

Formation of d -wave superconducting order in a randomly doped lattice

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We consider the interplay between superconducting coupling and dopant impurity scattering of charge carriers in planar square lattice systems and examine the physical conditions (doping level, temperature, local symmetry of coupling and scattering potentials) necessary in this model system to obtain a d -wave superconducting order, like that observed in real doped cuprate HTSC materials. Using the Lifshitz model for the disorder introduced into system by dopants, we analyze also the nonuniform structure of such a d -wave parameter, including both its magnitude and phase variation. The results indicate that d -wave superconductivity becomes possible in a doped metal until it is destroyed at too high doping levels.

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1. Introduction

Studies of the effect of impurities and defects on superconducting (SC) properties of metals (including SC alloys) began practically as early as the BCS theory had been constructed. In particular, the classical papers by Anderson [1] and by Abrikosov and Gor'kov [2] indicated a substantial difference between magnetic and nonmagnetic impurities in superconductors. While the addition of nonmagnetic impurities has practically no effect on the value of transition critical temperature T_c , the presence of spin on the impurity atom (leading to the Kondo effect in a normal metal) results in pair-breaking, that is, it transforms a singlet Cooper pair into an unstable triplet and rapidly suppresses T_c . All of the known studies have considered the s -type, or isotropic, SC order (apart from heavy-fermion systems, where it is the p -type order and T_c is extremely low) and, correspondingly, an isotropic gap near the Fermi level.

The discovery of high- T_c superconductivity (HTSC) in copper oxides confronted physicists with a number of problems which still remain a challenge for the theory. Undoubtedly, this includes the issue of the HTSC mechanism, the strong dependences of many (both SC and normal) proper-

ties of copper oxides on the charge-carrier concentration, the specifics of weakly doped systems (first of all, the existence of a pseudogap at temperatures above T_c), the formation of stripe structures, etc. (see, e.g., the review articles [3–6]). Such a problem is also presented by the impurity effect on the SC properties of HTSC systems. These differ from the «old» or «conventional» superconductors not only in higher T_c and d -wave anisotropy of the order parameter but also in the fact that here magnetic and nonmagnetic impurities change their roles: the former are weak suppressors for T_c [7,8], while the latter (in particular, Zn substituting for Cu in cuprate layers) lead to a fast decay of HTSC [7,10,11]. Many aspects of impurity effects in superconductors with anisotropic (including d -wave) pairing have already been studied theoretically in Refs. 12–17, using a range of models and approximations. However, these (and many other) papers did not include one of the most essential features of HTSC systems, the fact that they cannot be non-impure.

In other words, most of theoretical approaches to HTSC are based on the concept, formulated and applied in the pioneering works [1,2]: one starts from an ideal (2D or quasi-2D) metal with given Fermi energy ε_F , defined by the density of free

carriers, and then considers the perturbation of an independently existing SC condensate by some extrinsic (magnetic or nonmagnetic) impurities. Their action, local or global, affects the preformed and condensed singlet pairs. Of course, this formulation is reasonable but it lacks an essential element for the conductance in copper oxides: almost all HTSCs are doped metals, where (like the doped semiconductors) each carrier is provided by insertion of a donor or acceptor into the system. In turn, this implies that HTSCs are intrinsically impure systems with an inherent disorder*, and the number of impurity («foreign» included) atoms can not be less than at least the number of charge carriers. While in normal metals one has the condition $k_F l \gg 1$ (k_F is the Fermi momentum, and l is the carrier mean free path between collisions with impurity atoms) [18], it turns to $k_F l \sim 1$ in HTSCs, and they belong to the family of «*bad*» metals with both k_F and l defined by the doping.

Perhaps the first attempt to consider in a self-consistent way the characteristic tendencies for HTSC, pairing of the carriers and their localization on impurity atoms, was made in the authors' work [19]. It discussed the phase diagram of doped 2D metal in presence of *s*-wave pairing and showed that SC is possible neither at low impurity concentrations $c < c_0 \sim \epsilon_0/W$ (when all the carriers are localized near impurities with localization energies ϵ_0 much less of the bandwidth W , so that c_0 is typically few percent) nor at too high c (when the pair inverse lifetime times \hbar exceeds the SC gap). There, in general, the self-consistency is related either to the SC order parameter (like the common Bardeen–Cooper–Schrieffer or Bogolyubov–de Gennes treatments) and to the chemical potential.

The present work is aimed at extending the approach of Ref. 19 to the case of *d*-wave SC coupling and to trace the formation of the corresponding order parameter. It is motivated, not least, by an apparent controversy between the experimental evidence for *d*-symmetry of the order parameter in HTSCs [20–22] and the theoretical claim that anisotropic pairing should not survive in the presence of chaotically distributed isotropic scatterers [23]. For the sake of simplicity, we restrict consideration to the doping range $c > c_0$,

where the self-consistency is only relevant for the SC order parameter, while the chemical potential can be put in the form** $\mu \approx \epsilon_F \approx 3cW/4$. Then we distinguish between two types of impurity effects by doping. The first, the so-called *homogeneous effects*, are displayed by translationally invariant *single-particle* Green functions (SPGF). They have been studied earlier by various means [24] but, as a rule, by introducing the disorder through a single parameter V_A of Anderson's model [24]. In contrast, we employ the Lifshitz' model of disorder [25], characterized by two independent parameters: c and the impurity potential V_L . They produce an equivalent $V_A \sim \sqrt{c(1-c)}V_L$, but not vice versa. Within this model, more adequate for doped HTSC systems, we conclude the persistence of the *d*-wave order parameter under homogeneous impurity effects. Also we explicitly consider the other type of effects, inhomogeneous, due to local variations of the order parameter near impurity centers. This involves *two-particle* Green functions (TPGF) besides the usual SPGF, and yields a possible limitation on SC at high enough dopant concentrations.

At least, we would like to acknowledge the great honor and pleasant opportunity for us to publish this work in the Low Temperature Physics issue dedicated to the memory of the outstanding physicist L. V. Shubnikov, whose contribution to low-temperature physics in general and to superconductivity in particular cannot be overestimated.

2. Hamiltonian and Green functions

We start from the model electronic Hamiltonian in the band representation

$$H = \sum_{\mathbf{k}} \left\{ \sum_{\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^+ c_{\mathbf{k},\sigma} - \frac{1}{N} \sum_{\mathbf{k}'} \left[V \gamma_{\mathbf{k}} \gamma_{\mathbf{k}'} c_{\mathbf{k},\uparrow}^+ c_{-\mathbf{k},\downarrow}^+ c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow} - V_L \sum_{\mathbf{p},\sigma} e^{i(\mathbf{k}'-\mathbf{k})\mathbf{p}} c_{\mathbf{k}',\sigma}^+ c_{\mathbf{k},\sigma} \right] \right\}, \quad (1)$$

where $c_{\mathbf{k},\sigma}$ and $c_{\mathbf{k},\sigma}^+$ the Fermi operators for a charge carrier with wave vector \mathbf{k} and spin σ . The simplest

* Here we don't consider the possible formation of stripe structures, where an ordered or disordered distribution of dopants cannot yet be confirmed by any reliable data.

** However, it is known that μ can differ substantially from the Fermi energy ϵ_F in the limit of very low doping (see, e.g., [4,6]).

band energy $\varepsilon_{\mathbf{k}} = 4t - 2t(\cos ak_x + \cos ak_y)$, with full bandwidth $W = 8t$, is expressed through the amplitude t of carrier hopping between nearest-neighbor sites* (of the total N in the lattice, with a lattice constant a). The parameter V models the attraction between two carriers with opposite spins on such sites, the factor $\gamma_{\mathbf{k}} = (\cos ak_x - \cos ak_y) \times \theta(\varepsilon_D^2 - \xi_{\mathbf{k}}^2)$ has the d -wave symmetry and is effective only for quasiparticle energies $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \varepsilon_F$ smaller than the «Debye energy» ε_D . The latter is understood as a characteristic energy of the intermediate (Froelich) boson, and in what follows we suppose the condition $\varepsilon_D < \mu$ to hold and a BCS shell to exist (the alternative $\mu < \varepsilon_D$, possible for underdoped HTSC systems, will be considered elsewhere). The impurity perturbation V_L expresses the shift of the on-site electronic energy at a random dopant site \mathbf{p} , where the negative sign takes explicit account of the carrier attraction to the ionized dopant, and, for simplicity, we consider this perturbation localized on a single site. With the usual BCS ansatz: $c_{-\mathbf{k},\downarrow} c_{\mathbf{k}\uparrow} = \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle + \phi_{\mathbf{k}}$, and in neglect of terms quadratic in the pair fluctuations $\phi_{\mathbf{k}}$, Eq. (1) leads to a bilinear form $H' = H - \mu N$:

$$H' = \sum_{\mathbf{k}} \left[\sum_{\sigma} \xi_{\mathbf{k}} c_{\mathbf{k},\sigma}^+ c_{\mathbf{k},\sigma} - (\Delta_{\mathbf{k}} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} + \text{h.c.}) - \frac{V_L}{N} \sum_{\mathbf{p},\mathbf{k}',\sigma} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{p}} c_{\mathbf{k}',\sigma}^+ c_{\mathbf{k},\sigma} \right]. \quad (2)$$

Here the gap function is defined by the self-consistency relation

$$\Delta_{\mathbf{k}} = \frac{V\gamma_{\mathbf{k}}}{N} \sum_{\mathbf{k}'} \gamma_{\mathbf{k}'} \langle c_{\mathbf{k}',\uparrow} c_{-\mathbf{k}',\downarrow} \rangle, \quad (3)$$

extending the common BCS gap equation to the d -wave case. A nonuniform system can be treated within the formalism used formerly for impurity problems in SC [14,19] by passing to the Nambu spinors $\psi_{\mathbf{k}}^+ = (c_{\mathbf{k},\uparrow}^+, c_{-\mathbf{k},\downarrow})$ and $\psi_{\mathbf{k}}$ and defining the Fourier-transformed matrix Green function (GF)

$$\hat{G}_{\mathbf{k},\mathbf{k}'}(\varepsilon) \equiv \langle\langle \psi_{\mathbf{k}} | \psi_{\mathbf{k}'}^+ \rangle\rangle_{\varepsilon} = \int_{-\infty}^0 e^{i(\varepsilon-i0)t} \langle\langle \psi_{\mathbf{k}}(t), \psi_{\mathbf{k}'}^+(0) \rangle\rangle dt. \quad (4)$$

* So, we do not take into account next-neighbor hoppings.

Here \hat{A} denotes a 2×2 matrix in Nambu indices, $\langle \dots \rangle$ is the quantum statistical average, and $\{a(t), b(0)\}$ is the anticommutator of Heisenberg operators. In the GFs below we omit their explicit dependence on energy ε but distinguish between their diagonal and nondiagonal forms in the Nambu (N) and momentum (M) indices. Then, applying the Heisenberg equation of motion $i\hbar \partial \psi_{\mathbf{k}} / \partial t = [H', \psi_{\mathbf{k}}]$ in Eq. (4), we arrive at an equation of motion of the Dyson type for the SPGFs:

$$\hat{G}_{\mathbf{k},\mathbf{k}'} = \hat{G}_{\mathbf{k}}^{(0)} \delta_{\mathbf{k},\mathbf{k}'} - \hat{G}_{\mathbf{k}}^{(0)} \hat{V} \sum_{\mathbf{p},\mathbf{k}''} e^{i(\mathbf{k}-\mathbf{k}'')\cdot\mathbf{p}} \hat{G}_{\mathbf{k}'',\mathbf{k}'} \quad (5)$$

where the unperturbed SPGF $\hat{G}_{\mathbf{k}}^{(0)} = (\varepsilon - \xi_{\mathbf{k}} \hat{\tau}_3 - \Delta_{\mathbf{k}} \hat{\tau}_1 + i0)^{-1}$, and the scattering matrix $\hat{V} = V_L \hat{\tau}_3$ includes the Pauli matrices $\hat{\tau}_i$.

For a disordered system, the relevant (observable) characteristics are described by the so-called self-averaging GFs, whose values for all particular realizations of disorder turn practically nonrandom, equal to those averaged over disorder [26]. The most important example of such a function is the M-diagonal SPGF, $\hat{G}_{\mathbf{k}} \equiv \hat{G}_{\mathbf{k},\mathbf{k}}$. The general solution for Eq. (5) in this case can be written (see Appendix E) as

$$\hat{G}_{\mathbf{k}} = \left\{ [\hat{G}_{\mathbf{k}}^{(0)}]^{-1} - \hat{\Sigma}_{\mathbf{k}} \right\}^{-1}, \quad (6)$$

where the self-energy matrix $\hat{\Sigma}_{\mathbf{k}}$ is given by the so-called fully renormalized group expansion (GE) [14,19,27,28]

$$\hat{\Sigma}_{\mathbf{k}} = -c \hat{V} [1 + \hat{G} \hat{V}]^{-1} \times \left\{ 1 + c \sum_{\mathbf{n} \neq 0} [\hat{A}_{0\mathbf{n}} e^{-i\mathbf{k}\cdot\mathbf{n}} + \hat{A}_{0\mathbf{n}} \hat{A}_{\mathbf{n}0}] [1 - \hat{A}_{0\mathbf{n}} \hat{A}_{\mathbf{n}0}]^{-1} + \dots \right\}. \quad (7)$$

Here the integrated SPGF matrix $\hat{G} = N^{-1} \Sigma_{\mathbf{k}} \hat{G}_{\mathbf{k}}$, and the matrices $A_{0\mathbf{n}}$ of indirect interaction between scatterers at sites 0 and \mathbf{n} are

$$\hat{A}_{0\mathbf{n}} = -\hat{V} \sum_{\mathbf{k}' \neq \mathbf{k}} e^{i\mathbf{k}'\cdot\mathbf{n}} \hat{G}_{\mathbf{k}'} [1 + \hat{G} \hat{V}]^{-1}. \quad (8)$$

The restriction to $\mathbf{k}' \neq \mathbf{k}$ in the single summation in \hat{A}_{0n} should be complemented by $\mathbf{k}'' \neq \mathbf{k}, \mathbf{k}'$ for double summation in the product $\hat{A}_{0n} \hat{A}_{n0}$, but such restrictions can be already ignored in $\hat{A}_{0n} \hat{A}_{0n} \hat{A}_{n0}$ and the higher-degree terms [27] resulting from expansion of the right-hand side of Eq. (7).

Many observable characteristics of the SC state follow from the GFs, in the spectral theorem representation

$$\langle ab \rangle = \int_{-\infty}^{\infty} \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} \text{Im} \langle\langle b | a \rangle\rangle_{\varepsilon}, \quad \beta = \frac{1}{T}, \quad (9)$$

where the chemical potential μ is defined by the overall electron concentration

$$c = \frac{1}{N} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} \text{Im Tr} \hat{\tau}_3 \hat{G}_{\mathbf{k}}. \quad (10)$$

On the other hand, c is just the concentration of dopant centers which give rise to carrier scattering: $c = N^{-1} \sum_{\mathbf{p}} 1$ and the *carrier* concentration only gets close to (but never exceeds) c in the regime of the doped metal, for c above a certain metallization threshold c_0 (for a quasi-2D dispersed $\varepsilon_{\mathbf{k}}$ it is $c_0 \sim \exp(-\pi W/4V_L) \ll 1$ [19]). Under this condition, the self-consistency implied by Eq. (10) is not necessary, and a good approximation* for the chemical potential is $\mu \approx 3cW/4$ (see Appendix A). Then the gap equation (3) takes the form

$$\Delta_{\mathbf{k}} = \frac{V\gamma_{\mathbf{k}}}{2N} \sum_{\mathbf{k}'} \gamma_{\mathbf{k}'} \int_{-\infty}^{\infty} \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} \text{Im Tr} \hat{\tau}_1 \hat{G}_{\mathbf{k}}, \quad (11)$$

and its solution, discussed in Appendix C for the uniform case ($V_L = 0$), is simply $\Delta_{\mathbf{k}} = \Delta\gamma_{\mathbf{k}}$, with the ratio $r = 2\Delta/k_B T_c$ being $e^{1/3}$ times the s -wave BCS value $r_{BCS} \approx 3.52$.

Another important self-averaging quantity is the integrated SPGF matrix \hat{G} itself, since the density of states $\rho(\varepsilon)$ is just

$$\rho(\varepsilon) = \frac{1}{\pi} \text{Im Tr} \hat{G}. \quad (12)$$

* This approximation is actually justified by the fact that for $c > c_0$ the Fermi level ε_F of metallic phase is well higher than the conduction band edge, and one can hardly suppose the existence of local pairs and the related inequality $\mu < \varepsilon_F$ at these concentrations. Therefore, in what follows we do not distinguish between μ and ε_F .

For an unperturbed system $V_L \rightarrow 0$, $\hat{G} \rightarrow \hat{G}^{(0)} = N^{-1} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}}^{(0)}$, and calculation of the imaginary part of $\hat{G}^{(0)}$ within the nodal point approximation (Appendix B) leads to the standard d -wave density of states:

$$\rho(\varepsilon) \rightarrow \rho^{(0)}(\varepsilon) = \frac{1}{\pi} \text{Im Tr} \hat{G}^{(0)} = \frac{2\varepsilon\rho_0}{\Delta} \arcsin \left[\min \left(1, \frac{\Delta}{\varepsilon} \right) \right], \quad (13)$$

where $\rho_0 \approx 4/(\pi W)$ is the normal Fermi density of states of a doped (quasi-2D) metal with $\varepsilon_F < W/2$. Respectively, the real part of $\hat{G}^{(0)}$ is

$$\text{Re} \hat{G}^{(0)} = \varepsilon\rho_0 \left[\frac{W}{\mu(W-\mu)} - \frac{\pi}{\Delta} \theta(\Delta - \varepsilon) \text{arccosh} \frac{\Delta}{\varepsilon} \right]. \quad (14)$$

Then Eqs. (13) and (14) can be unified into a single analytic form:

$$\hat{G}^{(0)} = \varepsilon\rho_0 \left[\frac{W}{\mu(W-\mu)} - \frac{\pi}{\Delta} \left(\text{arccosh} \frac{\Delta}{\varepsilon} - i \frac{\pi}{2} \right) \right], \quad (15)$$

since at $\varepsilon > \Delta$ one has $\arccos(\Delta/\varepsilon) = i[\pi/2 - \arcsin(\Delta/\varepsilon)]$, thus restoring Eq. (13). But it is just the growth of the (real) arccosh term at $\varepsilon < \Delta$ that permits the existence of a low-energy ($\varepsilon_{\text{res}} \ll \Delta$) resonance feature in $\text{Re}(1 + \hat{G}V)^{-1}$ and hence in $\rho(\varepsilon)$. Such a resonance was discussed previously for a d -wave SC with low enough concentration c (so that $\hat{G} \approx \hat{G}^{(0)}$) of «foreign» impurities producing strong enough perturbation V_L [14], and it is similar to the known low-frequency resonance by heavy impurities in acoustic phonon spectra [29]. However, in the situation of interest here, when both V_L and c are not small, \hat{G} can be substantially modified compared to $\hat{G}^{(0)}$, and this is expressed in a very complicated way by Eq. (7). To simplify the task, certain self-consistent procedures, like the CPA method, quite useful in the theory of normal metals [30], can be employed. A similar approach was previously proposed for an s -wave SC doped system [19], and here we begin with the analysis of a self-consistent solution for Eq. (5) in the d -wave case.

3. Uniform doping effects in the self-consistent approach

If the GE series (7) is restricted to its first term, the self-energy matrix $\hat{\Sigma}_{\mathbf{k}}$ in fact becomes independent of \mathbf{k} :

$$\hat{\Sigma}_{\mathbf{k}} \rightarrow \hat{\Sigma} = -c\hat{V} [1 + \hat{G}\hat{V}]^{-1}, \quad (16)$$

and substitution of Eq. (16) into Eq. (6) defines the self-consistent approximation $\hat{G}_{\mathbf{k}}^{(sc)}$ for the M-diagonal SPGF:

$$\hat{G}_{\mathbf{k}}^{(sc)} = \left\{ [\hat{G}_{\mathbf{k}}^{(0)}]^{-1} - \hat{\Sigma}^{(sc)} \right\}^{-1}, \quad (17)$$

$$\hat{\Sigma}^{(sc)} = -c\hat{V} [1 + \hat{G}^{(sc)}\hat{V}]^{-1}, \quad (18)$$

$$\hat{G}^{(sc)} = \frac{1}{N} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}}^{(sc)}. \quad (19)$$

To solve this system, we first parametrize the self-energy matrix (18):

$$\hat{\Sigma}^{(sc)} = \Sigma_0 + \Sigma_1 \hat{\tau}_1 + \Sigma_3 \hat{\tau}_3, \quad (20)$$

where the Σ_i are some complex-valued functions of energy. Then the integration in Eq. (19) within the nodal-point approximation (Appendix D) results in

$$\hat{G}^{(sc)} = G_0 + G_1 \hat{\tau}_1 + G_3 \hat{\tau}_3 \quad (21)$$

with the coefficients

$$G_0 = (\varepsilon - \Sigma_0) \rho_0 \times \left[-\frac{\pi}{2\Delta} \left(\operatorname{arccosh} \frac{\Delta + \Sigma_1}{\varepsilon - \Sigma_0} + \operatorname{arccosh} \frac{\Delta - \Sigma_1}{\varepsilon - \Sigma_0} - i\pi \right) + \frac{W}{\mu(W - \mu)} \right], \quad (22)$$

$$G_1 = \Sigma_1 \rho_0 \left[-\frac{2i\pi}{\sqrt{(\varepsilon - \Sigma_0)^2 - (\Delta + \Sigma_1)^2} + \sqrt{(\varepsilon - \Sigma_0)^2 - (\Delta - \Sigma_1)^2}} + \frac{W}{\mu(W - \mu)} \right], \quad (23)$$

$$G_3 = \rho_0 \left[\ln \frac{\mu}{W - \mu} + 2\Sigma_3 \frac{(\varepsilon - \Sigma_0)^2 - \Delta^2/3 - \Sigma_1^2}{\varepsilon_D^3} \right]. \quad (24)$$

Substituting Eq. (21) into Eq. (18), we arrive at

$$\hat{\Sigma}^{(sc)} = \frac{cV_L [V_L(G_0 + G_1 \hat{\tau}_1) - (1 + V_L G_3) \hat{\tau}_3]}{(1 + V_L G_3)^2 - V_L^2(G_0^2 - G_1^2)}. \quad (25)$$

Comparing Eqs. (25), and (22)–(24) with Eq. (20), we immediately conclude that $\Sigma_1 = G_1 = 0$, or that $\hat{\Sigma}^{(sc)}$ is in fact *N-diagonal*, which is extremely important. Physically, this means that (within the self-consistent, linear in c approximation) the scattering by dopants does not influence the d -wave order parameter, and this can be directly related to the fact that the s -symmetry of the impurity perturbation V_L is orthogonal to the d -symmetry of the SC pairing V . It also applies to more realistic models of dopant perturbation in HTSC (e.g., with plaquette- or dumbbell-like anisotropy [31]), provided that their symmetries do not coincide with that of the order parameter. Complications arise when they do coincide, as was found for an isotropic perturbation on s -wave order with all three Σ_i being nonzero [19]; hence the apparently «harder» d -wave system in fact turns «easier»!

Using the fact that $\Sigma_1 = 0$ and the relation $\cosh(x + i\pi/2) = \sin x$, Eq. (22) is brought to a very simple form:

$$\frac{\Delta}{\varepsilon - \Sigma_0} = \sin \left(\alpha - \frac{G_0}{\pi\rho_0} \frac{\Delta}{\varepsilon - \Sigma_0} \right), \quad (26)$$

with $\alpha = W\Delta/[\pi\mu(W - \mu)] \ll 1$, while the same comparison for the two nonzero components of $\hat{\Sigma}^{(sc)}$: Σ_0 and Σ_3 , gives:

$$\Sigma_0 [(1 + V_L G_3)^2 - V_L^2 G_0^2] = cV_L^2 G_0, \quad (27)$$

$$\Sigma_3 [(1 + V_L G_3)^2 - V_L^2 G_0^2] = -cV_L(1 + V_L G_3). \quad (28)$$

From Eq. (28) we estimate $|\Sigma_3| \sim cV_L$; hence, within the relevant energy region $|e| \ll \varepsilon_D$ the function G_3 from Eq. (24) is reasonably well approximated by a (negative) constant $g_3 = \rho_0 \times \ln[\mu/(W - \mu)]$. Then Eq. (27) turns quadratic for G_0 :

$$G_0^2 + \frac{c}{\Sigma_0} G_0 - \left(\frac{1}{\tilde{V}} \right)^2 = 0, \quad (29)$$

with $\tilde{V} = V_L/(1 + V_L g_3) \approx V_L \ln(1/c_0)/\ln(3c/4c_0)$. The system of equations (26), (29) fully defines the self-energy Σ_0 and other uniform physical properties

of a disordered d -wave system, and its solution can be found (in principle, numerically) within the whole relevant energy range. It turns especially simple if $|\Sigma_0| \ll c\tilde{V}$ (this proves to hold at least for $\varepsilon \ll \varepsilon_{\text{res}}$); then the proper solution to Eq. (29) is: $G_0 \approx \Sigma_0 / c\tilde{V}^2$, and from Eq. (26) we obtain the following equation for a single important function Σ_0 :

$$\frac{\Delta}{\varepsilon - \Sigma_0} = \sin \left(\alpha - \frac{\tilde{\alpha}\Sigma_0}{\varepsilon - \Sigma_0} \right) \quad (30)$$

with $\tilde{\alpha} = \Delta / [\pi c \tilde{V}^2 \rho_0] \ll 1$. It defines the self-consistent density of states

$$\rho^{(sc)}(\varepsilon) = \frac{1}{\pi} \text{Im Tr } \hat{G}^{(sc)}(\varepsilon) = \frac{2 \text{Im } \Sigma_0(\varepsilon)}{\pi c \tilde{V}^2}, \quad (31)$$

at lowest energies. The results of this approach are free of the infrared logarithmic divergences that appear in the integrals of perturbation theory [32] and thus allows one to avoid applying heavy field-theoretic methods for a white-noise scattering potential [15], whose adequacy to the case of discrete random dopants is not clear.

The exact value of the density of states at the very center of the gap, $\rho(0) = \rho(\varepsilon \rightarrow 0)$, is also of a particular interest in view of the known claim about existence of a nonzero «universal» value $\rho(0) \sim c / \ln(1/c)$ if V_L is sufficiently strong [12,17]. However, we conclude from Eq. (30) that in the limit $\varepsilon \rightarrow 0$:

$$\Sigma_0 \rightarrow \varepsilon \left[1 + i \frac{\tilde{\alpha}}{\ln(2\Delta/\tilde{\alpha}|\varepsilon|)} \right],$$

and hence the self-consistent density of states at $\varepsilon \rightarrow 0$:

$$\rho^{(sc)}(\varepsilon) \rightarrow \frac{4\tilde{\alpha}^2 \rho^{(0)}(\varepsilon)}{\pi \ln(2\Delta/\tilde{\alpha}|\varepsilon|)}, \quad (32)$$

vanishes even faster than the unperturbed function $\rho^{(0)}(\varepsilon)$ of Eq. (13). This produces a certain narrow «quasi-gap» (not to be confused with the pseudogap observed at $T > T_c$ in the underdoped regime) around the center. For comparison, the estimated $\rho(\varepsilon)$ from the two first terms of Eq. (7) tends to zero linearly in ε with corrections $\sim \varepsilon^2$ [14], while the field-theoretical analysis [15] predicts $\rho(\varepsilon) \rightarrow \varepsilon^\omega$, with the nonuniversal exponent being

* Except for the special case $1/\tilde{V} = 0$, which corresponds to $c \approx 4c_0/3$, while the actual consideration is for $c \gg c_0$.

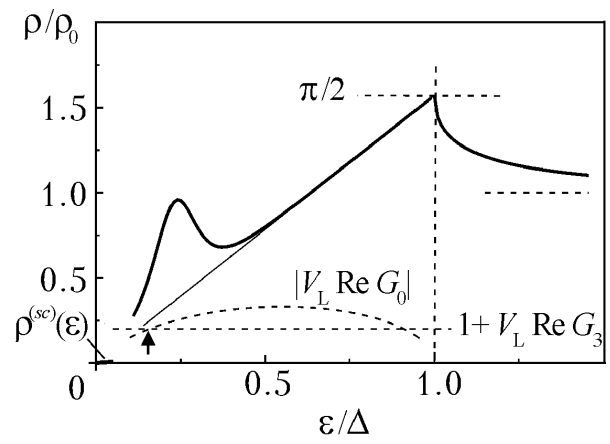


Fig. 1. Density of states in a d -wave SC system (heavy solid line). The thin solid line shows the unperturbed $\rho^{(0)}(\varepsilon)$, and the arrow indicates the solution for $\text{Re} [(1 + V_L G_3)^2 - V_L^2 G_0^2] = 0$, corresponding to the low-energy resonance (the other solution at $\varepsilon \approx \Delta$ is not resonant) for the choice of parameters $W = 2 \text{ eV}$, $V_L = 0.5 \text{ eV}$, $c = 0.1$.

(in our notation) $\omega = \tanh \ln \sqrt{\pi^2 \Delta W / 2cV_L^2}$, which is always < 1 and can even be < 0 .

The discrepancy between our results and the aforementioned «universal» behavior originates in the improper use of the unitary limit $V_L \rightarrow \infty$ in neglect of the $1 + V_L G_3$ term in Eq. (27), leading to the relation $\Sigma_0 = -c/G_0$. But the true limiting relation is inverse: $\Sigma_0 = c\tilde{V}^2 G_0$, with \tilde{V} finite for $V_L \rightarrow \infty$, and also the unitary limit fails at any* finite V_L when $\varepsilon \rightarrow 0$. Finally, the existing experimental data do not confirm the «universal» $\rho(0)$ value, but seem to favor the conclusion about existence of a strong low-energy resonance in $\rho(\varepsilon)$ [11], with a possible quasi-gap at the very center [33], though experimental observations at such low energies of course need extremely low temperatures.

Note, however, that the self-consistent treatment of the low-energy resonance, at $\varepsilon_{\text{res}} \sim \Delta \ln(3c/4c_0) / (\pi \ln 2\pi)$ for the case of self-impurities (Fig. 1), already requires solution of the full system of equations (26), (29), and, in view of a probable underestimate of this hump (like that in normal systems [28,30]), it should be better described by the exact GE (7).

The obtained $\Sigma^{(sc)}$ can be in principle directly inserted in Eq. (17), in order to use the resulting $G_{\mathbf{k}}^{(sc)}$ for correction of the gap equation (11). However, at the quasiparticle energies $\xi_{\mathbf{k}} \sim \varepsilon_D$ important there, renormalization effects are negligible,

and thus Δ remains well approximated by the result of Appendix C.

4. Nonuniform effects

The SPGFs considered in the previous Section describe the uniform self-averaging characteristics of the SC state. The next important question is the behavior of fluctuations of the order parameter (both its amplitude and phase) in an inhomogeneous system, which should be closely related to the breakdown of superconductivity in the overdoped regime. A strong local suppression of d -wave order close to a single «foreign» impurity has been predicted theoretically [14] and observed experimentally [11]. In the general case of a finite concentration of scatterers, the local d -wave order can be characterized by the operator

$$\Omega_{\mathbf{n}} = \frac{V}{N} \sum_{\mathbf{k}, \mathbf{k}'} \gamma_{\mathbf{k}} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{n}} c_{-\mathbf{k}, \downarrow} c_{\mathbf{k}', \uparrow}, \quad (33)$$

such that its mean value (generally complex) defines the uniform gap parameter: $N^{-1} \sum_{\mathbf{n}} \langle \Omega_{\mathbf{n}} \rangle = N^{-1} \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \Delta_{\mathbf{k}} = \Delta$ [14]. On the other hand, it is natural to characterize local fluctuations of the order parameter by the variance of $\Omega_{\mathbf{n}}$ (identified with the variance of the gap parameter):

$$\delta^2 = \frac{1}{N} \sum_{\mathbf{n}} (\langle \Omega_{\mathbf{n}}^2 \rangle - \langle \Omega_{\mathbf{n}} \rangle^2). \quad (34)$$

Using Eq. (33), we write

$$\delta^2 = \frac{V^2}{N^3} \sum_{\mathbf{n}} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} e^{i(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{n}} \gamma_{\mathbf{k}_1} \gamma_{\mathbf{k}_2} [\langle c_{-\mathbf{k}_1, \downarrow} c_{\mathbf{k}_3, \uparrow} c_{-\mathbf{k}_2, \downarrow} c_{\mathbf{k}_4, \uparrow} \rangle - \langle c_{-\mathbf{k}_1, \downarrow} c_{\mathbf{k}_3, \uparrow} \rangle \langle c_{-\mathbf{k}_2, \downarrow} c_{\mathbf{k}_4, \uparrow} \rangle], \quad (35)$$

or, summing over \mathbf{n} to close the sum of 4 momenta, and using the spectral representation (9) for $T = 0$:

$$\delta^2 = \frac{V^2}{N^2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} \gamma_{\mathbf{k}_1} \gamma_{\mathbf{k}_2} \left[\int_0^{\infty} d\varepsilon \text{Im} \langle\langle c_{-\mathbf{k}_1, \downarrow} c_{\mathbf{k}_2, \uparrow} | c_{-\mathbf{k}_2 + \mathbf{q}, \downarrow} c_{\mathbf{k}_1 - \mathbf{q}, \uparrow} \rangle\rangle - \int_0^{\infty} d\varepsilon \text{Im} \langle\langle c_{-\mathbf{k}_1, \downarrow} | c_{\mathbf{k}_2, \uparrow} \rangle\rangle \int_0^{\infty} d\varepsilon \text{Im} \langle\langle c_{-\mathbf{k}_2 + \mathbf{q}, \downarrow} | c_{\mathbf{k}_1 - \mathbf{q}, \uparrow} \rangle\rangle \right]. \quad (36)$$

Here, besides the previously used SPGFs, the TPGF $\langle\langle c_{-\mathbf{k}_1, \downarrow} c_{\mathbf{k}_2, \uparrow} | c_{-\mathbf{k}_2 + \mathbf{q}, \downarrow} c_{\mathbf{k}_1 - \mathbf{q}, \uparrow} \rangle\rangle$ appears. An explicit calculation of this function for the unperturbed ($V_L = 0$) SC system (see Appendix E) gives the following result

$$\begin{aligned} & \langle\langle c_{-\mathbf{k}_1, \downarrow} c_{\mathbf{k}_2, \uparrow} | c_{-\mathbf{k}_2 + \mathbf{q}, \downarrow} c_{\mathbf{k}_1 - \mathbf{q}, \uparrow} \rangle\rangle = \\ & = \delta_{0, \mathbf{q}} \frac{4\varepsilon \Delta_{\mathbf{k}_1} \Delta_{\mathbf{k}_2} + \dots}{(\varepsilon^2 - E_{\mathbf{k}_1}^2 - E_{\mathbf{k}_2}^2)^2 - 4E_{\mathbf{k}_1}^2 E_{\mathbf{k}_2}^2}. \quad (37) \end{aligned}$$

Here $E_{\mathbf{k}}^2 = \xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2$, and three other terms in the numerator are not mutually odd in $\gamma_{\mathbf{k}_1}$ and $\gamma_{\mathbf{k}_2}$ and thus do not contribute to δ^2 . Then it is easy to see that the resulting contribution to Eq. (36) from the M-diagonal ($\mathbf{q} = 0$) and N-nondiagonal TPGFs by Eq. (37) exactly cancels with that from the SPGFs, which confirms the uniformity of d -wave order in this case. The most important contribution to δ^2 at

$V_L \neq 0$ comes from two consecutive scattering processes in the left-hand sides of an N- and M-nondiagonal ($\mathbf{q} \neq 0$) TPGF, first $c_{-\mathbf{k}_1, \downarrow} c_{\mathbf{k}_2, \uparrow} \rightarrow c_{-\mathbf{k}_1 + \mathbf{q}, \downarrow} c_{\mathbf{k}_2, \uparrow}$ and

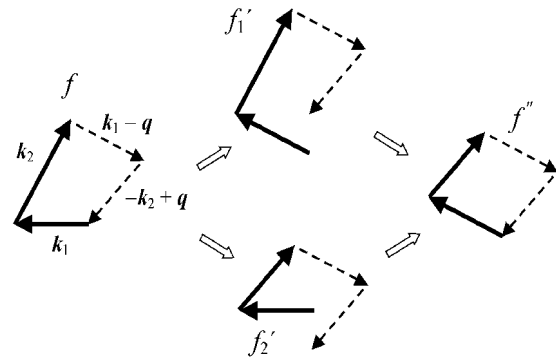


Fig. 2. Schematic of consecutive scattering processes (see Appendix E), bringing an M-nondiagonal TPGF f , through intermediate, partly M-diagonal f'_1 and f'_2 to fully M-diagonal f'' : the solid vectors standing for the operators of the left-hand side get fully nested with the dashed vectors for the right-hand side.

then $c_{-\mathbf{k}_1+\mathbf{q},\downarrow} c_{\mathbf{k}_2,\uparrow} \rightarrow c_{-\mathbf{k}_1+\mathbf{q},\downarrow} c_{\mathbf{k}_2-\mathbf{q},\uparrow}$ (or vice versa, Fig. 2), on the same scattering center \mathbf{p} . It is linear in c , while the contribution from SPGFs in this order, $-\Delta V \int_0^\infty d\varepsilon \text{Im Tr } \hat{\tau}_1 \hat{\Sigma}$, is zero, accordingly to

the N-diagonal form of $\hat{\Sigma}$ established in the previous Section. Hence we generally estimate the variance of the gap to grow with c as $|\delta| = \Delta\sqrt{c/c_1}$, where $c_1 \sim (V/V_L)^2$ defines the upper critical concentration for SC at $T = 0$.

A more detailed analysis, resolving amplitude and phase fluctuations, can be done in a similar way, but considering separately the two operators:

$$\Omega_{\mathbf{n},+} = \frac{\Omega_{\mathbf{n}} + \Omega_{\mathbf{n}}^+}{2}, \quad \text{and} \quad \Omega_{\mathbf{n},-} = \frac{\Omega_{\mathbf{n}} - \Omega_{\mathbf{n}}^+}{2i},$$

such that their mean values $\langle \Omega_{\mathbf{n},\pm} \rangle$ lead to real and imaginary parts of the order parameter, and constructing the corresponding variances:

$$\delta_{\pm}^2 = \frac{1}{N} \sum_{\mathbf{n}} (\langle \Omega_{\mathbf{n},\pm}^2 \rangle - \langle \Omega_{\mathbf{n},\pm} \rangle^2).$$

This approach should be particularly important upon extension of the theory to finite temperatures, in order to establish the dominant type of fluctuations due to the static disorder, responsible for breakdown of SC order at $T = T_c$, and its possible role in the persistence of a pseudogap in the density of states ρ at $T > T_c$.

5. Conclusions

The analysis presented above shows that the disordered structure of doped HTSC systems is crucial for many of their characteristic properties and for the existence of SC order itself. The interplay between doping and disorder effects can be briefly summarized as follows. Superconductivity sets in with the metallization of the system, at a critical concentration $c \sim c_0$ resulting from the competition between the kinetic energy of the charge carriers in the regular lattice and their attraction to random dopant centers. The uniform d -wave order parameter Δ increases with increasing number of charge carriers as $\Delta \sim \sqrt{c}$ [6] and saturates at a certain optimum doping $c_{\text{opt}} \sim \varepsilon_D / W$, when the relation $\mu > \varepsilon_D$ comes to hold. With further increase in c , the increasing local fluctuations of Δ bring it to collapse at some upper critical concentration $c_1 \sim (V/V_L)^2$, resulting from the competition

between the pairing and scattering potentials. This picture is quantitatively satisfied with a very natural choice of parameters $W \sim 2$ eV, $V_L \sim 0.5$ eV, $V \sim 0.22$ eV, $\varepsilon_D \sim 0.2$ eV, giving plausible estimates: $c_0 \sim 5\%$, $c_{\text{opt}} \sim 15\%$, $T_{c,\text{max}} \sim 100$ K, $c_1 \sim 20\%$. Our forthcoming work should specify such important aspects, left beyond the scope of this paper, as the disorder effects on the cusp of density of states $\rho(\varepsilon)$ at $\varepsilon = \Delta$, the matching conditions between the self-consistent and GE descriptions of SPGF, the exact numerical coefficient for the critical value c_1 , etc. And, of course, it is of fundamental interest to extend the present self-consistent treatment to the case of finite temperatures up to T_c , in order to obtain a quantitative estimate for the bell-like $T_c(c)$ shape, and further to $T > T_c$, to study the role of doping disorder versus d -wave SC coupling in the formation and subsequent merging (at $c \sim c_{\text{opt}}$) of the pseudogap in the normal density of states.

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Appendix A

For the normal phase, we consider the dispersion relation $\varepsilon_{\mathbf{k}} = 4t - 2t(\cos ak_x + \cos ak_y)$ and relate the dopant concentration c to the number (per unit cell) of occupied states below μ :

$$\begin{aligned} c &= \frac{2a^2}{(2\pi)^2} \int_{\varepsilon_{\mathbf{k}} \leq \mu} d\mathbf{k} = \\ &= \frac{2a^2}{\pi^2} \int_0^{\arccos\left(1 - \frac{4\mu}{W}\right)} dk_x \int_0^{\arccos\left(2 - \frac{4\mu}{W} - \cos ak_x\right)} dk_y = \\ &= \frac{2}{\pi^2} \int_{1 - \frac{4\mu}{W}}^1 \frac{du}{\sqrt{1-u^2}} \int_{2 - \frac{4\mu}{W} - u}^1 \frac{dv}{\sqrt{1-v^2}} = \frac{2}{\pi^2} F\left(\frac{4\mu}{W}\right). \end{aligned} \quad (\text{A.1})$$

Here the dependence of the integral

$$F(x) = \int_{1-x}^1 \frac{\arccos(2-x-u) du}{\sqrt{1-u^2}}$$

is very well approximated by a simple linear function $F(x) \approx 5x/3$ in the whole physically important range $0 \leq x = 4\mu/W \leq x_{\max}$ (where $x_{\max} \approx 0.6$) corresponds to $\mu_{\max} \approx 0.15W$ at the maximum physical doping $c_{\max} \approx 0.2$). Then we readily arrive at the estimate cited above:

$$\mu \approx \frac{3\pi^2}{40} cW \approx \frac{3cW}{4}.$$

Appendix B

For the uniform SC system with d -wave gap, we perform integration over the Brillouin zone with the parametrization: $\mathbf{k} - \mathbf{k}_i = a^{-1}(\rho_0 \xi \mathbf{e}_i + \Delta^{-1} \eta \mathbf{e}_i \times \mathbf{e}_z)$, $\mathbf{e}_i = (\pm 1/\sqrt{2}, \pm 1/\sqrt{2}, 0)$, $\mathbf{e}_z = (0, 0, 1)$, near 4 nodal points $\mathbf{k}_i = \arccos(1 - \mu/W) \mathbf{e}_i$ of the gap function $\Delta_{\mathbf{k}} = \Delta \gamma_{\mathbf{k}}$. This integration for $\hat{G}^{(0)}$ becomes

$$\hat{G}^{(0)} = \frac{1}{N} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}}^{(0)} = \rho_0 \left[\frac{1}{2\Delta} \int_{-\Delta}^{\Delta} d\eta \int_{-\varepsilon_D}^{\varepsilon_D} d\xi \hat{g}(\varepsilon, \xi, \eta) + \int_{-\mu}^{-\varepsilon_D} d\xi \hat{g}(\varepsilon, \xi, 0) + \int_{\varepsilon_D}^{W-\mu} d\xi \hat{g}(\varepsilon, \xi, 0) \right], \quad (\text{B.1})$$

where we have defined the matrix function (cp. $\hat{G}_{\mathbf{k}}^{(0)}$ in (5))

$$\hat{g}(\varepsilon, \xi, \eta) = (\varepsilon - \xi \hat{\tau}_3 - \eta \hat{\tau}_1)^{-1} = \frac{\varepsilon + \xi \hat{\tau}_3 + \eta \hat{\tau}_1}{\varepsilon^2 - \xi^2 - \eta^2}.$$

The integration in ξ (normal to the Fermi surface) in Eq. (B.1) treats the BCS shell, $[-\varepsilon_D, \varepsilon_D]$, separately from the out-of-shell segments, $[-\mu, -\varepsilon_D]$ and $[\varepsilon_D, W-\mu]$, where the gap parameter Δ becomes zero (together with $\gamma_{\mathbf{k}}$) and no integration over $\eta = \Delta \gamma_{\mathbf{k}}$ is needed. Equation (B.1) permits one to define explicitly the coefficient functions g_i in the general form $\hat{G}^{(0)} = g_0 + g_1 \hat{\tau}_1 + g_3 \hat{\tau}_3$. Let us denote $z^2 = \varepsilon^2 - \eta^2$, and then the shell contribution to g_0 results from the integral:

$$\int_{-\varepsilon_D}^{\varepsilon_D} \frac{d\xi}{z^2 - \xi^2} = \frac{2}{z} \left(\operatorname{arctanh} \frac{z}{\varepsilon_D} + i\pi \right) \approx \frac{2}{\varepsilon_D} + \frac{2i\pi}{z}, \quad (\text{B.2})$$

which is followed for its last term by:

$$\int_{-\Delta}^{\Delta} \frac{d\eta}{\sqrt{\varepsilon^2 - \eta^2}} = 2 \arccos \frac{\Delta}{\varepsilon}. \quad (\text{B.3})$$

The out-of-shell contributions are:

$$\int_{-\mu}^{-\varepsilon_D} \frac{d\xi}{\varepsilon^2 - \xi^2} = \frac{1}{\varepsilon} \left(\operatorname{arctanh} \frac{\varepsilon}{\mu} - \operatorname{arctanh} \frac{\varepsilon}{\varepsilon_D} \right) \approx \frac{1}{\mu} - \frac{1}{\varepsilon_D} \quad (\text{B.4})$$

and

$$\int_{\varepsilon_D}^{W-\mu} \frac{d\xi}{\varepsilon^2 - \xi^2} \approx \frac{1}{W-\mu} - \frac{1}{\varepsilon_D}. \quad (\text{B.5})$$

To find g_1 and g_3 , we use the obvious equations

$$\int_{-\varepsilon_D}^{\varepsilon_D} \frac{\xi d\xi}{z^2 - \xi^2} = \int_{-1}^1 \eta d\eta = 0$$

and

$$\int_{-\mu}^{-\varepsilon_D} \frac{\xi d\xi}{\varepsilon^2 - \xi^2} + \int_{\varepsilon_D}^{W-\mu} \frac{\xi d\xi}{\varepsilon^2 - \xi^2} = \frac{1}{2} \ln \frac{\mu^2 - \varepsilon^2}{(W-\mu)^2 - \varepsilon^2} \approx \ln \frac{\mu}{W-\mu}. \quad (\text{B.6})$$

Summing up Eqs. (B.2)–(B.6) we obtain

$$g_0 = \varepsilon \rho_0 \left[\frac{W}{\mu(W-\mu)} - \frac{\pi}{\Delta} \left(\operatorname{arccosh} \frac{\Delta}{\varepsilon} - \frac{i\pi}{2} \right) \right];$$

in accordance with Eq. (15), $g_1 = 0$ and $g_3 = \rho_0 \times \ln [\mu/(W-\mu)]$.

Appendix C

The gap equation (11) for a uniform ($V_L = 0$) d -wave system at $T = 0$ transforms into:

$$\frac{1}{\lambda} = \frac{16}{\pi\Delta^3} \text{Im} \int_0^{\Delta} \eta^2 d\eta \int_0^{\varepsilon_D} d\xi \int_0^{\infty} \frac{d\varepsilon}{\varepsilon^2 - \xi^2 - \eta^2 - i0}, \quad (\text{C.1})$$

with coupling constant $\lambda \equiv V\rho_0$. The quantity sought is the gap amplitude Δ . On the right-hand side of Eq. (C.1) we perform the elementary integration over ε , using the relation $\text{Im}(x - i0)^{-1} = \pi\delta(x)$:

$$\begin{aligned} \frac{16}{\pi} \text{Im} \int_0^{\Delta} \eta^2 d\eta \int_0^{\varepsilon_D} d\xi \int_0^{\infty} \frac{d\varepsilon}{\varepsilon^2 - \xi^2 - \eta^2 - i0} &= \\ &= 8 \int_0^{\Delta} \eta^2 d\eta \int_0^{\varepsilon_D} \frac{d\xi}{\sqrt{\xi^2 + \eta^2}}. \end{aligned} \quad (\text{C.2})$$

Then, integrating out in ξ and passing from η to $y = \hbar\varepsilon_D/\eta$, we present Eq. (C.2) as

$$\begin{aligned} 8 \left(\frac{\varepsilon_D}{\Delta} \right)^3 \int_{\varepsilon_D/\Delta}^{\infty} \frac{\text{arcsinh } y \, dy}{y^4} &= \\ &= \frac{8}{3} \text{arcsinh} \frac{\varepsilon_D}{\Delta} + 4 \frac{\varepsilon_D \sqrt{\varepsilon_D^2 + \Delta^2}}{3\Delta^2} - \\ &- \frac{4}{3} \left(\frac{\varepsilon_D}{\Delta} \right)^3 \text{arcsinh} \frac{\Delta}{\varepsilon_D} \approx \frac{8}{3} \left(\ln \frac{2\varepsilon_D}{\Delta} + \frac{1}{3} \right). \end{aligned}$$

The equation for critical temperature T_c , corresponding to $\Delta = 0$, in this case reads

$$\begin{aligned} \frac{1}{\lambda} &= \frac{16}{3\pi} \text{Im} \int_0^{\varepsilon_D} d\xi \tanh \left(\frac{\xi}{2k_B T_c} \right) \int_0^{\infty} \frac{d\varepsilon}{\varepsilon^2 - \xi^2 - i0} \approx \\ &\approx \frac{8}{3} \ln \left(\frac{2\gamma_E \varepsilon_D}{\pi k_B T_c} \right), \end{aligned}$$

with the Euler constant $\gamma_E \approx 1.781$. Hence for the d -wave case the effective coupling constant is

$\tilde{\lambda} = 8\lambda/3$, which is $8/3$ times the «Hamiltonian» value λ , which can serve as one more explanation for high T_c itself. Also, the ratio $r = 2\Delta/k_B T_c$ here turns out to be $\exp(1/3)$ times the common s -wave BCS value $r_{BCS} = 2\pi/\gamma_E \approx 3.52$, reaching values as high as $r_d \approx 4.92$. In turn, this means that, for other conditions (say, ρ_0 and V) equal, the s -condensate turns out more stable to thermal fluctuations and requires a higher T_c to destroy it than the d -condensate. Of course, this is directly related to the absence of a gap in the latter case, permitting quasi-particles to exist at any $T < T_c$.

Appendix D

Calculation of the self-consistent SPGF $\hat{G}^{(sc)} = G_0 + G_1 \hat{\tau}_1 + G_3 \hat{\tau}_3$ generalizes the scheme of Appendix B:

$$\begin{aligned} \hat{G}^{(sc)} &= \frac{1}{N} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}}^{(sc)} = \\ &= \rho_0 \left[\frac{1}{2\Delta} \int_{-\Delta}^{\Delta} d\eta \int_{-\varepsilon_D}^{\varepsilon_D} d\xi \hat{g}(\varepsilon - \Sigma_0, \xi + \Sigma_3, \eta + \Sigma_1) + \right. \\ &\quad \left. \int_{-\varepsilon_D}^{-\varepsilon_D} d\xi \hat{g}(\varepsilon - \Sigma_0, \xi + \Sigma_3, \Sigma_1) + \int_{-\mu}^{W-\mu} d\xi \hat{g}(\varepsilon - \Sigma_0, \xi + \Sigma_3, \Sigma_1) \right]. \end{aligned} \quad (\text{D.1})$$

Next we set $z^2 = (\varepsilon - \Sigma_0)^2 - (\eta + \Sigma_1)^2$ and $z = r + ip$, and pass from ξ to $x = \xi + \Sigma_3$, where Σ_3 can be taken real (as seen, e.g., from the final result (28)). Then the analog to Eq. (B.2) is:

$$\begin{aligned} &\int_{-\varepsilon_D + \Sigma_3}^{\varepsilon_D + \Sigma_3} \frac{dx}{z^2 - x^2} = \frac{1}{2z} \times \\ &\times \left\{ \frac{1}{2} \ln \frac{[(\varepsilon_D + \Sigma_3 + r)^2 + p^2][(\varepsilon_D - \Sigma_3 + r)^2 + p^2]}{[(\varepsilon_D - \Sigma_3 - r)^2 + p^2][(\varepsilon_D + \Sigma_3 - r)^2 + p^2]} - \right. \\ &\quad \left. - i \left[\arctan \frac{\varepsilon_D + \Sigma_3 + r}{p} + \arctan \frac{\varepsilon_D + \Sigma_3 - r}{p} + \right. \right. \end{aligned}$$

$$\left. + \arctan \frac{\varepsilon_D - \Sigma_3 + r}{p} + \arctan \frac{\varepsilon_D - \Sigma_3 - r}{p} \right\} \approx \\
\approx \frac{2}{\varepsilon_D} - i \frac{\pi + 2p/\varepsilon_D}{z}, \quad (D.2)$$

where the small term $2p/\varepsilon_D$ can be safely dropped. The next integration, over $y = \eta + \Sigma_1$, is done only on the $i\pi/z$ term accordingly to

$$\int_{-\Delta+\Sigma_1}^{\Delta+\Sigma_1} \frac{dy}{\sqrt{(\varepsilon-\Sigma_0)^2 - y^2}} = \arccos \frac{\Delta+\Sigma_1}{\varepsilon-\Sigma_0} + \arccos \frac{\Delta-\Sigma_1}{\varepsilon-\Sigma_0}, \quad (D.3)$$

which is relevant for G_0 , supplemented with

$$\int_{-\Delta+\Sigma_1}^{\Delta+\Sigma_1} \frac{y dy}{\sqrt{\varepsilon - \Sigma_0^2 - y^2}} = \\
= - \frac{4\Delta\Sigma_1}{\sqrt{(\varepsilon - \Sigma_0)^2 - (\Delta + \Sigma_1)^2} + \sqrt{(\varepsilon - \Sigma_0)^2 - (\Delta - \Sigma_1)^2}} \quad (D.4)$$

for G_1 . The out-of-shell integration of the components mentioned is much easier, giving:

$$\int_{\varepsilon_D - \Sigma_3}^{\mu - \Sigma_3} \frac{dx}{(\varepsilon - \Sigma_0)^2 - x^2} = \\
= \frac{1}{\varepsilon - \Sigma_0} \left(\operatorname{arctanh} \frac{\varepsilon - \Sigma_0}{\mu - \Sigma_3} - \operatorname{arctanh} \frac{\varepsilon - \Sigma_0}{\varepsilon_D - \Sigma_3} \right) \approx \\
\approx \frac{1}{\mu - \Sigma_3} - \frac{1}{\varepsilon_D - \Sigma_3}, \quad (D.5)$$

and

$$\int_{\varepsilon_D - \Sigma_3}^{W - \mu - \Sigma_3} \frac{dx}{(\varepsilon - \Sigma_0)^2 - x^2} \approx \frac{1}{W - \mu - \Sigma_3} - \frac{1}{\varepsilon_D - \Sigma_3}. \quad (D.6)$$

Here Σ_3 can also be disregarded besides W , μ , ε_D , and then the two $-1/\varepsilon_D$ terms cancel with that from Eq. (D.2). Now, combining Eqs. (D.2)–(D.6), we obtain

$$G_0 = (\varepsilon - \Sigma_0) \rho_0 \left[\frac{W}{\mu(W - \mu)} - \right. \\
\left. - \frac{\pi}{2\Delta} \left(\operatorname{arccosh} \frac{\Delta + \Sigma_1}{\varepsilon - \Sigma_0} + \operatorname{arccosh} \frac{\Delta - \Sigma_1}{\varepsilon - \Sigma_0} - i\pi \right) \right], \quad (D.7)$$

and

$$G_1 = \Sigma_1 \rho_0 \left[\frac{W}{\mu(W - \mu)} - \right. \\
\left. - \frac{2i\pi}{\sqrt{(\varepsilon - \Sigma_0)^2 - (\Delta + \Sigma_1)^2} + \sqrt{(\varepsilon - \Sigma_0)^2 - (\Delta - \Sigma_1)^2}} \right].$$

At least, G_3 is obtained after

$$\int_{-\varepsilon_D + \Sigma_3}^{\varepsilon_D + \Sigma_3} \frac{x dx}{z^2 - x^2} = \frac{1}{2} \ln \frac{(\varepsilon_D - \Sigma_3)^2 - z^2}{(\varepsilon_D + \Sigma_3)^2 - z^2}, \\
\int_{\varepsilon_D + \Sigma_3}^{W - \mu + \Sigma_3} \frac{x dx}{z^2 - x^2} = \frac{1}{2} \ln \frac{(\varepsilon_D + \Sigma_3)^2 - z^2}{(W - \mu + \Sigma_3)^2 - z^2}, \\
\int_{-\mu + \Sigma_3}^{-\varepsilon_D + \Sigma_3} \frac{x dx}{z^2 - x^2} = \frac{1}{2} \ln \frac{(\mu - \Sigma_3)^2 - z^2}{(\varepsilon_D - \Sigma_3)^2 - z^2}, \\
\frac{1}{2\Delta} \int_{-\Delta + \Sigma_1}^{\Delta + \Sigma_1} y^2 dy = \frac{\Delta^2}{3} + \Sigma_1^2,$$

in the form

$$G_3 = \rho_0 \left\{ \ln \frac{\mu}{W - \mu} + 2\Sigma_3 \frac{(\varepsilon - \Sigma_0)^2 - \Delta^2/3 - \Sigma_1^2}{\varepsilon_D^3} \right\}. \quad (D.8)$$

Appendix E

Search for solutions of Eq. (5) in the form of GE consists in consecutive iterations of its right-hand side, separating systematically the GFs already present in previous iterations [27]. Let us start from the M-diagonal SPGF $\hat{G}_{\mathbf{k}}$, and then the iteration sequence begins with singling out the scattering term with $\hat{G}_{\mathbf{k}}$ itself from those with $\hat{G}_{\mathbf{k}',\mathbf{k}}$, $\mathbf{k}' \neq \mathbf{k}$:

$$\begin{aligned} \hat{G}_{\mathbf{k}} &= \hat{G}_{\mathbf{k}}^{(0)} + \hat{G}_{\mathbf{k}}^{(0)} \frac{1}{N} \sum_{\mathbf{k}',\mathbf{p}} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{p}} \hat{V} \hat{G}_{\mathbf{k}',\mathbf{k}} = \\ &= \hat{G}_{\mathbf{k}}^{(0)} + c \hat{G}_{\mathbf{k}}^{(0)} \hat{V} \hat{G}_{\mathbf{k}} + \hat{G}_{\mathbf{k}}^{(0)} \hat{V} \frac{1}{N} \sum_{\mathbf{k}' \neq \mathbf{k}, \mathbf{p}} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{p}} \hat{G}_{\mathbf{k}',\mathbf{k}}. \end{aligned} \quad (\text{E.1})$$

Then for each $\hat{G}_{\mathbf{k}',\mathbf{k}}$ we again write down Eq. (5) and separate the scattering terms with $\hat{G}_{\mathbf{k}}$ and $\hat{G}_{\mathbf{k}',\mathbf{k}}$ in their right-hand sides:

$$\begin{aligned} \hat{G}_{\mathbf{k}',\mathbf{k}} &= \hat{G}_{\mathbf{k}'}^{(0)} \hat{V} \frac{1}{N} \sum_{\mathbf{k}'',\mathbf{p}'} e^{i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{p}'} \hat{G}_{\mathbf{k}'',\mathbf{k}} = \\ &= c \hat{G}_{\mathbf{k}'}^{(0)} \hat{V} \hat{G}_{\mathbf{k}',\mathbf{k}} + \hat{G}_{\mathbf{k}'}^{(0)} \hat{V} \frac{1}{N} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{p}'} \hat{G}_{\mathbf{k}} + \\ &\quad + \hat{G}_{\mathbf{k}'}^{(0)} \hat{V} \frac{1}{N} \sum_{\mathbf{p}' \neq \mathbf{p}} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{p}'} \hat{G}_{\mathbf{k}} + \\ &\quad + \hat{G}_{\mathbf{k}'}^{(0)} \hat{V} \frac{1}{N} \sum_{\mathbf{k}'' \neq \mathbf{k}, \mathbf{k}'; \mathbf{p}'} e^{i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{p}'} \hat{G}_{\mathbf{k}'',\mathbf{k}}. \end{aligned} \quad (\text{E.2})$$

Note that the $\mathbf{p}' = \mathbf{p}$ term which gives the phase factor $e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{p}}$ in the right-hand side of Eq. (E.2), coherent to that already figured in the last sum in Eq. (E.1), is explicitly separated from incoherent ones, $e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{p}'}$, $\mathbf{p}' \neq \mathbf{p}$ (but there will be no such separation when doing 1st iteration of Eq. (5) for the M-nondiagonal SPGF $\hat{G}_{\mathbf{k}',\mathbf{k}}$ itself). Continuing the sequence, we shall explicitly collect the terms with the initial function $G_{\mathbf{k}}$, resulting from: i) all multiple scatterings on the same site \mathbf{p} and ii) on the same pair of sites \mathbf{p} and $\mathbf{p}' \neq \mathbf{p}$. Then the summing of i) in \mathbf{p} produces the first term of GE, and, if the pair processes are neglected, it will coincide with the well-known CPA result [30]. The second term of the GE, obtained by summing of ii) in \mathbf{p} , $\mathbf{p}' \neq \mathbf{p}$, contains interaction matrices $\hat{A}_{\mathbf{p},\mathbf{p}'}$ generated by multiply scattered functions $\hat{G}_{\mathbf{k}',\mathbf{k}}$, $\mathbf{k}' \neq \mathbf{k}$ etc. (including their own renormalization). For instance, the iteration for a function $\hat{G}_{\mathbf{k}'',\mathbf{k}}$ with $\mathbf{k}'' \neq \mathbf{k}$, \mathbf{k}' in the last term in Eq. (E.2) will give:

$$\begin{aligned} \hat{G}_{\mathbf{k}'',\mathbf{k}} &= \hat{G}_{\mathbf{k}''}^{(0)} \hat{V} \frac{1}{N} \sum_{\mathbf{k}''',\mathbf{p}''} e^{i(\mathbf{k}''-\mathbf{k}''')\cdot\mathbf{p}''} \hat{G}_{\mathbf{k}''',\mathbf{k}} = \\ &= \hat{G}_{\mathbf{k}''}^{(0)} \hat{V} \frac{1}{N} e^{i(\mathbf{k}''-\mathbf{k})\cdot\mathbf{p}} \hat{G}_{\mathbf{k}} + \hat{G}_{\mathbf{k}''}^{(0)} \hat{V} \frac{1}{N} e^{i(\mathbf{k}''-\mathbf{k})\cdot\mathbf{p}'} \hat{G}_{\mathbf{k}} + \\ &\quad + \text{terms with } \hat{G}_{\mathbf{k}',\mathbf{k}} \text{ and } \hat{G}_{\mathbf{k}'',\mathbf{k}} + \text{terms with } \hat{G}_{\mathbf{k}''',\mathbf{k}} \\ &\quad (\mathbf{k}''' \neq \mathbf{k}, \mathbf{k}', \mathbf{k}''). \end{aligned} \quad (\text{E.3})$$

Consequently, the GE for $\hat{G}_{\mathbf{k}}$ obtains the form given by Eq. (6).

Now turn to TPGF

$$\langle\langle c_{-\mathbf{k}_1,\downarrow} c_{\mathbf{k}_2,\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle,$$

beginning from the equations of motion in the absence of scattering, which develop into a 4×4 matrix form:

$$\hat{B}(\xi_1, \xi_2, \Delta_1, \Delta_2) f = \delta_{0,\mathbf{q}} d, \quad (\text{E.4})$$

$$\begin{aligned} \hat{B}(\xi_1, \xi_2, \Delta_1, \Delta_2) &= \\ &= \begin{pmatrix} \varepsilon - \xi_1 - \xi_2 & \Delta_1 & \Delta_2 & 0 \\ \Delta_1 & \varepsilon + \xi_1 - \xi_2 & 0 & \Delta_2 \\ \Delta_2 & 0 & \varepsilon - \xi_1 + \xi_2 & \Delta_1 \\ 0 & \Delta_2 & \Delta_1 & \varepsilon + \xi_1 + \xi_2 \end{pmatrix}, \end{aligned}$$

with 4-vectors:

$$\begin{aligned} f &= \begin{pmatrix} \langle\langle c_{-\mathbf{k}_1,\downarrow} c_{\mathbf{k}_2,\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{\mathbf{k}_1,\uparrow}^+ c_{\mathbf{k}_2,\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{-\mathbf{k}_1,\downarrow} c_{-\mathbf{k}_2,\downarrow}^+ | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{\mathbf{k}_1,\uparrow}^+ c_{-\mathbf{k}_2,\downarrow}^+ | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \end{pmatrix}, \\ d &= \begin{pmatrix} 2\Delta_1 \Delta_2 \\ \Delta_1 \\ \Delta_2 \\ 2 \end{pmatrix}, \end{aligned}$$

and $\xi_1 \equiv \xi_{\mathbf{k}_1}$, $\xi_2 \equiv \xi_{\mathbf{k}_2}$, $\Delta_1 \equiv \Delta_{\mathbf{k}_1}$, $\Delta_2 \equiv \Delta_{\mathbf{k}_2}$. The solution to Eq. (E.4):

$$f = \delta_{0,\mathbf{q}} B^{-1}(\xi_1, \xi_2, \Delta_1, \Delta_2) d,$$

gives just the result of Eq. (37) for the 1st component of f .

In the presence of scattering, we consider only the M-nondiagonal ($\mathbf{q} \neq 0$) case, and then Eq. (E.4) turns into

$$\begin{aligned} & \hat{B}(\xi_1, \xi_2, \Delta_1, \Delta_2)f = \\ & = -\frac{1}{N} \sum_{\mathbf{p}} \left(e^{-i\mathbf{q}\cdot\mathbf{p}} \hat{A}_1 f'_1 + e^{i\mathbf{q}\cdot\mathbf{p}} \hat{A}_2 f'_2 \right), \quad (\text{E.5}) \end{aligned}$$

where the vectors of «single scattered» TPGFs are

$$f'_1 = \begin{pmatrix} \langle\langle c_{-\mathbf{k}_1+\mathbf{q},\downarrow} c_{\mathbf{k}_2,\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{\mathbf{k}_1-\mathbf{q},\uparrow}^+ c_{\mathbf{k}_2,\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{-\mathbf{k}_1+\mathbf{q},\downarrow} c_{-\mathbf{k}_2,\downarrow}^+ | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{\mathbf{k}_1-\mathbf{q},\uparrow}^+ c_{-\mathbf{k}_2,\downarrow}^+ | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \end{pmatrix},$$

$$f'_2 = \begin{pmatrix} \langle\langle c_{-\mathbf{k}_1,\downarrow} c_{\mathbf{k}_2-\mathbf{q},\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{\mathbf{k}_1,\uparrow}^+ c_{\mathbf{k}_2-\mathbf{q},\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{-\mathbf{k}_1,\downarrow} c_{-\mathbf{k}_2+\mathbf{q},\downarrow}^+ | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \\ \langle\langle c_{\mathbf{k}_1,\uparrow}^+ c_{-\mathbf{k}_2+\mathbf{q},\downarrow}^+ | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle \end{pmatrix},$$

and the 4×4 matrices:

$$\hat{A}_1 = \begin{pmatrix} \hat{V} & 0 \\ 0 & \hat{V} \end{pmatrix}, \quad \hat{A}_2 = \begin{pmatrix} \hat{V}\tau_3 & 0 \\ 0 & -\hat{V}\tau_3 \end{pmatrix}.$$

Next, the equations of motion for $f'_{1,2}$:

$$\begin{aligned} & \hat{B}(\xi'_1, \xi_2, \Delta'_1, \Delta_2) f'_1 = -\frac{1}{N} e^{-i\mathbf{q}\cdot\mathbf{p}} \hat{A}_1 f'' , \\ & \hat{B}(\xi_1, \xi'_2, \Delta_1, \Delta'_2) f'_2 = -\frac{1}{N} e^{-i\mathbf{q}\cdot\mathbf{p}} \hat{A}_2 f'' , \end{aligned} \quad (\text{E.6})$$

with

$$\xi'_1 \equiv \xi_{\mathbf{k}_1-\mathbf{q}}, \quad \xi'_2 \equiv \xi_{\mathbf{k}_2-\mathbf{q}}, \quad \Delta'_1 \equiv \Delta_{\mathbf{k}_1-\mathbf{q}}, \quad \Delta'_2 \equiv \Delta_{\mathbf{k}_2-\mathbf{q}},$$

contain the «double scattered» TPGF $f'' \equiv \langle\langle c_{-\mathbf{k}_1+\mathbf{q},\downarrow} c_{\mathbf{k}_2-\mathbf{q},\uparrow} | c_{-\mathbf{k}_2+\mathbf{q},\downarrow} c_{\mathbf{k}_1-\mathbf{q},\uparrow} \rangle\rangle$, which is already M-diagonal and hence can be taken just in the form of Eq. (37). Finally, the solution

$$\begin{aligned} & f = \hat{B}^{-1}(\xi_1, \xi_2, \Delta_1, \Delta_2) \times \\ & \times \left\{ \delta_{0,\mathbf{q}} + \frac{c}{N} [\hat{A}_1 \hat{B}^{-1}(\xi'_1, \xi_2, \Delta'_1, \Delta_2) \hat{A}_1 + \right. \end{aligned}$$

$$\left. + \hat{A}_2 \hat{B}^{-1}(\xi_1, \xi'_2, \Delta_1, \Delta'_2) \hat{A}_2] \hat{B}^{-1}(\xi'_1, \xi'_2, \Delta'_1, \Delta'_2) \right\} d, \quad (\text{E.7})$$

defines the contribution $\sim c(V_L \Delta/V)^2$ to δ^2 , Eq. (36), the factor Δ^2 being due to Δ_1, Δ_2 -odd terms from $\hat{B}^{-1}(\xi'_1, \xi_2, \Delta_1, \Delta_2)$ and $1/V^2$ due to the dominanting, zeroth order in Δ_1, Δ_2 , terms from $\hat{B}^{-1}(\xi'_1, \xi_2, \Delta'_1, \Delta'_2) \hat{B}^{-1}(\xi'_1, \xi'_2, \Delta'_1, \Delta'_2)$ and $\hat{B}^{-1}(\xi_1, \xi'_2, \Delta_1, \Delta'_2) \hat{B}^{-1}(\xi'_1, \xi'_2, \Delta'_1, \Delta'_2)$.

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