Nonzero Fermi Level Density of States for a Disordered d-Wave Superconductor in Two Dimensions

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In 3D, arbitrarily weak disorder in superconductors with line nodes gives rise to a nonzero Fermi level density of states $N(0)$, leading to characteristic low-temperature thermodynamics similar to that observed in cuprate and heavy-fermion systems. In a strictly 2D model, possibly appropriate for the cuprates, it has been argued that $N(0)$ vanishes. We perform an exact calculation for a 2D d-wave superconductor with Lorentzian disorder and find a nonzero $N(0)$. For other continuous distributions we obtain a nonzero lower bound for $N(0)$. We discuss the reasons for this discrepancy. [S0031-9007(96)01309-9]

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A large amount of evidence [1] has accumulated recently suggesting that the order parameter in the cuprate superconductors vanishes linearly at lines on the Fermi surface. Frequently, these experiments have been interpreted in terms of a $d_{x^2-y^2}$ pairing state, but states of "extended-s" symmetry with nodes have also been considered. One of the most interesting consequences of such nodes in three spatial dimensions is the creation of a nonzero density of zero-energy quasiparticle states $N(0)$ for infinitesimal disorder [2,3]. Such a residual density of states (DOS) is, of course, reflected in many experimental observables, and may be shown [4] to lead, in particular, to a T^2 term in the London penetration depth $\lambda(T) - \lambda(0)$, and more generally to low-temperature thermodynamic and transport properties characteristic of a normal Fermi system with strongly reduced DOS. Systematic *Zn* doping and electron damage experiments have been found to lead to precisely these types of temperature dependences in YBCO single crystals [5], and in certain cases quantitative fits [6] have been obtained to the "dirty d-wave" model, in which the effects of potential scatterers on a 2D d-wave superconductor are calculated using a t-matrix approximation [7,8] assuming large electronic phase shifts.

Recently, Nersesyan, Tsvelik, and Wenger [9] have questioned the accuracy of the t-matrix approximation when applied to a strictly 2D disordered d-wave system, pointing out that, in 2D, logarithmic divergences in multisite scattering processes, some of which are neglected in the t-matrix approach, prevent a well-controlled expansion in impurity concentration. These authors avoided perturbation theory by using bosonization together with the replica trick, and predicted a power law DOS $N(E) \sim |E|^{\alpha}$, $\alpha \simeq 1/7$, for sufficiently small energy E and disorder, rather than the analytic behavior $N(E) \sim \text{const} + aE^2$ expected in 3D. They also argued that a nonzero DOS at $E = 0$, a quantity indicating spontaneous symmetry breaking, may not occur because of the Mermin-Wagner theorem [10].

Although the physical systems in question are in reality highly anisotropic 3D systems, the possibility of a 2D-3D crossover at low temperatures could conceivably invalidate some of the results of the usual dirty d-wave approach. This would render the description of the low-temperature transport properties of the cuprate superconductors considerably more complicated even if the order parameter corresponds to the very simple 2D $d_{x^2-y^2}$ form usually assumed.

It is therefore of considerable importance to check the results of Ref. [9] by other methods. In this paper we show that, for certain types of disorder, *exact* results can be obtained for the DOS of strictly 2D disordered superconductors. We show that, for *any* disorder diagonal in position and particle-hole space, the DOS of a classic isotropic s-wave superconductor has a rigorous threshold at the (unrenormalized) gap edge Δ, as expected from Anderson's theorem [11]. Within the same general method, we show that the residual DOS $N(0)$ of a superconductor with line nodes (e.g., d or extended-s wave) is nonzero for arbitrarily small disorder, in disagreement with Ref. [9]. We believe that the DOS in a disordered system is not an order parameter which belongs to the class of order parameters covered by the Mermin-Wagner theorem. This is supported by the fact that a nonzero DOS occurs also in other tight-binding models (e.g., model for two-dimensional Anderson localization [12]), which are described by a field theory with continuous symmetry.

As exact results are only obtainable for Lorentzian disorder, we discuss ways [13] of obtaining information on the effects of other distributions, including models where the randomness has a compact domain. Finally, we compare our results to those arising from alternative methods, and comment on possible origins of the current disagreement.

Density of states.—Here, we introduce a general method of calculating exactly the DOS of a superconductor for certain types of disorder, motivated by the analysis

of Dirac fermions in 2D [14]. The BCS Hamiltonian is given by

$$H = (-\nabla^2 - \mu)\sigma_3 + \Delta\sigma_1\,, \tag{1}$$

which describes quasiparticles in the presence of the spin singlet order parameter Δ. The σ_i are the Pauli matrices in particle-hole space. The disorder is modeled by taking $\mu = \mu_x$ as a random variable distributed according to a probability distribution $P(\mu_x)$.

The kinetic energy operator $-\nabla^2$ is taken to act as $\nabla^2\Psi(x) = \Psi(x + 2e_1) + \Psi(x - 2e_1) + \Psi(x + 2e_2) + \Psi(x - 2e_2)$ on a function $\Psi(x)$ of the sites x of a 2D square lattice spanned by the unit vectors e_1 and e_2. Note that this function involves displacements of two lattice sites rather than one, as would be the case in the simplest tight-binding representation of the lattice kinetic energy. For a system of fermions in the thermodynamic limit, the bare kinetic energy will then have a band representation quite similar to the usual tight-binding form, with no particular distinguishing features near the Fermi level. The reason for this choice will become clear below. It obeys, of course, the same global continuous symmetries discussed for the model in Ref. [9]. The bilocal lattice operator $\hat{\Delta} \equiv \Delta_{x,x'}$ is taken to act as a c-number in the isotropic s-wave case, $\hat{\Delta}\Psi(x) = \Delta\Psi(x)$, whereas to study extended pairing we define $\hat{\Delta}^s_d\Psi(x) = \Delta^s_d[\Psi(x + e_1) + \Psi(x - e_1) \pm \Psi(x + e_2) \pm \Psi(x - e_2)]$.

We consider the single-particle Matsubara Green function defined as $G(iE) = (iE\sigma_0 - H)^{-1}$. We are primarily interested in calculating the DOS $N(E) \equiv -\frac{1}{\pi}\,\mathrm{Im}\,\sum_{\vec{k}}\langle G_{11}(iE \to E + i\epsilon)\rangle$, where $\langle\cdots\rangle$ denotes the disorder average. The problem now is how to perform this disorder average over the probability measure $P(\mu_x)d\mu_x$ of the random variable μ_x. Exact results for the disorder-averaged propagator in noninteracting systems can frequently be obtained for Lorentzian disorder, $P(\mu_x)d\mu_x = (\gamma/\pi)[(\mu_x - \mu_0)^2 + \gamma^2]^{-1}\,d\mu_x$, by exploiting the simple pole structure of $P(\mu_x)$ in the complex μ_x plane. μ_0 is the chemical potential of the averaged system. For convenience, we set $\mu_0 = 0$. The averaged Green function is $\langle G(iE)\rangle \equiv \int \prod_x d\mu_x P(\mu_x) G(iE;\,\mu_x)$, which may then be trivially evaluated *if* G can be shown to be analytic in either the upper or lower μ-half plane.

In a superconductor, the Green function depends on the random variable μ_x via $\mu_x \pm iE$, as a consequence of the particle-hole structure. Therefore, the averaging of G with respect to Lorentzian disorder is not trivially possible. However, we will show below that it is possible to reformulate the problem so that G consists of terms which are analytic in one of the half-planes. This allows us to perform the averaging of the Green function for Lorentzian disorder.

Isotropic s-wave superconductor.—We first assume a homogeneous s-wave order parameter, neglecting the response of the superconducting condensate to the random potential. The Matsubara Green function may be written $G(iE) = -(iE\sigma_0 + H)(E^2 + H^2)^{-1}$, where we note that $H^2 = (-\nabla^2 - \mu)^2\sigma_0 + \Delta^2\sigma_0$ since, in the isotropic s-wave case, $(-\nabla^2 - \mu)\sigma_3$ anticommutes with $\Delta\sigma_1$ even for random μ due to the locality of the order parameter.

The expression $H^2 + E^2$ is proportional to the unit matrix; as a consequence, the Green function can be written in the simple form,

$$G(iE) = -\frac{iE\sigma_0 + H}{2i\sqrt{\Delta^2 + E^2}} \times [(-\nabla^2 - \mu - i\sqrt{\Delta^2 + E^2})^{-1} - (-\nabla^2 - \mu + i\sqrt{\Delta^2 + E^2})^{-1}]\sigma_0\,. \tag{2}$$

It is straightforward to show that the imaginary part of this expression (after analytic continuation, $iE \to E + i\epsilon$) for *any given configuration of impurities* is vanishing for $|E| < \Delta$. Therefore, the DOS shows a gap of size Δ *independent* of the distribution function $P(\mu)$. Thus, our model reproduces the famous Anderson theorem [11] which states that the thermodynamics of an isotropic s-wave superconductor are not affected by diagonal, nonmagnetic disorder. The situation is different if the order parameter itself is random, in which case all quasiparticle states are broadened and $N(E) > 0$ for all $E \geq 0$ [13,15]. Here we neglect these effects, as did Nersesyan *et al.* [9].

d-wave and extended-s symmetry superconductors.—The second class of examples includes the d-wave and extended-s "bond" order parameters $\hat{\Delta}^s_d$ defined above. The corresponding pure systems in momentum space fulfill the condition $\sum_k \Delta_k = 0$, so that nonmagnetic disorder must cause significant pair breaking [2]. The behavior of the imaginary part of the Green's function can be studied using a method analogous to that used for the s-wave case. However, the main difference is that the nonlocal order parameter term $\hat{\Delta}^s_d\sigma_1$ does not anticommute with $(-\nabla^2 - \mu)\sigma_3$ anymore if μ is random.

This requires a different type of transformation. We introduce a diagonal matrix (or staggered field) $D_{x,x'} = (-1)^{x_1+x_2}\delta_{x,x'}$ (note D^2 is the unit matrix). Now we may write

$$H^2 = HD\sigma_3^2DH = [(-\nabla^2 - \mu)D\sigma_0 - i\hat{\Delta}^s_dD\sigma_2] \times [D(-\nabla^2 - \mu)\sigma_0 + iD\hat{\Delta}^s_d\sigma_2]. \tag{3}$$

Because D commutes with $-\nabla^2$ (as defined above) and μ, but anticommutes with the order parameter $\hat{\Delta}^s_d$, we have simply $H^2 = \tilde{H}^2$, with $\tilde{H} \equiv (-\nabla^2 - \mu)D\sigma_0 - i\hat{\Delta}^s_dD\sigma_2$. Therefore, the quantity $H^2 + E^2\sigma_0 = (\tilde{H} + iE\sigma_0)(\tilde{H} - iE\sigma_0)$ can be used to write

$$G(iE) = \frac{i(iE\sigma_0 + H)}{2E} \times [(\tilde{H} - iE\sigma_0)^{-1} - (\tilde{H} + iE\sigma_0)^{-1}]. \tag{4}$$

Observe that both H and $\tilde{H}$ appear in this expression, but H appears only in the numerator.

Defining $z_x \equiv \mu_x D_x$, we now note that for $E > 0$ *and* $\mathrm{Im}(z_x) \geq 0$, the matrix $iE\sigma_0 - \tilde{H}$ is nonsingular (i.e., $\det(iE\sigma_0 - \tilde{H}) \neq 0$). Therefore, the transformed Green's function $(iE\sigma_0 - \tilde{H})^{-1}$ can be expanded as a Taylor series with nonzero radius of convergence around any z_x in the upper half z-plane, and is consequently analytic there. Using this fact and $P(z) = P(\mu)$, we can now perform the disorder integration, as defined above. The disorder-averaged Matsubara Green function is translationally invariant. Performing a spatial Fourier transform, we replace $-\nabla^2$ by $\xi = \epsilon_{\vec{k}} - \mu_0$ and find

$$\langle G(iE)\rangle = -\frac{(iE + i\gamma)\sigma_0 + \xi\sigma_3 + \Delta_d^s\sigma_1}{(E + \gamma)^2 + \xi^2 + (\Delta_d^s)^2} \equiv G(iE + i\gamma)\,. \tag{5}$$

This is the Matsubara Green function of the pure system with the frequency iE shifted by the disorder parameter, $iE \rightarrow iE + i\gamma$. It should be noted that, for the local (isotropic) s-wave order parameter discussed before, the average over a Lorentzian distribution in Eq. (2) implies a shift $i\sqrt{\Delta^2 + E^2} \rightarrow i\sqrt{\Delta^2 + E^2} + i\gamma$.

To obtain the DOS for the d-wave case we approximate the sum over the momenta $\vec{k}$ in standard fashion as $N_0 \int_{-\infty}^{\infty} d\xi \int_0^{2\pi} \frac{d\phi}{2\pi}$, where N_0 is the density of states of the normal metal at the Fermi level, with the tetragonal Fermi surface approximated by a circle. The result is

$$N(E) = N_0 \int_0^{2\pi} \frac{d\phi}{2\pi}\, \mathrm{Im}\left(\frac{E + i\gamma}{[\Delta_d^2(\phi) - (E + i\gamma)^2]^{1/2}}\right), \tag{6}$$

where the d-wave order parameter is approximated by $\Delta_d(\phi) = \Delta_d \cos(2\phi)$. At $E = 0$, $N(0) = N_0 \frac{2\gamma}{\pi\Delta_d} \times \ln(4\Delta_d/\gamma)$ for $\gamma \ll \Delta_d$. Thus, the DOS is nonzero at the Fermi level for arbitrarily small disorder. For small E, $N(E)$ varies as E^2.

For more general continuous distributions $P(\mu)\,d\mu$, the averaged DOS can be estimated using again the analytic structure of $\tilde{G}$. Applying the ideas of Ref. [13], one can derive a lower bound by a decomposition of the lattice into finite subsquares. The average DOS on an isolated subsquare can be estimated easily. Moreover, the contribution of the connection between the subsquares to the average DOS can also be estimated. A combination of both contributions leads to $\langle N(0)\rangle \geq c_1 \min_{-\mu_1 \leq \mu \leq \mu_1} P(\mu)$, where c_1 and μ_1 are distribution dependent positive constants. In particular, μ_1 must be chosen such that the spectrum of $H(\mu_0 = 0) = -\nabla^2\sigma_3 + \hat{\Delta}_d^s\sigma_1$ is inside the interval $[-\mu_1, \mu_1]$. For all unbounded distributions, such as the Gaussian distribution used in Ref. [9], as well as compact distributions with sufficiently large support, this estimate leads to a nonzero DOS at the Fermi level.

The major result in the d-wave (extended-s-wave) case with Lorentzian disorder is the presence of a finite purely imaginary self-energy $\Sigma_0 = -i\gamma\sigma_0$ due to nonmagnetic disorder which leads to a *nonzero* DOS at the Fermi level. The latter is in qualitative agreement with standard theories based on the self-consistent t-matrix approximation [7,8] as well as with exact diagonalization studies in 2D [16,17]. In contrast to such theories, our self-energy has no dependence on $\hat{\Delta}_d^s$, i.e., it is the same as in the normal state. In Fig. 1 we show a comparison of the self-energies of our theory and the limits of the t-matrix approximation.

A drawback of the model with Lorentzian disorder is that impurity concentration does not appear explicitly in the theory. Whereas in the t-matrix approach we have with the impurity concentration and the scattering strength (or phase shift) two parameters associated with disorder, in the present model we have only γ, the width of the Lorentzian. A way of making a connection is by comparing the variance of the Lorentzian distribution (γ) and the variance of the distribution underlying the t-matrix approximation, which is a bimodal distribution of a chemical potential $\mu = \mu_0$ with probability $1 - \delta$ (δ being the dimensionless impurity concentration) and $\mu = \mu_0 + V$ with probability δ (V being the scattering potential). The variance Var_μ of this distribution is determined by

$$\mathrm{Var}_\mu^2 = \langle\mu^2\rangle - \langle\mu\rangle^2 = V^2(\delta - \delta^2)\,. \tag{7}$$

For small concentrations of impurities, $\delta \ll 1$, we find $\mathrm{Var}_\mu = V\delta^{1/2}$. The $\delta^{1/2}$ behavior is also found for $\mathrm{Im}\ \Sigma_0(E = 0)$ in the t-matrix approach for strong scattering. Since in our model the variance of the distribution is also the imaginary part of the self-energy, this suggests that our model is closer to the strong scattering limit of the t-matrix approximation than the Born limit.

Finally, we comment on the discrepancies between our result and the calculation of Nersesyan *et al.* [9], who found a power law for the averaged DOS with Gaussian disorder.

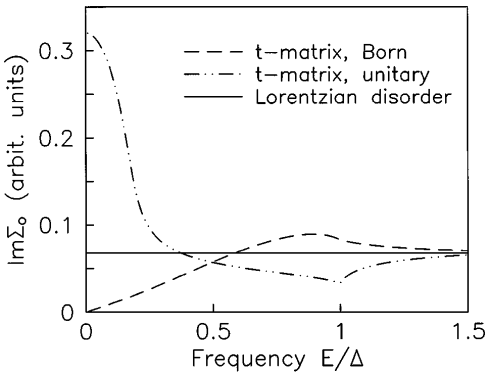

FIG. 1. Imaginary part of the self-energy vs frequency. For Lorentzian disorder (solid line) the self-energy is constant $i\gamma$. The self-energy of the self-consistent t-matrix approximation in the unitary scattering limit (dashed-dotted line) behaves $\propto(\delta\Delta)^{1/2}$ at zero frequency. For Born scattering (dashed line) the value at zero frequency is nonzero, but exponentially small. We have adjusted the impurity concentration to obtain equal normal state self-energies for the t-matrix results.

One might question the analysis of Nersesyan *et al.* because of the use of the replica trick, which is a dangerous procedure in a number of models [18]. However, Mudry, Chamon, and Wen [19] have obtained identical results for the *continuum* problem of Dirac fermions in the presence of a random gauge field using supersymmetry methods. We therefore believe that the crucial difference between our results and those of Ref. [9] occurs in the passage to the continuum and concomitant mapping of the site disorder in the original problem onto the random gauge field. Only in the continuum case is there a direct analogy between disorder in the chemical potential and a gauge field; on the lattice, gauge fields and chemical potential terms enter quite differently. Chemical potential terms are local while gauge fields are defined on bonds. Furthermore, chemical potential disorder enters linearly in the Hamiltonian while gauge fields enter through the Peierls prescription as a phase in the exponential multiplying the kinetic energy.

Disorder of the gauge field type is furthermore nongeneric even in the continuum, as discussed by Mudry *et al.* [19], who showed that the critical points of the system with random gauge field are *unstable* with respect to small perturbations by other types of disorder [20]. We expect that a proper mapping of the lattice Dirac fermion or d-wave superconductor problems to continuum models will inevitably generate disorder other than random gauge fields. Therefore, we believe that our result of a finite DOS at the Fermi level is the generic case for a d-wave superconductor in two dimensions.

We have computed the single-particle Green function and DOS for a model of a superconductor with nonmagnetic impurities. For an isotropic s-wave superconductor, we recover standard results; in particular, Anderson's theorem is reproduced. Furthermore, our calculations for the disorder-averaged d- and extended-s-wave propagators show that the DOS is nonzero for all energies, provided the distribution of the chemical potential is continuous and of sufficient width. The disorder average has been performed exactly in the case of a Lorentzian distribution. In this approach, we have neglected spatial order parameter disorder, but believe that, since this effect by itself leads to pairbreaking at all energies [13,15,17], we have provided strong evidence for a finite Fermi level density of states in a disordered 2D d-wave superconductor. Our calculation suggests that the standard t-matrix approach to disordered d-wave superconductors is qualitatively sufficient and casts doubt on the result by Nersesyan *et al.,* who found a power law for the averaged DOS with Gaussian disorder.

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