Coherent potential approximation for *d*-wave superconductivity in disordered systems

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A coherent-potential approximation CPA is developed for *s*-wave and *d*-wave superconductivity in disordered systems. We show that the CPA formalism reproduces the standard pair breaking formula, the self-consistent Born approximation and the self-consistent *T*-matrix approximation in the appropriate limits. We implement the theory and compute T_c for *s*-wave and *d*-wave pairing using an attractive nearest-neighbor Hubbard model featuring both binary-alloy disorder and a uniform distribution of scattering site potentials. We determine the density of states and examine its consequences for low-temperature heat capacity.
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I. INTRODUCTION

A treatment of disorder is an essential part of the theory of superconductivity. After all, one must explain why impurity scattering does not cause resistance. Thus it is natural that as evidence for novel superconducting states multiplies the foundations of the subject, due mainly to Anderson[1] and Abrikosov and Gorkov,[2,3] are being reexamined. The experiments which stimulate most strongly the current revival of interest in the problem are those on the high-temperature superconductors,[4] which are now universally regarded as ''*d*-wave superconductors,''[5] and those involving some of the heavy fermion systems which display signs of ''*p*-wave'' pairing.[6] In what follows, we wish to contribute to the theoretical discussion[7–14] of the issues raised by these very interesting developments.

The case of classic, ''*s*-wave,'' superconductors is by now well understood. If the perturbation does not break time-reversal symmetry and the coherence length is sufficiently long, so that the pairing potential Δ does not fluctuate, the Anderson theorem[1] guarantees that there is an absolute gap in the quasiparticle spectrum and the main effect of disorder is that the density of normal states in the gap equation is replaced by its average over configurations.[15] On the other hand, if the perturbation breaks time-reversal invariance, as is the case with paramagnetic impurities, the effect is more dramatic. For instance, the transition temperature T_c is reduced from its clean limit value T_{c0}, according to the well-known pair breaking formula

$$\ln\left(\frac{T_c}{T_{c0}}\right)=\psi\left(\frac{1}{2}\right)-\psi\left(\frac{1}{2}+\rho_c\right), \tag{1}$$

where $\psi(x)$ is the digamma function and $\rho_c=(2\pi\tau T_c)^{-1}$ is a measure of the strength of the scattering and τ^{-1} is the scattering rate.[2,7]

By contrast in the case of superconductors whose Cooper pairs are of exotic *p*-wave or *d*-wave character even simple potential scattering, which does not break time-reversal symmetry, causes pair breaking.[7] This fact was noted already in the early contributions to the field,[16] but has become a subject of intense scrutiny only recently.[7–14] Of particular interest are two-dimensional models featuring *d*-wave pairing as these may be relevant to experiments on high-T_c superconductors. Notably, for cuprates many experiments have explored the variation of T_c, the density of states and other properties as a function of Ni and Zn substitutions on the copper sites[17–24] or irradiation damage.[25–27] Although a wide variety of theoretical ideas[28–32] and methods[33–38] have been applied to interpret the experiments, a comprehensive picture of the role of disorder is far from complete. On a more formal level, an intriguing problem arises from the observation of Gorkov and Kalugin[10] that the scattering in models where the order parameter has a line of zeros on the Fermi surface is highly singular and this may be a manifestation of interesting new physics. Indeed in two dimensions, Nersesyan and co-workers[14] predict that the quasiparticle density of states $N(E)$ approaches zero, even in the disordered state, as power law $\sim|E|^{\alpha}$, with positive exponent α, instead of going to a finite value as was found by Gorkov and Kalugin.[10] Another interesting and controversial issue is the relative importance of the self-consistent Born approximation (SCBA) and resonant scattering in the unitarity limit.[11,12] Our aim here is to explore the subject systematically on the basis of explicit calculations, albeit for a simple, extended Hubbard model with attractive interactions and site diagonal randomness only.

In short, we will examine the problem of disordered unconventional superconductors making use of the coherent-potential approximation (CPA). The CPA is the most reliable approximation developed for the theory of electronic structure of random metallic alloys in the normal state.[39,40] Notably, it has been shown to be exact in both the weak and the strong scattering limits, and applicable to systems with low as well as high concentration of impurities. Significantly, the CPA reduces to the self-consistent Born approximation (SCBA) for weak scattering impurities, and agrees with the self-consistent *T*-matrix approximation (SCTA) results for strongly scattering impurities of low concentrations. Indeed, it remains a good approximation in the unitarity limit of resonant scattering.[11,12] Finally, on account of the fact that it becomes exact as the number of nearest neighbors goes to infinity, the CPA is often referred to as a mean-field theory of disorder.[41]

Given these desirable features, it is clearly worthwhile to explore the consequences of the CPA for disordered superconductors. For the case of conventional *s*-wave pairing this has already been done, generating many useful results.[42,43] The case of superconductors with Cooper pairs of *d* symmetry will be treated here within CPA, developing in detail the method introduced in our earlier paper[44] and the limited discussion in Ref. 45.

We will demonstrate that in various limits our formalism reproduces many of the well-known results for disordered superconductors, and examine in detail the phase diagram of the local and nonlocal attractive two-dimensional Hubbard models. In particular, we study the variations of T_c with impurity scattering strength and with impurity concentration for the case of local *s*-wave pairing as well as nonlocal (extended) *s*-wave and *d*-wave pairing. We also contrast the cases for a binary alloy, *A*-*B* type, disorder with the case of uniformly distributed scattering potentials on each site. Finally, we investigate the density of states (DOS), $N(E)$, at low energies and its consequences for measurements of the specific heat.

II. INCORPORATING CPA INTO BOGOLIUBOV-DE GENNES EQUATION

Our starting point is the single band Hubbard model with an attractive extended interaction which is described by the following Hamiltonian:

$$H=\sum_{ij\sigma} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}+\frac{1}{2}\sum_{ij} U_{ij}\hat{n}_i\hat{n}_j-\sum_{i}(\mu-\varepsilon_i)\hat{n}_i, \quad (2)$$

where $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are, respectively, the usual creation and annihilation operators for electrons on site i with spin σ, and the local charge operator is $\hat{n}_i=\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}$ with $\hat{n}_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$. The chemical potential is μ, t_{ij} are the hopping integrals (for $i\neq j$) and ϵ_i is the local site energy. The interaction term U_{ij} can be either a local attractive interaction ($U_{ii}<0$) giving rise to *s*-wave pairing, or a nonlocal attractive interaction ($U_{ij}<0$ for $i\neq j$) giving rise to *d*-wave or extended *s*-wave pairing. Disorder is introduced into the problem by allowing the site energies ε_i to vary randomly from site to site.

Starting from Eq. (2) we apply the Hartree-Fock-Gorkov[46,47] approximation, which results in the following Bogoliubov-de Gennes equation:

$$\sum_{l}\begin{pmatrix}(\imath\omega_n-\varepsilon_i+\mu)\delta_{il}+t_{il} & \Delta_{ij}\\ \Delta^{*}_{ij} & (\imath\omega_n+\varepsilon_i-\mu)\delta_{il}-t_{il}\end{pmatrix}\times\begin{pmatrix}G_{11}(l,j;\imath\omega_n) & G_{12}(l,j;\imath\omega_n)\\ G_{21}(l,j;\imath\omega_n) & G_{22}(l,j;\imath\omega_n)\end{pmatrix}=\delta_{ij}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \quad (3)$$

for the Green's-function matrix $\boldsymbol{G}(i,j;\imath\omega_n)$ at the Mastusbara frequency $\omega_n=(2n+1)\pi k_BT$, in units where $\hbar=1$. For computational convenience we shall take the hopping integral t_{ij} to be nonzero only when the sites i and j are nearest neighbors. The mean-field pairing potential Δ_{ij} can either be local ($i=j$) or nearest-neighbor nonlocal. Of course, the above equations are completed by the self-consistency condition that

$$\Delta_{ij}=|U_{ij}|\frac{1}{\beta}\sum_{n} e^{\imath\omega_n\eta}G_{12}(i,j;\imath\omega_n), \quad (4)$$

where η is a positive infinitesimal. To simplify matters we have assumed that the normal Hartree and exchange terms can be absorbed into the definitions of the chemical potential μ or the hopping integrals t_{ij}. As usual, Eqs. (3) and (4) are to be solved subject to the requirement on the chemical potential that

$$n_i=\frac{2}{\beta}\sum_{n} e^{\imath\omega_n\eta}G_{11}(i,i;\imath\omega_n), \quad (5)$$

where n_i is the number of electrons at site i. Clearly, the Green's-function matrix $\boldsymbol{G}(i,j;\imath\omega_n)$ determined by the above equations depends on the set of site energies $\{\varepsilon_i\}$. Our task is to find the configurationally averaged Green's-function matrix $\langle\boldsymbol{G}(i,j;\imath\omega_n)\rangle$. Evidently, this is made much easier if we assume that the pairing potential does not fluctuate from configuration to configuration. As was argued by Györffy, Litak, and Wysokiński[15] for *s*-wave superconductors this is a good approximation when the $T=0$ coherence length ξ_0 is large. Thus our specific results will have to be treated with appropriate care when applied to superconductors with *d*-wave symmetry or short coherence length such as superconducting cuprates.

Let us now proceed to deploy the CPA strategy for calculating the averaged Green's function matrix $\langle\boldsymbol{G}(i,j;\imath\omega_n)\rangle$ subject to the self-consistency conditions:

$$\overline{\Delta}_{ij}=|U_{ij}|\frac{1}{\beta}\sum_{n} e^{\imath\omega_n\eta}\langle G_{12}(i,j;\imath\omega_n)\rangle, \quad (6)$$

$$\overline{n}=\frac{2}{\beta}\sum_{n} e^{\imath\omega_n\eta}\langle G_{11}(i,i;\imath\omega_n)\rangle. \quad (7)$$

The first move in deriving the fundamental equations of the coherent potential approximation is to define a coherent medium Green's-function matrix $\boldsymbol{G}^{c}(i,j;\imath\omega_n)$ by

$$\sum_{l}\begin{pmatrix}[\imath\omega_n+\mu-\Sigma_{11}(\imath\omega_n)]\delta_{il}+t_{il} & \overline{\Delta}_{il}\\ \overline{\Delta}^{*}_{il} & [\imath\omega_n-\mu-\Sigma_{22}(\imath\omega_n)]\delta_{il}-t_{il}\end{pmatrix}\boldsymbol{G}^{c}(l,j;\imath\omega_n)=\delta_{ij}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \quad (8)$$

As will be clear later, $\boldsymbol{G}^c(i,j;\imath\omega_n)=\langle \boldsymbol{G}(i,j;\imath\omega_n)\rangle$ and hence $\Sigma_{11}(\imath\omega_n)$ and $\Sigma_{22}(\imath\omega_n)$ are the diagonal components of the usual self-energy. Note that we did not introduce any off-diagonal self-energies such as $\Sigma_{12}(\imath\omega_n)$ and $\Sigma_{21}(\imath\omega_n)$, because for the single site perturbations of our model they are zero. The next step is to consider the scattering of the quasiparticles, propagating according to $\boldsymbol{G}^c(i,j;\imath\omega_n)$ by the defects described by the potentials:

$$\boldsymbol{V}^l(\imath\omega_n)=\begin{pmatrix} \varepsilon_l & 0 \\ 0 & -\varepsilon_l \end{pmatrix}-\begin{pmatrix} \Sigma_{11}(\imath\omega_n) & 0 \\ 0 & \Sigma_{22}(\imath\omega_n) \end{pmatrix}, \tag{9}$$

where l labels one of the m different site energies we wish to consider.

In a straightforward application of the CPA principles,[40] $\Sigma(\imath\omega_n)$ and therefore $\boldsymbol{G}^c(i,j;\imath\omega_n)$ is determined by the condition that these defects do not scatter on the average, i.e.,

$$\sum_{l=1}^{m} c_l \boldsymbol{T}^l(\imath\omega_n)=0, \tag{10}$$

where

$$\boldsymbol{T}^l(\imath\omega_n)=\boldsymbol{V}^l(\imath\omega_n)[\mathbf{1}-\boldsymbol{G}^c(i,i;\imath\omega_n)\boldsymbol{V}^l]^{-1} \tag{11}$$

and the concentration of sites of energy ε_l is c_l, obeying

$$\sum_{l=1}^{m} c_l=1. \tag{12}$$

From Eqs. (10) and (11) it is now possible, in conjunction with Eqs. (6)–(8), to calculate $\Sigma(\imath\omega_n)$ and $\boldsymbol{G}^c(i,j;\imath\omega_n)$. The numerical methodology for calculating $\boldsymbol{G}^c(i,j;\imath\omega_n)$ and $\Sigma(\imath\omega_n)$ closely follows that in Ref. 48.

A number of recent studies of superconductors with unconventional pairing suggest that the consequences of disorder depend sensitively on the models used to describe the randomness.[49,50] Thus we are going to investigate two different models. The first corresponds to binary-alloy disorder, where $m=2$. Namely, we consider two *types* of sites with site energies ε_1 and ε_2 and concentrations of c and $1-c$, respectively. The second model is described by a uniform distribution of site energies. Here we shall have in mind the limit where $m\to\infty$ with $\varepsilon_l\in[-\delta/2,\ \ \delta/2]$. Consequently, in Eq. (10) the sum Σ_l becomes the integral $(1/\delta)\int d\varepsilon_l$.

In the bimodal case, where $m=2$, we can simplify Eq. (10) to find

$$\Sigma_{11}(\imath\omega_n)=(2c-1)\frac{\delta}{2}-\left(\frac{\delta}{2}-\Sigma_{11}(\imath\omega_n)\right) \times G^c_{11}(\imath\omega_n)\left(-\frac{\delta}{2}-\Sigma_{11}(\imath\omega_n)\right), \tag{13}$$

where $|\varepsilon_1-\varepsilon_2|=\delta$, while for uniform distribution one gets

$$\Sigma_{11}(\imath\omega_n)=-\frac{1}{G^c_{11}(\imath\omega_n)}+\frac{\delta}{2}\frac{1}{\tanh\left(\dfrac{\delta G^c_{11}(\imath\omega_n)}{2}\right)}. \tag{14}$$

Thus our CPA calculations will consist of solving numerically either Eq. (13) for the bimodal distribution of the site energies, or Eq. (14) for the case of uniform distribution, to determine the self-energies $\Sigma_{11}(\imath\omega_n)$ and $\Sigma_{22}(\imath\omega_n)$.

III. PAIR BREAKING FORMULA IN CPA

We now relate the CPA formulas derived above to the usual results of disordered superconductors, corresponding to the well-known pair breaking formula Eq. (1). As is well known,[7] the pair breaking formula was first derived for magnetic impurities in *s*-wave superconductors[2] but it also applies in many other interesting circumstances such as our present concern, namely, the case of nonmagnetic impurities in *d*-wave superconductors.[16]

To derive it within the CPA let us start with the gap equation

$$\Delta_{\vec{k}}=\frac{1}{N}\sum_{\vec{q}} U_{\vec{k}-\vec{q}}\frac{1}{\beta}\sum_{\omega_n} G^c_{12}(\vec{q};\imath\omega_n)e^{\imath\omega_n\delta}. \tag{15}$$

As a motivation for our argument we recall the method of Abrikosov and Gorkov[2] for solving the gap equation at T_c for a clean superconductor. In that case, to find T_c we linearize the analog of Eq. (15) by approximating the off-diagonal Green's function G^c_{12} as follows:

$$G^c_{12}(\vec{q};\imath\omega_n)\cong\frac{-\Delta_{\vec{q}}}{(\imath\omega_n-\xi_{\vec{q}})(\imath\omega_n+\xi_{\vec{q}})}, \tag{16}$$

where $\xi_{\vec{q}}=\varepsilon_{\vec{q}}-\mu$, and for our tight-binding model with a square lattice $\varepsilon_{\vec{q}}=-2t[\cos(q_x)+\cos(q_y)]$. Then, we note that the kernel of the linear integral equation for $\Delta_{\vec{k}}$ is a four-term degenerate kernel:

$$U(\vec{k}-\vec{q})=|U|\left(\frac{\eta_{\vec{k}}\eta_{\vec{q}}+\gamma_{\vec{k}}\gamma_{\vec{q}}}{4}+2\sin k_x\sin q_x +2\sin k_y\sin q_y\right), \tag{17}$$

where $\eta_{\vec{k}}=2[\cos(k_x)-\cos(k_y)]$ and $\gamma_{\vec{k}}=2[\cos(k_x)+\cos(k_y)]$. Consequently, the general $\Delta_{\vec{k}}$ will be a linear superposition of $\eta_{\vec{k}}$, $\gamma_{\vec{k}}$, $\sin k_x$, and $\sin k_y$. However, when the internal symmetry of the singlet Cooper pair is pure *d* wave we may take $\Delta_{\vec{k}}$ to be of the form

$$\Delta_{\vec{k}}=\Delta\,\eta_{\vec{k}}. \tag{18}$$

Then the condition for nonzero order parameter becomes

$$1=\frac{|U|}{N}\sum_{\vec{q}}\frac{\eta^2_{\vec{q}}}{4}T_{c0}\sum_{\omega_n}\frac{1}{\omega_n^2+\xi^2_{\vec{q}}}. \tag{19}$$

Let us now define a *d*-wave weighted density of states:

$$N_d(E)=\frac{1}{N}\sum_{\vec{q}}\frac{\eta^2_{\vec{q}}}{4}\delta(E-\xi_{\vec{q}}) \tag{20}$$

and write the above condition, which determines the transition temperature T_{c0}, as

$$1=|U|\int_{-\infty}^{\infty}dE N_d(E)T_{c0}\sum_{\omega_n>0}\frac{2}{\omega_n^2+E^2}, \tag{21}$$

where $\omega_n = \pi T_{c0}(2n+1)$. In the above equation the integral and the sum are divergent, so we need to introduce a cutoff, ω_n^c. In the usual way we assume the density of states $N_d(E)$ is slowly varying up to the cut-off energy, so we will make the approximation $N_d(E) = N_d(0)$. Then, considering that

$$N_d(0)\int_{-\infty}^{\infty} dE \frac{1}{\omega_n^2 + E^2} = \pi N_d(0)\frac{1}{\omega_n}, \tag{22}$$

we can write

$$1 = |U| N_d(0) 2\pi T_{c0} \sum_{\omega_n>0}^{\omega_n^c} \frac{1}{\omega_n} \tag{23}$$

and hence rewrite Eq. (21) as

$$\frac{1}{|U|N_d(0)} = \psi\left(\frac{1}{2} + \frac{\omega_n^c}{2\pi T_{c0}}\right) - \psi\left(\frac{1}{2}\right) \approx \ln\left(\gamma \frac{\omega_n^c}{2\pi T_{c0}}\right). \tag{24}$$

This is the BCS result for the superconducting transition temperature in the case of *d*-wave pairing.[46] It differs from the conventional result only in that the *d*-projected density of states $N_d(0)$ has replaced the usual full density of states $N(0)$.

Let us now return to disordered superconductors and examine how the above well-known argument is modified when the randomness is dealt with within the CPA. Using Eq. (8) it can be easily seen that instead of Eq. (16) we should use

$$G_{12}^c(\vec{q}; \imath\omega_n) = \frac{-\overline{\Delta}_{\vec{q}}}{(\imath\omega_n - \xi_{\vec{q}} - \Sigma_{11}(\imath\omega_n))[\imath\omega_n + \xi_{\vec{q}} - \Sigma_{22}(\imath\omega_n)]} \tag{25}$$

to linearize Eq. (15) at T_c. Thus noting that

$$\Sigma_{22}(\imath\omega_n) = -\Sigma_{11}(-\imath\omega_n), \tag{26}$$

the condition which determines T_c can be written as

$$1 = -|U|\int_{-\infty}^{\infty} dE N_d(E) T_c \times \sum_{\omega_n>0} \frac{2}{[\imath\omega_n - E - \Sigma_{11}(\imath\omega_n)][\imath\omega_n + E + \Sigma_{11}(-\imath\omega_n)]}. \tag{27}$$

Now, at this point we need to know the form of $\Sigma_{11}(\imath\omega_n)$ to progress any further. As a first approximation we assume that the most important component to the self-energy is the component at the Fermi energy $E = E_F = \mu$. Later on we will test the accuracy of this approximation by examining our numerical results for $\Sigma_{11}(\imath\omega_n)$. For now, however, let us proceed by taking

$$\Sigma_{11}(\imath\omega_n) = \imath|\Sigma_0|\mathrm{sgn}(\omega_n). \tag{28}$$

Evidently this leads to

$$1 = -|U|\int_{-\infty}^{\infty} dE N_d(E) T_c \times \sum_{\omega_n>0} \frac{2}{(\imath\omega_n - E + \imath|\Sigma_0|)(\imath\omega_n + E + \imath|\Sigma_0|)}. \tag{29}$$

Again taking $N_d(E)$ outside of the integration as $N_d(0)$ and performing the integration over E, we find

$$1 = |U| N_d(0) 2\pi T_c \sum_{\omega_n>0}^{\omega_n^c} \frac{1}{\omega_n + |\Sigma_0|}, \tag{30}$$

where again the sum is cut off, as in the clean limit, by ω_n^c. If we now add and subtract the terms corresponding to $\Sigma_0 = 0$ (the clean case) we find

$$\frac{1}{|U|N_d(0)} = 2\pi T_c \sum_{\omega_n>0}^{\omega_n^c} \frac{1}{\omega_n} + 2\pi T_c \sum_{\omega_n>0}^{\omega_n^c} \left(\frac{1}{\omega_n + |\Sigma_0|} - \frac{1}{\omega_n}\right). \tag{31}$$

Clearly the term $1/|U|N_d(0)$ on the left-hand side of Eq. (31) can be replaced by $\ln[\gamma(\omega_n^c/2\pi T_{c0})]$ on account of Eq. (24). With the same accuracy, the first sum on the RHS of Eq. (31) equals $\ln[\gamma(\omega_n^c/2\pi T_c)]$ and the second sum is convergent. Hence the cutoff ω_n^c can be extended to infinity. As has been noted frequently before, this infinite sum can be readily performed[2] and we find

$$\ln\left(\frac{T_c}{T_{c0}}\right) = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \rho_c\right), \tag{32}$$

where

$$\rho_c = \frac{|\Sigma_0|}{2\pi T_c}. \tag{33}$$

Equations (32) and (33) are the central results of this section. Reassuringly, while Eq. (32) is the standard pair breaking formula,[7] Eq. (33) is a very natural CPA expression for the pair breaking parameter ρ_c. Recall that our derivation of the above result from CPA involved the approximation $\Sigma_{11}(\imath\omega_n) \cong \imath\Sigma_0$. To test the validity of this approximation we wish to compare exact CPA numerical results with the predictions of the analytical expression: Eqs. (32) and (33). Using numerical solutions of the CPA equation, to be discussed latter, Fig. 1 plots the pair breaking strength ρ_c vs δ/t, the disorder strength for the binary alloy-type disorder. To find pair breaking parameter ρ_c we calculated T_c for each disorder strength δ/t and inverted Eq. (32) to obtain an effective ρ_c. The exact CPA ρ_c can then be compared to the solid line in Fig. 1 where we have taken our numerically calculated values for Σ_0 and directly calculated ρ_c, via Eq. (33). Finally, the dashed line in Fig. 1 corresponds to ρ_c obtained using the self-consistent Born approximation (SCBA). Evidently, the self-energy at the Fermi energy, $E - \mu = 0$, Σ_0, gives a good description of the pair breaking parameter ρ_c via Eq. (32). Also it is clear that, as expected, the self-consistent Born approximation $\Sigma_0 \equiv \hbar/\tau = \pi\delta^2 N(0)$ only works well in the weak scattering limit.

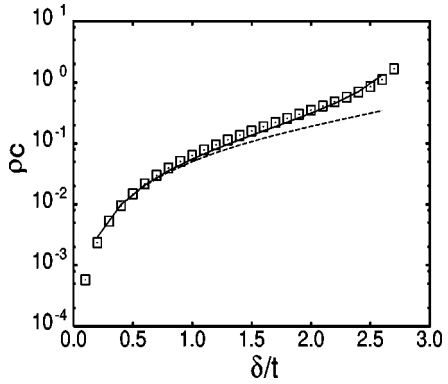


FIG. 1. The effective pair breaker ρ_c as calculated (i) by numerically finding T_c/T_{c0} and inverting Eq. (32) (squares), (ii) numerically finding $|\Sigma_0|$ and using this in Eq. (33) (solid line), and (iii) using the self-consistent Born approximation to find $|\Sigma_0|$ and then evaluating Eq. (33) (dashed line).

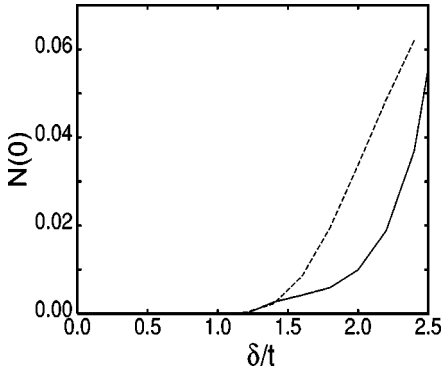


FIG. 2. A comparison of the density of states at the chemical potential vs different strengths of alloyed disorder $\epsilon_i = \pm \delta/2$. The solid line is the analytical form derived in Eq. (43) and the dashed one represents our self-consistent numerical calculations.

IV. ANALYTICAL FEATURES AND PREDICTIONS OF CPA EQUATIONS

In this section we examine various analytically accessible limits of the CPA formalism described above. First, we demonstrate that Anderson's theorem is obeyed for *s*-wave superconductors and the CPA equations are consistent with the results of Abrikosov and Gorkov.[2] Second, we show that for *d*-wave superconductors the quasiparticle density of states at the Fermi energy $N(0)$ is nonzero in the presence of nonmagnetic disorder scattering and is consistent with the results of Gorkov and Kalugin.[10]

A. Anderson's theorem in coherent-potential approximation

Formally, the CPA Eqs. (10) and (11) can be written in terms of renormalized Matsubara frequencies $\tilde{\omega}_n$, pairing parameter $\tilde{\Delta}_{\vec{k}}$, and particle energies $\tilde{\xi}_{\vec{k}}$. These quantities are defined as follows:

$$\tilde{\omega}_n = \omega_n \left(1 - \frac{\mathrm{Im}\,\Sigma_{11}(\imath\omega_n)}{\omega_n} \right), \tag{34}$$

$$\tilde{\Delta}_{\vec{k}} = \overline{\Delta}_{\vec{k}}, \tag{35}$$

$$\tilde{\xi}_{\vec{k}} = \xi_{\vec{k}} - \mu + \mathrm{Re}\,\Sigma_{11}(\imath\omega_n), \tag{36}$$

consequently

$$G_{11}(\imath\omega_n) = \frac{1}{N} \sum_{\vec{k}} \frac{\imath\tilde{\omega}_n + \tilde{\xi}_{\vec{k}}}{(\imath\tilde{\omega}_n)^2 - \tilde{\xi}_{\vec{k}}^2 - \tilde{\Delta}_{\vec{k}}^2} \tag{37}$$

and for the alloy-type disorder with $c = 0.5$ and $\varepsilon_l = \pm \delta/2$, the self-energy $\Sigma_{11}(\imath\omega_n)$ which renormalizes $\omega_n, \Delta_{\vec{k}}$, and $\xi_{\vec{k}}$, and is defined by Eq. (13), can be written as

$$\Sigma_{11}(\imath\omega_n) = \frac{(\delta^2/4) G^c_{11}(\imath\omega_n)}{1 + G^c_{11}(\imath\omega_n)\Sigma_{11}(\imath\omega_n)}. \tag{38}$$

The alternative expression for $\Sigma_{11}(\imath\omega_n)$ in the case of a uniform distribution of local potentials, $-\delta/2 < \varepsilon_l < \delta/2$, is given in Eq. (14).

Note that in the case of a nonisotropic, *d*-wave gap, $\Delta_{\vec{k}}$ is not renormalized if the disorder is diagonal both in site and Nambu space. This is different from the case of local *s*-wave pairing where, as can be readily shown, $\Delta_{\vec{k}}$ is renormalized by the same factor as $\tilde{\omega}_n$ in Eq. (34). Thus for conventional superconductors, in contradiction to Eqs. (34)–(37), we find that the CPA yields

$$\frac{\tilde{\omega}_n}{\omega_n} = \frac{\tilde{\Delta}}{\Delta}, \tag{39}$$

in agreement with Born approximation or Abrikosov-Gorkov theory.[2] As is widely appreciated,[2,15] the above equation implies the Anderson's theorem in *s*-wave superconductors. By contrast in the *d*-wave case represented by Eqs. (34), Eq. (39) does not hold and hence there is no Anderson theorem.

Finally, in concluding this section, we would like to stress that Eqs. (34)–(38) represent strictly a pure *d*-wave result. Even if we stick to the singlet case, a more general solution of the CPA equation will imply a renormalization of $\overline{\Delta}_{\vec{k}}$ to $\tilde{\Delta}_{\vec{k}}$. A good example of such a situation is a case where the symmetry of $\overline{\Delta}_{\vec{k}}$ is of extended *s*-wave symmetry $s^* \propto [\cos(k_x) + \cos(k_y)]$ type. We shall encounter this interesting circumstance later on in this paper.

B. Density of states $N(0)$ in *d*-wave superconductors

Moving on and returning to the *d*-wave case, we observe that the form of Eqs. (34)–(38) are the same as were found by Larkin.[16] Thus again the CPA reproduces the expected general form of the gap and frequency renormalizations, but with an improved description of the disorder. The most prominent feature of a conventional superconductor is vanishing of the quasiparticle density of states $N(E)$ for energies E measured from the Fermi energy E_F, less than Δ. In the case of clean, *d*-wave superconductors, the line of zeros of $\Delta_{\vec{k}}$ on the Fermi surface leads to finite $N(E)$ for all E except $E = 0$. In fact, as is well known,[7] $N(E)$ approaches zero linearly in E. In the present section we shall investigate what happens to $N(E)$ in the presence of disorder.

As it turns out for a given gap parameter $\overline{\Delta}_{\vec{k}} = \Delta\,\eta_{\vec{k}}$ and in the limit of small disorder $\delta \to 0$ the CPA equations can be solved analytically. To affect the solution note that in Eq.

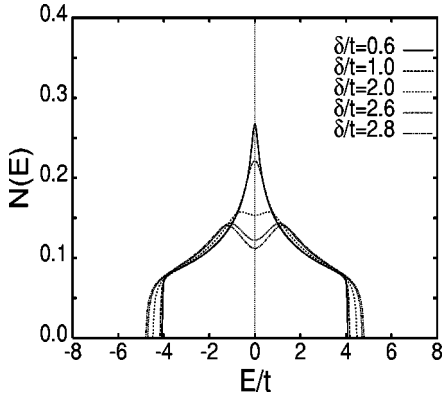


FIG. 3. Density of states $N(E)$ for a normal state with various alloyed disorder strengths δ/t and $n=1$.

(37) the major part of the summation is coming from the four singular points in the Brillouin zone where the denominator vanishes. Linearizing around these points and performing the summation over k analytically, we find that

$$G_{11}^{c}(0)=\frac{\imath\,\mathrm{Im}\,\Sigma_{11}(0)}{2\alpha}\ln\left|\frac{(4\Delta)^2+[\mathrm{Im}\,\Sigma_{11}(0)]^2}{[\mathrm{Im}\,\Sigma_{11}(0)]^2}\right|, \quad (40)$$

where $\alpha=2t\Delta\pi$. Clearly in the limit $|\mathrm{Im}\ \Sigma_{11}(0)|\ll 4\Delta$ this leads to

$$G_{11}^{c}(0)\approx\frac{\imath\,\mathrm{Im}\ \Sigma_{11}(0)}{\alpha}\ln\left|\frac{4\Delta}{\mathrm{Im}\ \Sigma_{11}(0)}\right|. \quad (41)$$

Moreover, when $\Sigma_{11}(\imath\omega_n)$ is small compared to the bandwidth, we can rewrite Eq. (38) as

$$\Sigma_{11}(\imath\omega_n)=\frac{\delta^2}{4}G_{11}^{c}(\imath\omega_n), \quad (42)$$

which is the result one gets in self-consistent Born approximation. On substituting this result into Eq. (41) the latter becomes an equation for $G_{11}^{c}(0)$ which determines the density of quasiparticles states $N(0)$ via the formula $N(0)=(1/\pi)G_{11}^{c}(\imath\omega_n=0)$. Indeed, we find

$$N(0)\approx\frac{4\Delta t}{\pi\delta^2}e^{-8\pi\Delta t/\delta^2} \quad (43)$$

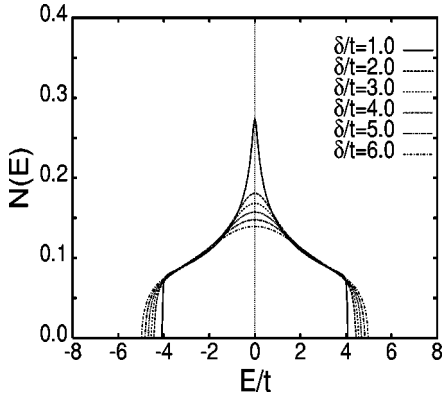
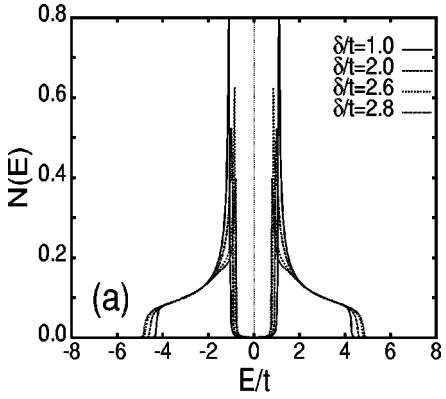


FIG. 4. Density of states $N(E)$ for a normal state with various uniform disorder strengths δ/t and $n=1$.



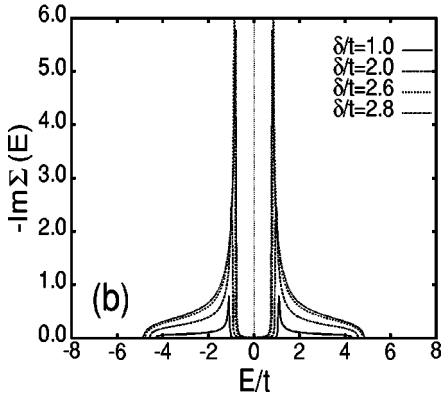


FIG. 5. (a) Density of states $N(E)$ and (b) self-energies $\mathrm{Im}\ \Sigma(E)$ for a superconducting state with various alloyed disorder strengths δ/t, calculated for a local interaction $|U|=3.5t$ and $n=1$.

and

$$-\mathrm{Im}\,\Sigma_{11}(0)\approx 4\Delta t e^{-8\pi\Delta t/\delta^2}. \quad (44)$$

These formulas agree with the results of Kalugin and Gorkov[10] and Haas *et al.*[28] and have been verified numerically. For example, Fig. 2 compares $N(0)$ as calculated from Eq. (43) and calculated using completely self-consistent CPA. As one can see, for $\delta/t\ll 1$ there is good agreement between the two results and thus we conclude that at $E=0$ the density of states, in CPA, becomes finite when an arbitrary small amount of disorder is introduced. For a more detailed description of what is happening to $N(0)$ and $-\mathrm{Im}\ \Sigma_{11}(0)$, in the presence of disorder, see Sec. VII of this paper, where we have analyzed their properties more closely and report, extensively, further numerical results.

V. LOCAL QUASIPARTICLE DENSITY-OF-STATES CALCULATIONS

In this section we present results for the single site local quasiparticle density-of-states calculations. As mentioned before, we consider two types of disorder: (i) binary alloys where we have two on-site potentials randomly distributed throughout the lattice and (ii) a uniform distribution of random on-site potentials. For both types of disorder we have solved, numerically, Eq. (8) in conjunction with its appropriate self-consistency conditions, for the order parameter Δ the average number density n, and the self-energy $\Sigma_{11}(\imath\omega_n)$.

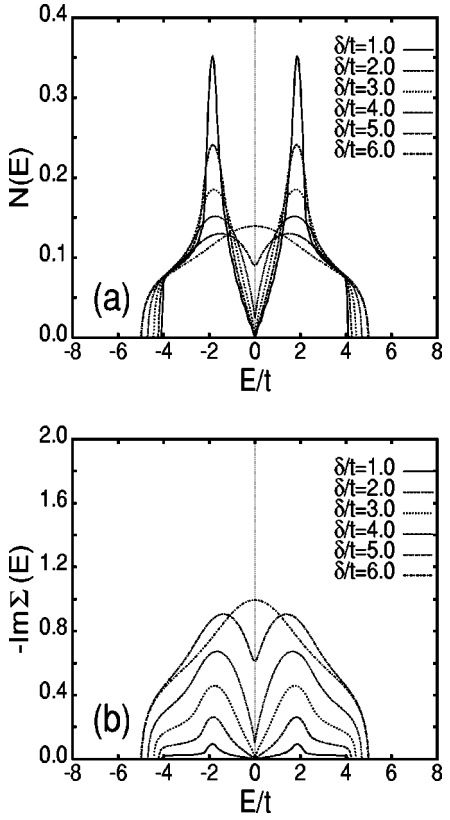


FIG. 6. (a) Density of states $N(E)$ and (b) self-energies Im $\Sigma(E)$ for a superconducting state with various uniform disorder strengths δ/t, calculated for a nonlocal interaction $|U|=3.5t$ and $n=1$.

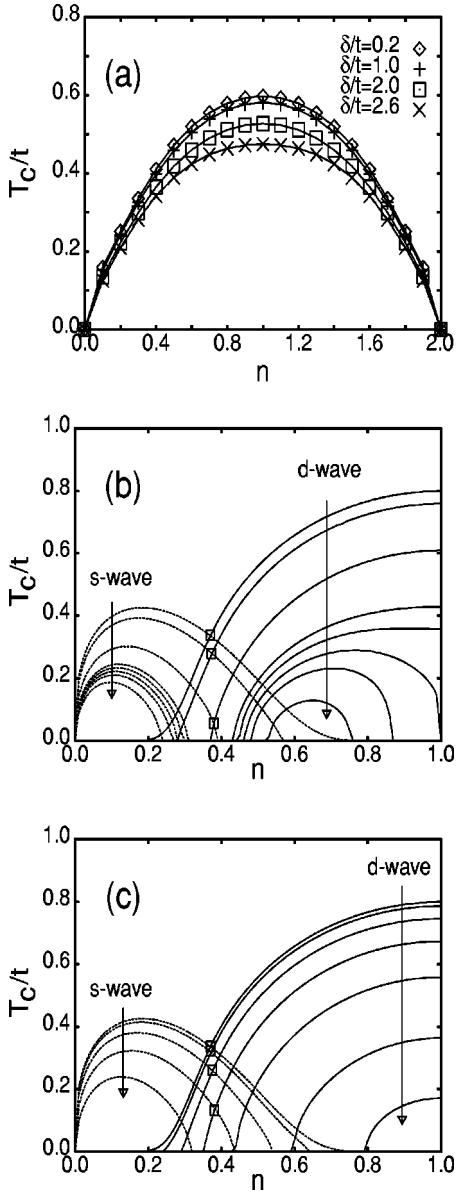


FIG. 7. Critical temperature T_c vs band filling n. (a) An *s*-wave superconductor with alloyed disorder, and a local interaction $|U|=3.5t$. (b) *d*-wave and extended *s*-wave critical temperature T_c with alloyed disorder, calculated for a nonlocal interaction $|U|=3.5t$ and $\delta/t=$ 0,1.2,2.0,2.5,2.6,2.7,2.8,3.0 from top to bottom curve. (c) As for (b) but for the case of uniform disorder ($\delta/t=0,1.0,2.0,3.0,$ 4.0,5.0,6.0 from top to bottom curve).

The first situation we consider is a binary alloy of random on-site energies ε_1 and ε_2 with equal concentration $c=1-c=0.5$. The parameter we have chosen to use to describe the strength of the disorder is $\delta=\varepsilon_1-\varepsilon_2$. Figure 3 shows the density of states in the normal state. The Van Hove singularity characteristic of a tight-binding model with nearest-neighbor hopping on a square lattice is clearly visible for small disorder ($\delta=0.6t$) in the middle of the band. As Fig. 3 shows, for more strongly disordered alloys this Van Hove peak is split into two peaks with some additional smearing. In the limit of δ being very large we get, as one would expect, band splitting of states associated with ε_1 and ε_2, respectively. On the other hand the disorder with uniform distribution of site energies, Fig. 4, gives only the smearing and flattening of density of states with, eventually, a complete flattening of the Van Hove peak.

Before turning to the problem of disordered *d*-wave superconductors for reference we have studied, briefly, the *s*-wave case. In short, we have introduced a site-diagonal, local, attractive interaction with strength U into the above model. As expected, such interaction leads to conventional *s*-wave pairing. When implementing the CPA we have assumed that in this case the pairing order parameter Δ, which is now site diagonal, does not vary from site to site. This is consistent with the Anderson theorem which was shown to be adequate for systems with a long coherence length.[15] Figure 5(a) shows the *s*-wave quasiparticle density of states as calculated for various values of the binary-alloy disorder strength δ. The results confirm that, for *s*-wave pairing, the gap is absolute and, while the edges may move, they remain well defined as required by Anderson's theorem.[1] In Fig. 5(b) we have also plotted the self-consistent self-energy as a function of the quasiparticle energy, for the same disorder strengths used to obtain Fig. 5(a). From this graph we can see that $-\mathrm{Im}\,\Sigma_{11}(E)$ is zero inside the gap and hence the normal disorder does not act as a pair breaker, for *s*-wave superconductivity.

The quasiparticle density of states for *d*-wave superconductors is dramatically different from the above BCS spectrum in the *s*-wave case even in the clean limit. As is well known, it has the characteristic v-like dip shown in Fig. 6(a),

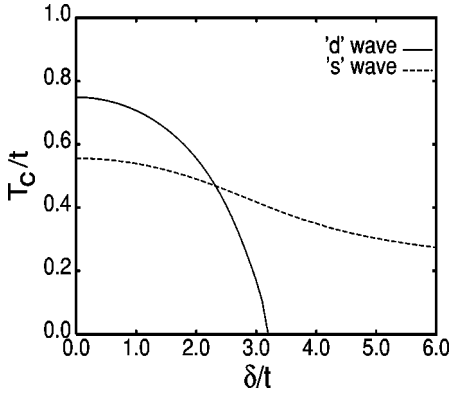


FIG. 8. Critical temperature of *d*-wave (solid line) and local *s*-wave (dashed line) superconducting pairing states as a function of alloyed disorder for $|U|=3.5t$, $n=0.6$, and $c=0.5$.

for E near the chemical potential ($\mu=0$). Upon introducing disorder into the *d*-wave system one would naturally expect similarly different behavior from that described above and in Fig. 5(a). As is clear from the results reported in Fig. 6 this is indeed the case. Strikingly, as the analytic results of the previous section suggested, $N(0)$ becomes nonzero for the slightest disorder. This implies gapless superconductivity in contrast to the gapped one in the *s*-wave case. These observations apply to both the uniform disorder case of Fig. 6(a) and the case of alloy disorder presented earlier.[44]

In Fig. 6(b) we have plotted the self-energies, corresponding to the quasiparticle density-of-states results presented in Fig. 6(a). This shows a complex evolution with disorder, for small δ the imaginary part of the self-energy $\Sigma(E)$ reflects the pure *d*-wave density of states (as expected in the SCBA limit) and hence $\mathrm{Im}[\Sigma(0)]\sim 0$. However, increasing δ leads to a finite $\Sigma(0)$, with a cusplike minimum in $\mathrm{Im}[\Sigma(E)]$ at $E=0$. Increasing the disorder even further, to $\delta=2.8t$, the *d*-wave pairing is completely destroyed, and $\mathrm{Im}\,\Sigma(E)$ reverts to the normal system self-energy. In this case $-\mathrm{Im}\,\Sigma(E)$ is a maximum at $E=0$, since the Fermi energy $E_F=\mu$ was set exactly to 0.

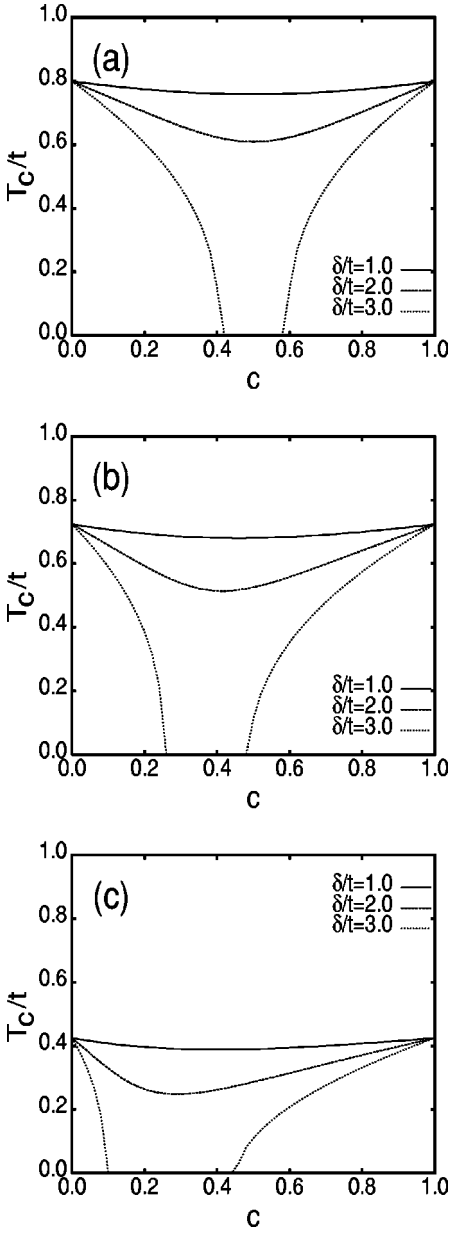


FIG. 9. Critical temperature vs concentration, at different alloyed disorder strengths, for a nonlocal interaction $|U|=3.5t$. (a) The case $n=1.0$, (b) $n=0.7$, (c) $n=0.1$.

VI. CRITICAL TEMPERATURE CALCULATIONS

To analyze the effect of the disorder upon T_c we have solved the gap equation together with the CPA equations. Again for the sake of comparison we have developed the analogous theory for the conventional *s*-wave superconductors based on the site-diagonal particle-particle interaction, of strength U_0, mentioned briefly in a previous section. In this case neglecting the spatial fluctuations of Δ_i, and linearizing the gap equation for the configurationally averaged single-site pairing potential $\overline{\Delta}$ we find the condition for the temperature T_c, below which $\overline{\Delta}\neq 0$, to be

$$1=|U_0|\int_{-\infty}^{\infty} dE\frac{\overline{N}(E)}{2E}\tanh\left(\frac{\beta_c E}{2}\right), \tag{45}$$

where $\overline{N}(E)$ is the averaged density of states in the normal state at energy E, as calculated within the CPA, and $\beta_c=1/k_B T_c$.

The solution of Eq. (45) for T_c as a function of band filling and strengths of alloyed disorder δ is shown in Fig. 7(a). From this figure we can see that the superconducting state exists for all band filling and the strength of disorder does little to suppress T_c. Again this is consistent with Anderson's theorem.

Now let us turn to the case where the interaction is nonlocal and the pairing potential Δ_{ij} connects nearest-neighbors sites. Near T_c, where the gap equation is linear, the solutions can be labeled by their symmetries. Indeed, we find two separate conditions on the temperature T_c for the instability

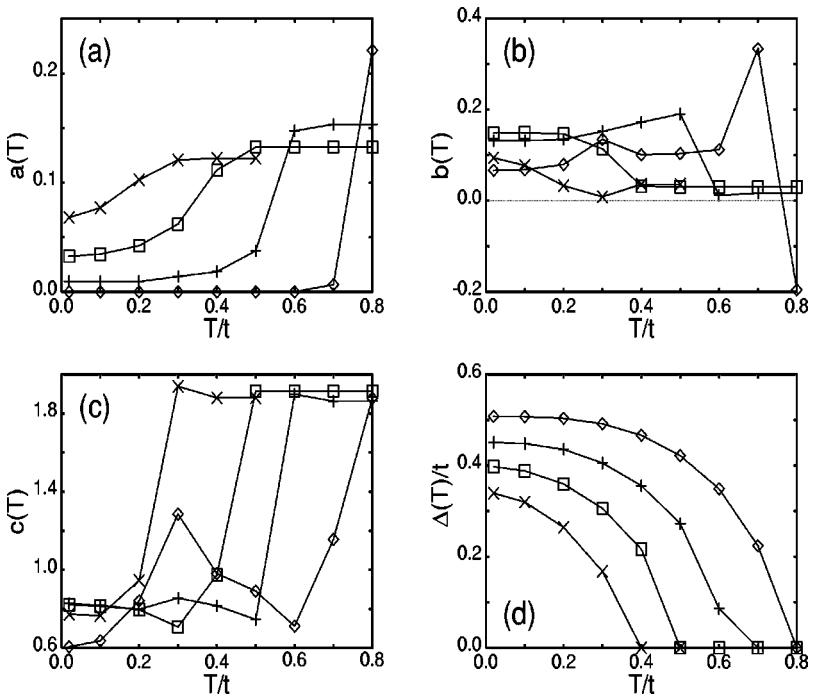


FIG. 10. The coefficients *a* (a), *b* (b), and *c* (c) which represent the local particle density of states in the region of the chemical potential as a function of temperature, for different alloyed disorder strengths δ [$\delta=0.6t$ (diamonds), $\delta=1.0t$ (+), $\delta=2.0t$ (squares), and $\delta=2.6t(\times)$]. In (d) we have also plotted the magnitude of the *d*-wave gap vs temperature, for the same alloyed disorder strengths as in figures (a), (b), and (c). In all four figures the interaction is nonlocal with $|U|=3.5t$, $n=1$, and $c=0.5$.

of the normal state to *d* and extended *s* symmetry breaking. In the first case T_c^d is determined by

$$1=-\frac{|U|}{4\pi}\frac{1}{N}\sum_{\vec{k}}\int_{-\infty}^{\infty}dE \times \mathrm{Im}\left(\frac{\eta_{\vec{k}}^2 G_{11}^c(\vec{k};E)}{2E-\Sigma_{11}(E)-\Sigma_{22}(E)}\right)\tanh\left(\frac{\beta_c^d E}{2}\right) \quad (46)$$

and in the second extended *s*-wave case, T_c^s is given by

$$1=-\frac{|U|}{4\pi}\frac{1}{N}\sum_{\vec{k}}\int_{-\infty}^{\infty}dE \times \mathrm{Im}\left(\frac{\gamma_{\vec{k}}^2 G_{11}^c(\vec{k};E)}{2E-\Sigma_{11}(E)-\Sigma_{22}(E)}\right)\tanh\left(\frac{\beta_c^s E}{2}\right), \quad (47)$$

where $\eta_{\vec{k}}$ and $\gamma_{\vec{k}}$ refer to *s*-wave- and *d*-wave-like ''harmonics'' defined previously following Eq. (17).

In Fig. 7(b) the critical temperature for both *d*-wave and extended *s*-wave pairing is shown as a function of band filling *n* for various strengths of alloyed disorder δ. Full lines correspond to *d*-wave T_c while dashed ones to extended *s*-wave solutions. In the clean limit ($\delta=0$) we can see that the extended *s*-wave solution exists mainly at the band edges and the *d*-wave solution is largely confined to the central portion of the band. For the interaction strength we have chosen, the two solutions cross at $n\approx 0.38$. Evidently for $n\leqslant 0.38$ the superconducting instability is at T_c^s while $n\geqslant 0.38$ the transition temperature is T_c^d. As we increase the strength of the alloyed disorder ($\delta/t=0,1.2,2.0,2.5,2.6,2.7,2.8,3.0$ from top to bottom curves) we see that both the T_c for the extended *s*-wave and *d*-wave solutions is reduced and for particularly strong disorder ($\delta=2.7t$ and $\delta=3.0t$) the maximum in the *d*-wave T_c is no longer at $n=1$. This is connected with the splitting of Van Hove singularities visible in Fig. 5(a), i.e., the maximum in the normal-state density of states corresponds to the maximum in the *d*-wave T_c^d.

On the other hand, for a uniform distribution of random site energies there is no splitting of Van Hove singularities and hence we see a different tendency [Fig. 7(c), $\delta/t=0,1.0,2.0,3.0,4.0,5.0,6.0$ from top to bottom curve]. The maximum value of T_c^d is located at $n=1$ no matter what the strength of disorder. For extended *s*-wave solutions and for relatively small disorder in the of *d*-wave case the decreasing tendency in $T_c^{s,d}$ with growing disorder are very similar for the two types of disorder. However, above a certain strength in either case we note that there is no crossing between the extended *s*-wave and *d*-wave solutions. This fact may be interpreted as the sign that the *s* and *d* states cannot coexist or mix in this case. The close look at the dependence of T_c on disorder, whether alloyed or uniform prompts the conclusion, which may, however, be premature,[50] that T_c is not very sensitive to the details of the fluctuation in the site energy.

Another interesting point to investigate concerns the relative robustness of T_c against degradation by disorder in the cases of conventional *s*- and *d*-wave pairing.[37] Figure 8 shows the results for T_c for intersite *d*-wave and on site *s*-wave superconductors versus alloyed disorder strength δ, where $n=0.6$. Here one can easily recognize a typical difference between these two superconducting states. Clearly in the case of a *d*-wave superconducting state disorder acts as an effective pair breaker while for *s*-wave superconductors it decreases T_c only slowly or not at all. An interesting physical consequence of this effect is that if both U_{ii} and U_{ij} ($i\neq j$) are attractive increasing disorder could lead to a transition from *d*-wave to *s*-wave pairing, as suggested by Abrikosov.[37]

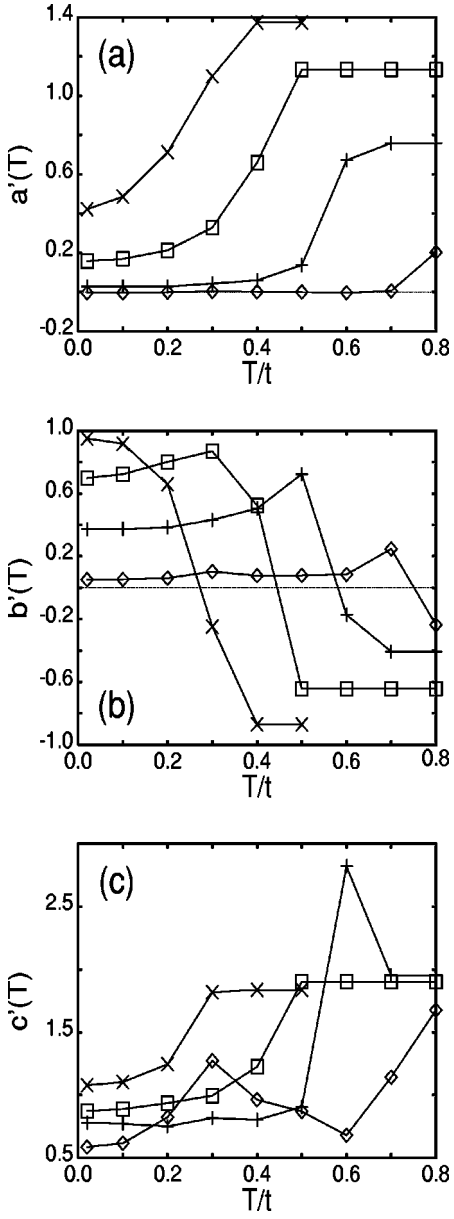


FIG. 11. The coefficients a' (a), b' (b), and c' (c) which represent the imaginary part of the self-energy, in the region of the Fermi energy, as a function of temperature, for different alloyed disorder strengths δ [$\delta=0.6t$ (diamonds), $\delta=1.0t$ (+), $\delta=2.0t$ (squares), and $\delta=2.6t$ ($\times$)]. The interaction is nonlocal with $|U|=3.5t$, $n=1$, and $c=0.5$.

To complete the discussion, Fig. 9 shows the critical temperature plotted versus concentration c for various strength of binary-alloy disorder δ with band fillings of $n=1$, $n=0.7$, and $n=0.1$. Figures 9(a) and (b) correspond to *d*-wave while Fig. 9(c) corresponds to intersite extended *s*-wave pairing. Again for large enough alloy disorder pair breaking phenomena takes place. If disorder is introduced by a fixed potential δ, but varying the concentration of scatters, $c \ll 1$, from 0 we see that the results are similar to the case of a fixed c and increasing δ from 0. This shows that CPA can work equally well, and indeed is asymptotically exact, in both the Born (small δ) and *T*-matrix (small c) and resonant scattering regimes.

VII. $N(E)$ AND $\Sigma_{11}(E)$ AS $E \to 0$ AND THE LOW-TEMPERATURE SPECIFIC HEAT

As mentioned earlier, the behavior of the quasiparticle density of states $N(E)$ and the imaginary part of the self-energy $\mathrm{Im}\,\Sigma_{11}(E)$ near $E=0$ is of general conceptual significance. For instance, the power-law behavior of $N(E) \propto |E|^{\alpha}$, for *d*-wave superconductors give rise to power-law dependence with temperature of many thermodynamic quantities, such as the specific heat $c_v(T)$, instead of the exponential cutoff characteristic of a gap in the quasiparticle spectrum.[5] Naturally, the dramatic changes in the low-energy behavior of $N(E)$ and $\mathrm{Im}\,\Sigma_{11}(E)$ as disorder is added to the problem are also of general interest and, as it turns out, of lively controversy.[10–14,51,52] In this section we wish to examine those predictions of the CPA calculations which are relevant to these issues in particular. Using the methods outlined in the previous sections we calculate numerically the quasiparticle local density of states $N(E)$ and the self-energy $\mathrm{Im}\ \Sigma_{11}(E)$, and then investigate how these two quantities change with both temperature and disorder.

For simplicity we have studied the half filled band ($\mu=0$, $n=1$). This is the band filling for which T_c, in the *d*-wave case, is a maximum. We will examine the effects of alloyed disorder on the system and show that as we increase the amount of scattering the specific heat vs temperature relation changes from T^2, in the clean limit, to T in the limit of strong scattering. As is widely recognized[5] this behavior is the consequence of $N(E) \sim |E|$ changing to $N(E)=$constant and is consistent with experiments.[8]

To get an impression of the form of $N(E)$ and $-\mathrm{Im}\,\Sigma_{11}(E)$ in the region of the chemical potential μ, we fit them to the function $a+b|E|^c$ in the energy range $-\Delta E < E < \Delta E$, where ΔE is small compared to the gap. Using the coefficients a, b, and c to fit the curves $N(E)$ and $-\mathrm{Im}\,\Sigma_{11}(E)$ in the region of μ gives us a tool to analyze their functional form. For example, a tells us if the curves are finite at $E=0$, b controls the gradient of the curve and c controls the curvature.

In Figs. 10(a)–(c) we have plotted these coefficients, for $N(E)$, as a function of T, for different values of δ. We also included in Fig. 10(d) plots of the magnitude of the *d*-wave superconducting order parameter $|\Delta|$ vs T, for the same values of alloyed disorder strength δ, to indicate the temperature where the order parameter goes to zero. Regarding these curves as a brief summary of what the CPA predicts about the low-energy behavior of $N(E)$ and $\Sigma(E)$ we now comment on their implications.

First we note that in Fig. 10(a) the parameter $a(T)$ tends to a finite limit as $T \to 0$ and this limit increases more and more rapidly as the disorder described by δ increases. Hence $N(0)$ is finite in agreement with our earlier discussion in Sec. IV where we derived for low scattering and low temperatures the dependence of $N(0)$ on δ [see Eq. (43)]. It lends credit to the general consistency of our results that the $a(T) \cong N(0,T)$ curves rise to their normal state values as $T \to T_c$. Interestingly, as can be seen in Fig. 10(b) the gradient of $N(E)$, namely b, changes dramatically only near T_c. In fact, for the case where δ is small (squares) the gradient even changes sign. This means that we go from having a gap in the density of states below T_c to having a Van Hove singu-

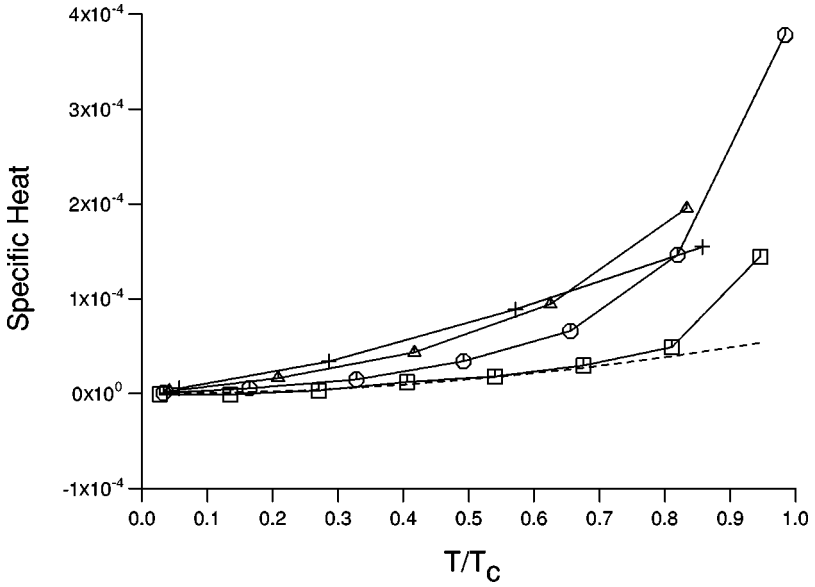


FIG. 12. The specific heat as a function of temperature for different strengths of alloyed disorder δ [$\delta=0.6t$ (squares), $\delta=1.0t$ (circles), $\delta=2.0t$ (triangles), and $\delta=2.6t$ (+)]; again the interaction is nonlocal with $|U|=3.5t$, $n=1$, and $c=0.5$.

larity above T_c. The curvature, represented by c and plotted in Fig. 10(c), shows that for low disorder (squares) as we increase the temperature we go from a curvature of $c\leqslant 1$, i.e., a cusp, to a curvature $c>1$. Finally, when the critical temperature is reached for each of the four different disorder types c goes to 2.

In the same manner, we now examine the corresponding coefficients a', b', and c' for $-\mathrm{Im}\,\Sigma_{11}(E)$. In Figs. 11(a)–(c) we have plotted the calculated coefficients for $-\mathrm{Im}\,\Sigma_{11}(E)$ at different values of δ as a function of the temperature. In Fig. 11(a) we can see that at low temperatures $-\mathrm{Im}\,\Sigma_{11}(0)$ increases with disorder; again this agrees with our results in Sec. IV where an analytical form for the dependence of $-\mathrm{Im}\,\Sigma_{11}(0)$ upon δ was derived at $T=0$, see Eq. (44). As we increase the temperature we can see the self-energy at the chemical potential also rises until the normal-state value is reached at the critical temperature. In Fig. 11(b) we can see how the gradient changes from being large for large δ and small for small δ at low T, and at temperatures greater than T_c to be large and negative for large δ and small and negative for small δ. Finally, Fig. 11(c) shows how the curvature c goes from being almost linear, $c=1$, at low temperatures, regardless of δ, to $c=2$ above T_c.

To illustrate the consequences of these results for the low-temperature thermodynamic properties we have calculated the effect of disorder upon the specific heat. Using the above temperature-dependent coefficients for the density of states near $E\sim 0$ we calculated the limiting behavior of the specific heat as $T\rightarrow 0$. The results are shown in Fig. 12 for different strengths of disorder δ. In the case where δ is small (squares) we can see that the specific heat has a T^2 dependence (the plotted continuous solid line with no points) and for large δ the dependence upon temperature is linear, as expected.[6]

VIII. CONCLUSIONS

We have compared and contrasted the effects of disorder on conventional *s*- and *d*-wave superconductors on the basis of an extended, negative U Hubbard model and a mean field, CPA treatment of disorder. On the one hand we have derived many of the well-known results, such as the pair breaking formula in Eq. (32) or that for the quasiparticle density of states $N(0)$, Eq. (43). On the other hand we have solved the Gorkov-CPA Eqs. (13) and (14) numerically and surveyed the salient features of their consequences by explicit calculations. The use of CPA in describing disordered *d*-wave superconductors is an advance in this very active field[4–14,49,50] because it allows us to avoid the usually delicate choice between methods, sets of diagrams, designed to deal with either weakly or strongly scattering perturbations. The CPA treats both kinds of problems equally accurately and it is known to provide a very credible interpolation between the two.[40] As an example where above feature of CPA may have a crucial role to play we recall the use of the resonant scatterer model in interpreting experimental data both on the cuprates[8,53] and some heavy fermion systems.[11,54] In short, note that in the impurity, $c\rightarrow 0$, limit the self-energy for the Green's function describing an electron moving on a lattice is given by

$$\Sigma(E)=cT(0,0;E), \tag{48}$$

where the T matrix is defined, in terms of the impurity ''potential'' V_{imp}, a real local shift in the site energy, as

$$T(0,0;E)=\frac{V_{imp}}{1-V_{imp}G(0,0;E)}. \tag{49}$$

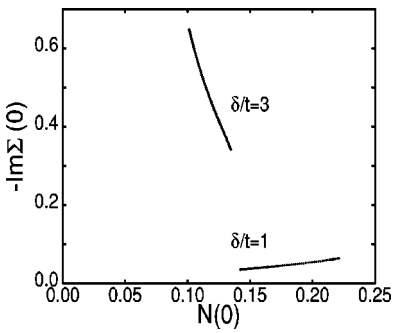


FIG. 13. Relations between Im $\Sigma(0)$ and $N(0)$ for weak $\delta/t=1.0$ and strong $\delta/t=3.0$ scatterers in binary alloys ($c=0.5$).

Evidently $T(0,0;E)$ is a complex number with an amplitude:

$$a(E) = V_{imp}/\sqrt{(1-[V_{imp}\ \mathrm{Re}\ G(0,0;E)]^2+[V_{imp}\ \mathrm{Im}\ G(0,0;E)]^2}$$

and a phase, the phase shift $\phi(E)$, given by

$$\tan\phi(E) = \frac{V_{imp}\,\mathrm{Im}\,G(0,0;E)}{1-V_{imp}\,\mathrm{Re}\,G(0,0;E)}. \tag{50}$$

Now, observe that while for weak scatterers

$$\mathrm{Im}\,\Sigma^B(E) = -c\pi|V_{imp}|^2 N(E) \tag{51}$$

for a resonant scatterer in the unitary limit, defined by $\phi(E)=\pi/2$,

$$\mathrm{Im}\,\Sigma^R(E) = -c\,\frac{1}{\pi N(E)}. \tag{52}$$

It is the above dramatic difference in the dependence of Im Σ^B and Im Σ^R on the density of states $N(E)$ that the cited authors rely on in interpreting the relevant experimental data. Evidently, since the individual scattering events described by the local T matrices are always treated exactly in the CPA, the CPA describes weak scatterers and resonant scatterers equally well. Moreover, since it is a reliable approximation not only in the impurity limit, $c\sim 0$, where we would be doing the same calculation as Fehrenbacher,[49] but also for arbitrary concentrations corresponding to our models it deals with resonance scatterers even when Eq. (52) no longer holds. Thus CPA should be the preferred treatment for models with strong, even resonant scattering.

Although we have not specifically concentrated on this aspect of the method, the principle feature of Eqs. (51) and (52), namely the dependence of $\Sigma(E)$ on $N(E)$, can be seen to be at work in our calculations of the previous section. To demonstrate this we have calculated $\Sigma(0)$ and $N(0)$ as functions of band filling n in the most interesting region $n\sim 1.0$, and compared in Fig. 13 their relationships for weak and strong scatterers at $c=0.5$. Clearly, for weak scatterers $\delta/t=1$, $-\mathrm{Im}\,\Sigma(0)$ is a more or less linear function of $N(0)$ as in Eq. (51), while for strong scatterers $\delta/t=3$, $\mathrm{Im}\,\Sigma(0)$ is inversely proportional to $N(0)$ as in the resonant scatterers model described by Eq. (52). Thus we conclude that the CPA employed in the calculation gives a reliable account of disorder in both the weak and strong scattering regimes.

Having listed the above desirable properties of the CPA we hasten to emphasize that it is a ''mean-field'' theory of disorder and hence does not describe such interesting phenomena as localization[53] even in the normal state.[54] Consequently, our result that $N(0)$ is finite for the smallest amount of disorder can not be taken as evidence against the conclusion that $N(E)\sim|E|^{\alpha}$ of Nersesyan and co-workers.[14] As this originates from the divergence of the vertex corrections in perturbation series for $\Sigma(E)$ we may conjecture that it has to do with localization effects not described by CPA. This very interesting point is in the need of further clarification, and indeed we shall return to it in a later publication.

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