

Nonmagnetic impurities in two-dimensional superconductors

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A numerical approach to disordered two-dimensional superconductors described by BCS mean-field theory is outlined. The energy gap and the superfluid density at zero temperature and the quasiparticle density of states are studied. The method involves approximate self-consistent solutions of the Bogolubov-de Gennes equations on finite square lattices. Where comparison is possible, the results of standard analytic approaches to this problem are reproduced. Detailed modeling of impurity effects is practical using this approach. The range of the impurity potential is shown to be of quantitative importance in the case of strong potential scatterers. We discuss the implications for experiments, such as the rapid suppression of superconductivity by Zn doping in copper oxide superconductors.

I. INTRODUCTION

It is well established that chemical substitutions on copper oxide superconductors can qualitatively alter the properties of these materials in both their normal and superconducting states.¹ In the normal state, impurity substitution can be used to test models of electronic transport. In the superconducting state, impurity scattering effects are sensitive to order parameter symmetry² as well as other properties. It is well known that nonmagnetic impurities are pair breakers in *d*-wave or other nontrivial pairing states with nodes of the energy gap on the Fermi surface. They produce a finite lifetime of the quasiparticles around the gap nodes and a finite density of states at low energy.

In order to parametrize impurity scattering, a physical picture for the normal state, the superconducting state, and the impurity is required. In this paper we are motivated by Zn-doping experiments in cuprates which we assume can be treated as a pure potential scatterer of fermions which obey Luttinger's theorem. Since *d* orbitals of Zn²⁺ are fully occupied, it is naively expected to behave as a nonmagnetic impurity. However, electronic correlations may modify this picture somewhat. Nuclear magnetic resonance measurements by Mahajan and co-workers³ show that the copper spin correlations are severely modified on neighboring Cu sites, which could in principle give rise to effects analogous to the spin-flip scattering process of conventional magnetic impurities. As discussed recently by Borkowski and Hirschfeld,⁴ the unknown relative strength of spin-flip and impurity scattering rates in Zn-doped systems poses an obstacle to the quantitative analysis of experiments involving Zn even within the conventional BCS formalism.

Even if spin-flip scattering is negligible, the modification of copper spin correlations in the vicinity of an impurity site has the effect of increasing the range of an effective scattering potential. Information about the effective potential in YBa₂(Cu_{1-x}Zn_x)₃O_{6.9} can be obtained from the residual sheet resistance estimated by

extrapolation from the normal state. The residual resistance from two-dimensional potential scattering is given by the approximate expression⁵

$$\Delta\rho = \frac{1}{\pi} x \frac{\hbar}{e^2} \sum_l \sin^2(\delta_l - \delta_{l+1}). \quad (1)$$

δ_l are the phase shifts which are constrained to satisfy the Friedel sum rule $\Delta Z = \frac{2}{\pi} \sum_{l=-\infty}^{\infty} \delta_l$. ΔZ is the difference in the number of conduction electrons in the system without impurities and with one impurity. If we assume Zn removes one electron from the conduction band (i.e., $\Delta Z = -1$) and the effective potential is an impenetrable disk of radius *a*, we estimate that the residual sheet resistance is ≈ 0.12 k Ω for $x = 0.01$ in the $l = 0$ dominant scattering channel ($a \sim 0.54/k_f$), which is a factor of 3 smaller than the experimental value 0.34 k Ω .⁶ This discrepancy may indicate appreciable phase shifts in one or more higher angular momentum channels. In fact the $l = 2$ "near-resonant channel," which requires a larger radius of the scattering potential ($a \sim 2.8/k_f$),⁷ yields ≈ 0.36 k Ω for $x = 0.01$. Recently, Poilblanc, Scalapino, and Hanke⁸ have investigated the effects of nonmagnetic impurities in antiferromagnetically correlated systems. They find that the scatterings in $l \leq 2$ channels are strong in that system.

The above discussion suggests that detailed structure of the impurity potential is important in making a quantitative study of Zn-doped materials. As seen below, lattice effects may also be of quantitative importance for short-coherence-length superconductors. Recently, in a brief report,⁹ we presented a numerical study of the disorder effect in two-dimensional superconductors of various pairing symmetries in the limit of strong impurity potentials. We demonstrated that a short- but finite-range potential has a much stronger effect than an on-site (" δ -function") potential. In fact the finite range of the potential may be the primary reason for the rapid suppression of pairing correlations with impurity concentration in YBa(Cu,Zn)O. The importance of finite potential

range has been pointed out recently by Balatsky *et al.*¹⁰ in connection with the nonuniversal behavior of the low-frequency conductance in *d*-wave superconductors.

In this paper we present a more detailed study of the disorder effect in two-dimensional superconductors. The model used here is a lattice BCS mean-field Hamiltonian with disorder defined by

$$H[\Delta_{\mathbf{r}\tau}] = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle \sigma} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + \sum_{\mathbf{r}\tau} (\Delta_{\mathbf{r}\tau} c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}+\tau\downarrow}^\dagger + \text{H.c.}) + \sum_{\mathbf{r}\sigma} \left(\sum_{\mathbf{r}_i} V_{\mathbf{r}_i, \mathbf{r}} - \mu \right) c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma}, \quad (2)$$

where $\langle \mathbf{r}\mathbf{r}' \rangle$ denotes nearest neighbors and μ is the chemical potential. $V_{\mathbf{r}_i, \mathbf{r}}$ is a scattering potential of an impurity at \mathbf{r}_i . Lacking detailed knowledge of the scattering potential in high- T_c cuprates, we assume a model potential form for it: $V_{\mathbf{r}_i, \mathbf{r}} = V_0 \delta_{\mathbf{r}_i, \mathbf{r}} + V_1 (\delta_{\mathbf{r}_i - \mathbf{r} \pm \hat{x}} + \delta_{\mathbf{r}_i - \mathbf{r} \pm \hat{y}})$. When $V_1 = 0$, it is a δ -function potential; otherwise, it is finite ranged. $\Delta_{\mathbf{r}\tau}$ is the superconducting gap parameter. For a given filling factor of electrons n_e , $\Delta_{\mathbf{r}\tau}$ and μ should be determined self-consistently from the relations

$$\Delta_{\mathbf{r}\tau} = J \langle c_{\mathbf{r}\uparrow} c_{\mathbf{r}+\tau\downarrow} \rangle_{\Delta_{\mathbf{r}\tau}}, \quad (3)$$

$$n_e = \frac{1}{N} \sum_{\mathbf{r}\sigma} \langle c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma} \rangle_{\Delta_{\mathbf{r}\tau}}, \quad (4)$$

where J is the coupling constant (assumed disorder independent), N is the system size, and $\langle A \rangle_{\Delta_{\mathbf{r}\tau}}$ means the average of A in the ground state of $H[\Delta_{\mathbf{r}\tau}]$. Without disorder $\Delta_{\mathbf{r}\tau}$ is independent of \mathbf{r} and has a particular symmetry with respect to τ . In this paper only the on-site *s*-wave pairing state $\Delta_{\mathbf{r}\tau} = \Delta \delta_{\tau\mathbf{0}}$ and the *d*-wave pairing state $\Delta_{\mathbf{r}\tau} = \Delta (\delta_{\tau\pm\hat{x}} - \delta_{\tau\pm\hat{y}})$ in two dimensions will be considered.

The Hamiltonian (2) is bilinear in fermion operators and can be diagonalized by solving a one-particle problem. $\Delta_{\mathbf{r}\tau}$ and μ should be determined self-consistently from Eqs. (3) and (4), which amount to solving the Bogolubov-de Gennes equations for the disordered superconductor. For simplicity in calculation, we perform a particle-hole transformation for the down-spin electrons, i.e., $c_{\mathbf{r}\downarrow} \longleftrightarrow c_{\mathbf{r}\downarrow}^\dagger$, and reexpress (2) as

$$H'[\Delta_{\mathbf{r}\tau}] = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} (c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}'\uparrow} - c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}'\downarrow}) + \sum_{\mathbf{r}\tau} (\Delta_{\mathbf{r}\tau} c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}+\tau\downarrow} + \text{H.c.}) + \sum_{\mathbf{r}} \left(\sum_{\mathbf{r}_i} V_{\mathbf{r}_i, \mathbf{r}} - \mu \right) (c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\uparrow} - c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}\downarrow}) + \text{const.} \quad (5)$$

H' has the usual tight-binding model form, but the hopping constant, the chemical potential, and the impurity potential have opposite signs for the up-spin electrons and the down-spin electrons.¹¹ In the remainder of the paper we set the hopping constant $t = 1$.

In Sec. II, the numerical method and essential approximation are outlined. Results for the disorder dependence of the zero-temperature gap and superfluid density ρ_s as well as the quasiparticle density of states ρ are presented. In Sec. III, a concluding remark is given.

II. NUMERICAL METHOD AND RESULTS

A. Gap parameter and superfluid density

In the presence of disorder, the energy gap is space dependent. We determine $\Delta_{\mathbf{r}\tau}$ by iteratively solving H' with the self-consistent conditions. We start from an initial gap function $\Delta_{\mathbf{r}\tau}$ with a certain pairing symmetry. After diagonalizing H' , we find a new gap function $\Delta_{\mathbf{r}\tau}$ from the self-consistent equations and then use it as input to repeat the above process until the self-consistent conditions are satisfied. This is a strict self-consistent iterative process. However, since the gap function at every site needs to be adjusted to satisfy the self-consistent equations, this is excessively time consuming when an average over a large number of impurity configurations is required. We shall, however, perform this strict self-consistent it-

eration procedure only for studying the properties of a single-impurity system and for checking the accuracy of the approximation used in many-impurity cases.

As mentioned above, to solve the self-consistent equations, the Hamiltonian needs to be exactly diagonalized. This can be done, however, only on small lattices in the presence of disorder. For a superconductor, a characteristic length scale is the superconducting correlation length $\xi \sim \hbar v_F / \pi \Delta$. If ξ is larger than the dimension of the system, the finite-size effect is large and the analysis of the disorder effect may be subtle. To avoid this situation, we shall limit our calculations only to cases where ξ is much smaller than the dimension of the system.

The existence of a finite superfluid density ρ_s is a defining property of superconductors. Experimentally ρ_s is determined from the microwave measurement of the penetration depth. ρ_s on a finite lattice can be evaluated directly from the current-current correlation function, using the eigenfunctions obtained from the iteration procedure described above,¹²

$$\frac{\rho_s}{4} = \langle -K_x \rangle - \Lambda_{xx}(q_x = 0, q_y \rightarrow 0, \omega = 0), \quad (6)$$

where $\langle A \rangle = \text{Tr}(Ae^{-\beta H}) / \text{Tr}e^{-\beta H}$, $\langle K_x \rangle$ is the kinetic energy along the x direction, and

$$\begin{aligned}\Lambda_{xx}(\mathbf{q}, \omega) &= \frac{i}{V} \int_{-\infty}^t dt' e^{i\omega(t-t')} \langle [J_x^p(-\mathbf{q}, t), J_x^p(\mathbf{q}, t')] \rangle \\ &= \frac{1}{V} \sum_{n_1 \neq n_2} \frac{A_{n_1, n_2}(-q) A_{n_2, n_1}(q)}{\omega + i\delta + E_{n_1} - E_{n_2}} (\langle c_{n_1}^\dagger c_{n_1} \rangle \\ &\quad - \langle c_{n_2}^\dagger c_{n_2} \rangle),\end{aligned}\quad (7)$$

with $c_n = \sum_{\mathbf{r}\sigma} \phi_n(\mathbf{r}, \sigma) c_{\mathbf{r}\sigma}$ the quasiparticle operator and

$$\begin{aligned}A_{n,m}(\mathbf{q}) &= \sum_{\mathbf{r}\sigma} e^{i\mathbf{q}\cdot\mathbf{r}} [\phi_n(\mathbf{r} + x\sigma) \phi_m(\mathbf{r}\sigma) \\ &\quad - \phi_n(\mathbf{r}\sigma) \phi_m(\mathbf{r} + x\sigma)].\end{aligned}\quad (8)$$

Before studying disordered systems, we consider a one-impurity system. We first consider the change of the gap function induced by an impurity. Figure 1 shows the self-consistent energy gap $\Delta_{\mathbf{r}\tau}$ for an *s*-wave superconducting state with one impurity on a 21×21 lattice. Since the scattering potential is short ranged, the gap function changes only in the vicinity of the impurity. Far away from the impurity, $\Delta_{\mathbf{r}\tau}$ approaches to the value of the energy gap without disorder. In a region with a length scale of the range of scattering potential around the impurity site, $\Delta_{\mathbf{r}\tau}$ is largely reduced due to the strong suppression of the probability of an electron hopping to this region by the impurity scattering. Beyond this region, there exists a relatively larger region with a length scale comparable with the superconducting correlation length ξ where a weak oscillation of $\Delta_{\mathbf{r}\tau}$ in space is observed. This oscillation is due to the interplay between the impurity scattering and the superconducting correlations. Because of the lattice effect, $\Delta_{\mathbf{r}\tau}$ is not isotropic in space. It is relatively strong along the diagonal direction. Along other directions, it is too weak to be resolved from the figure. For the *d*-wave state, similar results have been found. But the oscillation of $\Delta_{\mathbf{r}\tau}$ along two axes seems more apparent in this case.

For finite impurity doping systems where many impurity configurations are used in the disorder average we shall approximate $\Delta_{\mathbf{r}\tau}$ in (2) by the average of the pairing correlation functions $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$ in space, $\bar{\Delta}_\tau$, so that only a simplified self-consistent equation

$$\bar{\Delta}_\tau = \frac{1}{N} \sum_{\mathbf{r}} J \langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle \bar{\Delta}_\tau \quad (9)$$

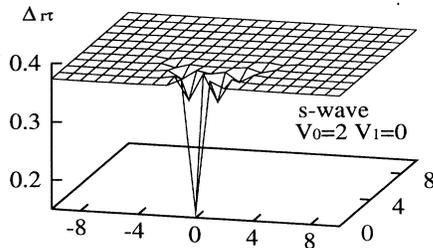


FIG. 1. Self-consistent gap function for the *s*-wave superconducting state on a 21×21 lattice. Only half of the lattice is shown. The impurity is located at the center of the lattice.

need be solved. This approximation is to ignore the fluctuation of $\Delta_{\mathbf{r}\tau}$ (but not $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$) in space.

The errors resulting from the above approximation can be found by directly comparing the results obtained with and without the approximation. We have calculated the errors for the pairing amplitude for several arbitrarily chosen configurations of impurities in both strong and weak scattering potential limits. For all the cases we have studied, we find that the relative errors in the average energy gap are small compared with the combined errors produced by the disorder average or the finite-size effect. For example, for a randomly chosen system of three impurities on a 14×14 lattice, the relative errors in the average energy gap are 0.1% (0.6%) in a weak potential $V_0 = 2$ and $V_1 = 0$ and 2% (2%) in a strong potential $V_0 = 20$ and $V_1 = 0$ for the *s*-wave (*d*-wave) pairing state. As the impurity concentration increases, the error increases slightly. The errors for the local pairing correlation functions $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$ are larger than that for the average gap, but still small. Figure 2, as an example, shows the relative error pattern for the local correlation function $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$ for a *s*-wave pairing state. We find that the errors for $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$ are largest (about 5%) at the impurity sites. Clearly $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$ is overestimated in the vicinity of impurities and underestimated far away from the impurities. Nevertheless, it is encouraging that the error made in neglecting off-diagonal disorder is small.¹³

Using the above approximation, we have evaluated the average gaps $\bar{\Delta}$ for both *s*- and *d*-wave pairing states in different scattering potentials. For all the cases we have studied, we find that $\bar{\Delta}$ decays almost linearly with x for small x . Figure 3 shows $\bar{\Delta}_\tau$ as a function of the impurity concentration x for both pairing states in a strong δ -function scattering potential $V_0 = 20$ on a 14×14 lattice. All four curves shown in the figure are nearly parallel to each other although their values at $x = 0$, i.e., $\bar{\Delta}(0)$, are quite different. This remarkable behavior indicates that the reduction of Δ by disorder ($d\bar{\Delta}/dx$) is determined only by the scattering potential to a first approximation and is independent of the pairing symmetries and the

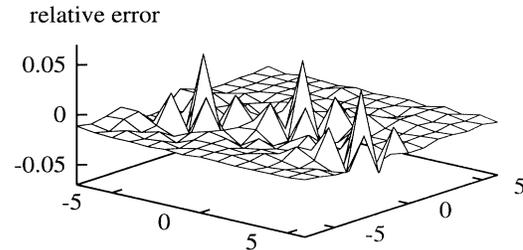


FIG. 2. Relative errors of the local pairing correlation function $(\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle_{\bar{\Delta}} - \langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle_{\Delta_{\mathbf{r}\tau}}) / \langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$ (where $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle_{\bar{\Delta}}$ and $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle_{\Delta_{\mathbf{r}\tau}}$ are the results obtained with and without approximation, and $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle$ is the average of $\langle c_{\mathbf{r}\downarrow} c_{\mathbf{r}+\tau\uparrow} \rangle_{\Delta_{\mathbf{r}\tau}}$ in space) for the *s*-wave pairing state on a 14×14 lattice with three impurities and a potential $V_0 = 20$ and $V_1 = 0$. The impurities are located on the sites where the three highest peaks emerge.

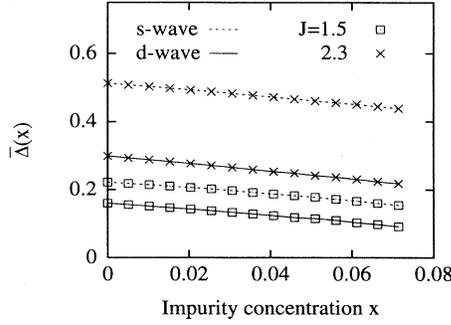


FIG. 3. Energy gap $\bar{\Delta}(x)$ vs x for both pairing states with the coupling constant $J = 1.5$ and 2.3 and the scattering potential $V_0 = 20$ and $V_1 = 0$ on a 14×14 lattice. Twenty-five impurity configurations are used in the disorder average.

values of the energy gaps for pure samples. This nearly universal property of the energy gap could be of use in future studies of disordered superconductors. For weak δ -function potentials or finite- but short-ranged potentials, similar results for $\bar{\Delta}$ have been found. But for a weak δ -function potential the slope of the decay of $\bar{\Delta}$ with x becomes smaller.

Our calculations for $\bar{\Delta}$ and ρ_s have been done mostly on lattices with sizes ranging from 10×10 to 18×18 sites. In general, $\bar{\Delta}$ and ρ_s are size dependent. However, for the quantities which are physically more interesting, the

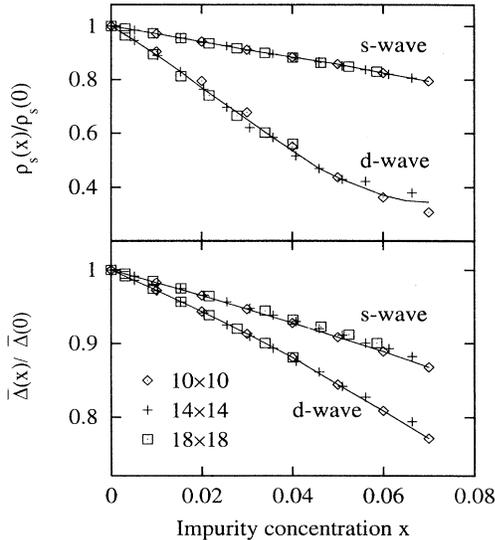


FIG. 4. Normalized energy gap $\bar{\Delta}(x)/\bar{\Delta}(0)$ and normalized superfluid density $\rho_s(x)/\rho_s(0)$ as functions of impurity concentration x on the square lattices of 10×10 , 14×14 , and 18×18 sites with $V_0 = 8$ and $V_1 = 0$. $\bar{\Delta}(0)$ is about 0.5 (0.3) for the s - (d -)wave pairing state, which is about a $1/20$ bandwidth. One hundred impurity configurations for a 10×10 lattice, and more than 25 impurity configurations for 14×14 and 18×18 lattices are used in the disorder average.

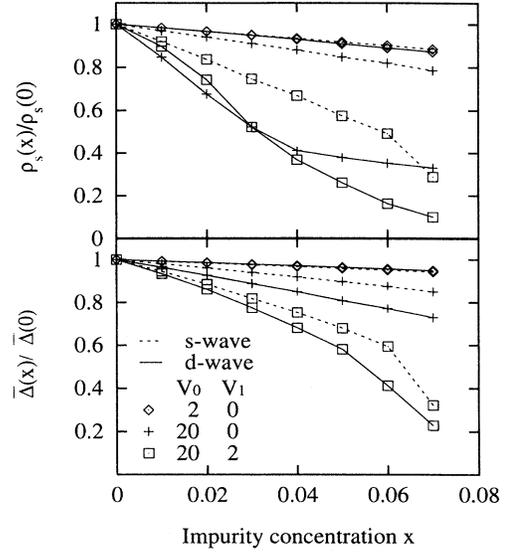


FIG. 5. Normalized energy gap $\bar{\Delta}(x)/\bar{\Delta}(0)$ and normalized superfluid density $\rho_s(x)/\rho_s(0)$ as functions of x for both s -wave and d -wave superconducting states with three different potentials on 10×10 lattices. $\bar{\Delta}(0)$ are the same as for Fig. 4. One hundred configurations of impurities are used in the disorder average.

relative energy gap $\bar{\Delta}(x)/\bar{\Delta}(0)$ and the relative superfluid density $\rho_s(x)/\rho_s(0)$, the finite-size effect is small. A comparison for $\bar{\Delta}(x)/\bar{\Delta}(0)$ and $\rho_s(x)/\rho_s(0)$ for the s - and d -wave states with a δ -function potential $V_0 = 8$ on lattices of 10×10 , 14×14 , and 18×18 sites is given in Fig. 4. Similar results have been found for other impurity potentials. In general, we find that the finite-size effect for ρ_s is larger than that for $\bar{\Delta}_\tau$ when $\bar{\Delta}_\tau$ is small (i.e., large ξ). Physically this is because that $\bar{\Delta}_{\tau\tau}$ is determined only by the local pair correlation function while ρ_s is determined by the current-current correlation function at long wave-

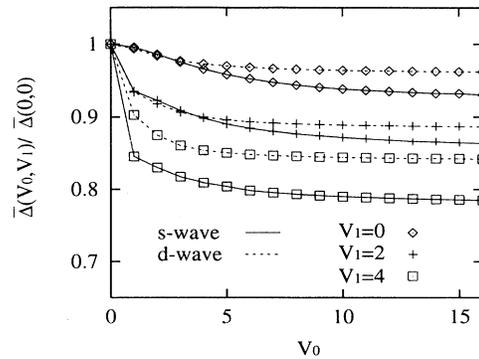


FIG. 6. Normalized energy gap $\bar{\Delta}(V_0, V_1)/\bar{\Delta}(0, 0)$ as functions of V_0 for the s - and d -wave pairing states with $x = 0.02$. The values of $\bar{\Delta}(0, 0)$ are the same as $\bar{\Delta}(0)$ used in Fig. 4. One hundred configurations of impurities are used in the disorder average.

lengths which in turn is determined by the properties of the eigenfunction on the whole lattice.

Figure 5 shows $\bar{\Delta}(x)/\bar{\Delta}(0)$ and $\rho_s(x)/\rho_s(0)$ as functions of x for the s - and d -wave pairing states in three potentials. For a weak δ -function potential, $\bar{\Delta}(x)/\bar{\Delta}(0)$ and $\rho_s(x)/\rho_s(0)$ decrease very slowly with x and the difference between the s - and d -wave pairing states is also small. With increasing V_0 , the difference between these two pairing states increases. The disorder has a stronger effect on the d -wave state than on the s -wave state; in particular, ρ_s falls much faster in the d -wave state than in the s -wave state. This property may be useful for distinguishing a d -wave pairing state from an s -wave pairing state in the unitary scattering limit from an experimental point of view. But if an off-site scattering potential (i.e., V_1 term) is present, this difference will be eventually reduced. The disorder effect is clearly strongly enhanced in a finite-range potential than in a δ -function potential.

Figure 6 shows $\bar{\Delta}(V_0, V_1)/\bar{\Delta}(0, 0)$ as functions of V_0 for the s - and d -wave pairing states with $x=0.02$. The qualitative behaviors of $\bar{\Delta}(V_0, V_1)/\bar{\Delta}(0, 0)$ are similar for all the cases shown in the figure. $\bar{\Delta}(V_0, V_1)/\bar{\Delta}(0, 0)$ decreases with V_0 for small V_0 , but soon becomes saturated when V_0 surpasses the bandwidth. $d\bar{\Delta}/dx$ for the s - and d -wave states can be very large depending on the value of V_1 .

B. Density of states

Now we consider the effect of disorder on the density of states of quasiparticles. We calculate the density of states using a recursion method.¹⁴ This method addresses the local density of states of an infinite lattice. In this method, the density of states $\rho(E)$ is obtained from the imaginary part of the one-particle Green's function $G(E)$,

$$\rho(E) = \lim_{\epsilon \rightarrow 0} -\frac{1}{\pi} \text{Im}G(E + i\epsilon). \quad (10)$$

Given a starting state $|0\rangle$, the recursion method is defined by the recurrence relations

$$H|0\rangle = a_0|0\rangle + b_1|1\rangle \quad (11)$$

and

$$H|n\rangle = b_n|n-1\rangle + a_n|n\rangle + b_{n+1}|n+1\rangle \quad (n > 0), \quad (12)$$

where $\{|n\rangle\}$ is a set of normalized bases generated automatically from Eqs. (11) and (12). From the a 's and b 's generated, $G(E)$ can be expressed in a continued fraction form

$$G(E) = \frac{1}{(E - a_0) - \frac{b_1^2}{(E - a_1) - \frac{b_2^2}{(E - a_2) - \dots}}} \quad (13)$$

In a real calculation, this continued fraction is truncated at a certain step and the remainder of the continued fraction is replaced by a parameter which is determined such

that the error is minimized. We truncate the continued fraction at a step when the difference between the result obtained at that step and that with five more steps is smaller than the error demanded. In using the recursion method, the values of $\Delta_{\mathbf{r}\mathbf{r}}$ and μ obtained previously on finite lattices will be used. When the impurity concentration is finite, the approximation $\Delta_{\mathbf{r}\mathbf{r}} = \bar{\Delta}_{\mathbf{r}}$ is assumed. For a one-impurity system, the strict self-consistent solution for $\Delta_{\mathbf{r}\mathbf{r}}$ on a small lattice around the impurity is used, while for the remainder of the lattice $\Delta_{\mathbf{r}\mathbf{r}}$ are approximated by the average value of $\Delta_{\mathbf{r}\mathbf{r}}$ on the edges of the small lattice.

As discussed by Byers *et al.*¹⁵ and Choi¹⁶ the densities of states in the vicinity of the impurity are in principle measurable via the spatial variation of the tunneling conductance around an impurity with a scanning-tunneling-microscope study of the surface of a superconductor. In continuum space, the local density of states (or the tunneling conductance) around an impurity has been calculated by Byers *et al.*¹⁵ for both the s - and d -wave pairing states and by Choi¹⁶ for the d -wave pairing state. They find that the density of states for a given energy oscillates in space and depends strongly on the anisotropy of the gap parameter. When the energy is larger than Δ , the oscillation is largest in the directions of the gap maxima and smallest in the directions of the gap minima. In lattice space, however, we find that their results are partly altered. Figure 7 shows the impurity-induced density of states as a function of distance from an impurity along two directions for the s - and d -wave pairing states. (Here the fully self-consistent isolated impurity result for the gap function on a 21×21 lattice shown in Fig. 1 is used as an input.) The density of states oscill-

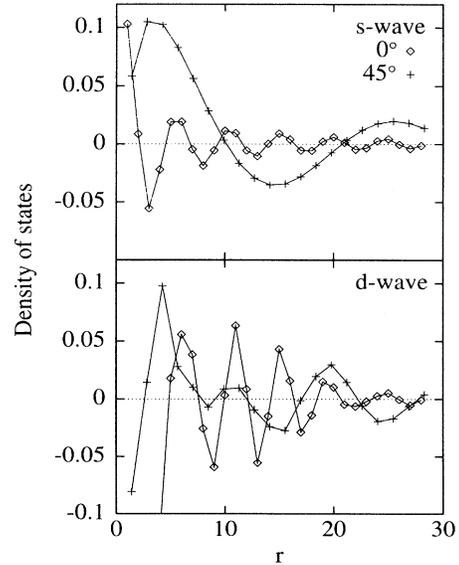


FIG. 7. The local density of states induced by an impurity as a function of distance r from an impurity along both the x -axis direction (0°) and the diagonal direction (45°) at energy $\omega = 1.5\Delta_{\text{max}}$. $V_0 = 2$ and $V_1 = 0$.

lates in space with an energy- and direction-dependent wavelength in agreement with the results of Ref. 15. In the s -wave case, the oscillation along the diagonal direction is much larger than that along the x -axis direction, in contrast to the isotropic s -wave pairing state in continuum space. Since the energy gaps are the same on the Fermi surface for s -wave states, this difference is purely a lattice effect. For the d -wave pairing state, the oscillations along two directions are not so different as shown in Refs. 15, 16. The impurity-induced density of states decays slightly faster along the x -axis direction than along the diagonal direction.

To compute the density of states with finite doping of impurities, we have used the results of the average gap $\bar{\Delta}$ obtained previously. The fluctuation of $\Delta_{\mathbf{r}\tau}$ in space is ignored in this calculation. Figure 8 shows the density of states for the s - and d -wave pairing states with different potentials and x . The main results are summarized as follows.

(a) For s -wave pairing with a weak or strong potential with very small x , ρ has no qualitative change with respect to the case without disorder. In particular, the energy gap still exists and is hardly changed by disorder in agreement with Anderson's theorem.¹⁷

(b) For the d -wave pairing state with a weak scattering potential, the change of ρ with respect to the case without disorder is small. But ρ at the Fermi energy E_F

becomes finite, consistent with the nonmagnetic impurity scattering theory in the Born scattering limit.¹⁸

(c) For the d -wave pairing state with a very strong on-site potential, ρ shows a peak around E_F . This result agrees very well with the self-consistent t -matrix theory for the d -wave superconductor in the unitary scattering limit.¹⁹ On the other hand it also shows that the approximations made in the self-consistent t -matrix theory, such as ignoring the vertex corrections and the energy dependence of the self-energy, are valid for the d -wave state.

(d) For the d -wave pairing state with a strong on-site potential or both pairing states with a finite-range potential, ρ at E_F grows quickly with increasing x and becomes comparable with the average density of states at some critical x . For the s -wave pairing state with a strong δ -function potential, a finite gap remains when x is smaller than a critical value x_c within numerical errors. When $x > x_c$, the gap vanishes (but ρ_s and $\bar{\Delta}$ are nonzero); ρ at E_f is small and increases slowly with increasing x .

(e) All singularities of ρ are suppressed by the disorder average in these calculations. We have not found any evidence for the singular behavior predicted recently by Nersisyan *et al.*²⁰ within numerical error.

III. CONCLUSION

We have discussed a straightforward numerical technique which allows detailed effects of various impurity potentials on superconductors to be investigated with a BCS mean-field framework. In particular we evaluated the gap parameter, the superfluid density, and the density of states for the s -wave and d -wave superconducting states with nonmagnetic impurities, as functions of impurity concentrations and scattering potentials. For one-impurity systems, the local density of states induced by impurity oscillates in space, in agreement with known analytic results. For s -wave pairing, the energy gap and the density of states are hardly affected by weak disorder (i.e., either weak scatterers or dilute strong scatterers), consistent with Anderson's theorem. In the dilute impurity limit, our results agree well with the self-consistent t -matrix theory in both the Born and unitary scattering limits, and in both s - and d -wave pairing states. For the d -wave pairing state, the density of states at E_F becomes finite even for the weak scattering potential, consistent with the Born scattering theory of the d -wave superconductor. For the d -wave pairing state with a strong on-site potential, the density of states is in good agreement with the self-consistent t -matrix theory for the d -wave superconductor in the unitary limit. For strong scatterers, the energy gap of the s -wave state disappears beyond a critical doping level which is sensitive to the range of the impurity potential. A finite-range potential is shown to have a stronger effect than a short-range potential in either pairing state. For Zn-doped YBaCuO, experiments find that T_c varies almost linearly with x and drops about 25% for 2% Zn doping.²¹ If we assume the change of T_c is equivalent to the change of $\bar{\Delta}$ at zero temperature, we

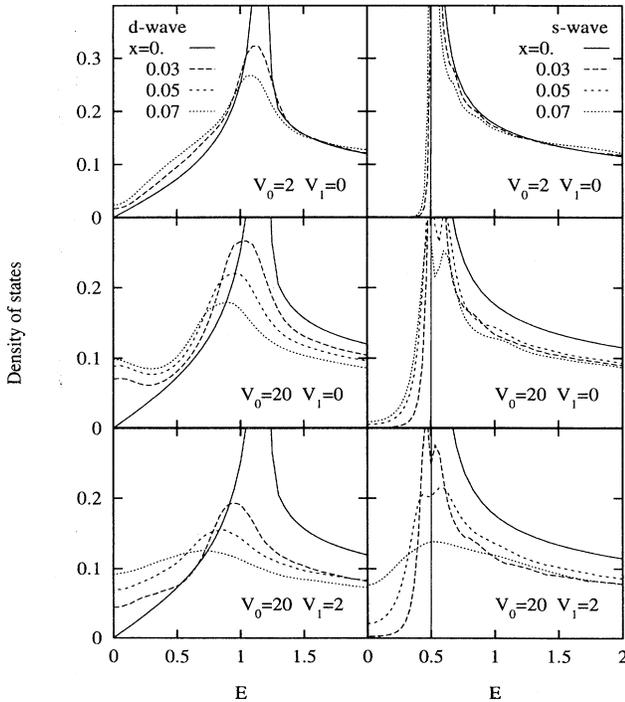


FIG. 8. Density of states as functions of energy E for s - and d -wave superconducting states with different impurity concentrations x . The parameters $\bar{\Delta}$ obtained in Fig. 5 are used in calculations here. More than 1000 configurations of impurities are used in the disorder average.

find that $d\bar{\Delta}/dx$ in a δ -function potential is too small to fit quantitatively with experiments even in the unitary scattering limit. However, for a finite-range potential, no such difficulty exists.

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