{u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{q}}v_{\mathbf{q}}v^2_{\mathbf{k}'}u^2_{\mathbf{q}'}}{|\tilde{\epsilon}_{\mathbf{k}}|+|\tilde{\epsilon}_{\mathbf{q}}|+|\tilde{\epsilon}_{\mathbf{k}'}|+|\tilde{\epsilon}_{\mathbf{q}'}|}\ . \tag{B19}$$

Now, from the condition

$$\frac{\partial\langle\hat{H}\rangle}{\partial\Delta}=0 \tag{B20}$$

we have

$$2\Delta\sum_{\mathbf{k}}\frac{1}{2E_{\mathbf{k}}}+2\frac{U\Delta}{N}\left[\sum_{\mathbf{k}}\frac{1}{2E_{\mathbf{k}}}\right]^2+2\beta\frac{U^2\Delta}{N}\left[\sum_{\mathbf{k}}\frac{1}{2E_{\mathbf{k}}}\right]^2=0\ , \tag{B21}$$

where

$$\beta=\frac{2}{N^2}\sum_{\mathbf{k}',\mathbf{q}'}\frac{v^2_{\mathbf{k}'}u^2_{\mathbf{q}'}}{|\tilde{\epsilon}_{\mathbf{k}'}|+|\tilde{\epsilon}_{\mathbf{q}'}|}\ . \tag{B22}$$

Finally, we have the following gap equation:

$$1=\frac{|U'|}{2}\sum_{\mathbf{k}}\frac{1}{E_{\mathbf{k}}}\ , \tag{B23}$$

where $U'=U+\beta U^2$. For the case of a half-filled band and a constant unperturbed density of states we have $\beta=2\ln2/B$ as in Eq. (44).

[1] J. G. Bernordz and K. A. Muller, Z. Phys. B **64**, 189 (1986).
[2] C. W. Chu *et al.*, Phys. Rev. Lett. **58**, 405 (1989).
[3] J. R. Schrieffer *et al.*, Phys. Rev. Lett. **60**, 944 (1988).
[4] P. W. Anderson, Science **235**, 1196 (1987).
[5] O. Labbe, Phys. Scr. **T29**, 82 (1989); C. C. Tsuei *et al.*, Phys. Rev. Lett. **65**, 2724 (1990).
[6] C. A. Balseiro, Phys. Rev. Lett. **62**, 2624 (1989).
[7] J. Ferrer *et al.*, Phys. Rev. B **44**, 415 (1991).
[8] R. Micnas *et al.*, Rev. Mod. Phys. **62**, 113 (1990).
[9] R. Micnas *et al.*, Phys. Rev. B **37**, 9410 (1988); R. Micnas *et al.*, Phys. Rev. B **39**, 11 653 (1989).
[10] A. A. Abrikosov *et al.*, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).
[11] J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964).
[12] R. D. Mattuck and B. Johansson, Adv. Phys. **17**, 509 (1968).
[13] G. D. Mahan, *Many Particle Physics* (Plenum, New York, 1981).
[14] V. J. Emery, Phys. Rev. B **14**, 2989 (1976).
[15] A. Georges and J. S. Yedidia, Phys. Rev. B **43**, 3475 (1991).
[16] B. Kjöllerström *et al.*, Phys. Rev. **148**, 665 (1966).