Details of Disorder Matter in 2D d-Wave Superconductors

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Within numerically exact solutions of the Bogoliubov–de Gennes equations, we demonstrate that discrepancies between predicted low-energy quasiparticle properties in disordered 2D d-wave superconductors occur because of the unanticipated importance of disorder model details and normal state particle-hole symmetry. For the realistic case, which is best described by a binary alloy model without particle-hole symmetry, we predict density-of-state suppression below an energy scale which appears to be correlated with the corresponding single impurity resonance.

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In metals, the many different analytic and numerical techniques used to study disorder and electron localization have led to a satisfyingly consistent understanding. The same cannot be said for the theory of disorder and quasiparticle localization in high T_c superconductors, which are widely believed to be correctly modeled as 2D systems with d-wave pairing. As pointed out some years ago by Nersesyan, Tsvelik, and Wenger [1], the standard perturbative approximation for the self-energy, the self-consistent T-matrix approximation (SCTMA), breaks down in 2D d-wave superconductors as $|E| \to 0$, even in the dilute impurity limit. In response, a variety of nonperturbative approaches have been applied [1–5], and have yielded apparently contradictory results. The purpose of this Letter is to demonstrate, by exact numerical calculation, that these discrepancies occur for the most part because, in contrast with the metallic case, details of the disorder model are qualitatively important. Moreover, for a physically important class of disorder models, the seemingly innocent assumption of particle-hole symmetric normal state bands leads to nongeneric results.

This work focuses on the quasiparticle density of states (DOS) $\rho(E)$, which is strongly affected by even small impurity concentrations. In pure materials, d-wave superconductivity is characterized by a gapless density of states $\rho(E) \sim |E|$ for $|E| < \Delta_0$ (Δ_0 is the d-wave gap amplitude). The SCTMA [6–8] predicts a finite DOS for disordered materials at $E = 0$. Nonperturbative approaches beyond the SCTMA have variously predicted that $\rho(E)$ vanishes according to universal [1,3] power laws, that $\rho(E)$ diverges as $|E| \to 0$ [4,5], and that there is a rigorous lower bound on $\rho(E)$ [2].

At first sight it seems impossible that these results could be mutually reconciled. We will undertake to show here, however, that most can be understood within a single framework, and that they differ primarily because of details in the treatment of disorder. It is natural to assume that such dramatic discrepancies for what *a priori* appear to be only slightly different physical models arise because the d-wave system is critical. We compare models by solving the Bogoliubov–de Gennes (BdG) equations numerically on large finite-size lattices. The model parameters we vary include disorder type (see below), disorder strength, normal state particle-hole symmetry, self-consistent renormalization of the local order parameter by disorder, and the so-called "Dirac cone anisotropy" v_F/v_Δ, where v_F is the Fermi velocity and v_Δ is the velocity of quasiparticles transverse to the nodes. We find that binary alloy and random site energy disorder models differ qualitatively. For strong scatterers, in particular, random site disorder models cannot describe the enhancement in the low-energy DOS predicted by Pépin and Lee [4], which we reproduce here. In addition, some of the present authors have recently shown that self-consistent treatment of the order parameter cannot be neglected in general [9]. We suggest that an appropriate model for disorder in the cuprates must involve a binary alloy treatment of strongly scattering impurities and self-consistency, and predict in this case a power law $\rho(E) \sim E^\alpha$ with disorder dependent α below an energy scale set by the single impurity resonance [9].

Method.—We consider a mean field Bogoliubov–de Gennes Hamiltonian for electrons hopping on a tight-binding square lattice with nearest neighbor hopping matrix element t, and bond mean field order parameter Δ_{ij},

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - \sum_{i,\sigma} [\mu - U_i] c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{\langle i,j \rangle} \{\Delta_{ij} c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} + \text{H.c.}\}, \quad (1)$$

where U_i is the impurity potential on site i. Energies will be measured in units of the hopping amplitude t and lengths in units of the lattice constant. We consider both random site energy models, in which the U_i are chosen randomly from a distribution $P(U)$, and binary alloy models, in which U_i takes the value U_0 on a fraction n_i of the sites and is zero elsewhere. The filling is chosen to stabilize a pure d-wave ground state in the absence of disorder,

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with homogeneous order parameter $\Delta_k = \Delta_0[\cos(k_x) - \cos(k_y)]$, where $\Delta_0 = \frac{1}{2}\sum_{\pm}(\Delta_{ii\pm x} - \Delta_{ii\pm y})$. In the tight-binding model, $v_F/v_\Delta = 2t/\Delta_0$.

For the d-wave system, Eq. (1) has been used to calculate DOS [10], superfluid density [11,12], and T_c suppression [11] numerically. It is widely assumed [10] that local fluctuations in Δ_{ij} produced by the impurity potential do not affect the DOS qualitatively. Recent numerical work [9,12] has suggested otherwise, and we therefore make a distinction between self-consistent (SC) solutions of the BdG equations, where $\Delta_{ij} \equiv V_{ij}\langle c_{j\downarrow}c_{i\uparrow}\rangle$ with nearest neighbor pairing interaction V_{ij}, and non-self-consistent (NSC) calculations, where Δ_{ij} has the homogeneous d-wave form. With Δ_{ij} determined, we can calculate the DOS from $\rho(E) = L^{-2}\sum_\alpha \delta(E - E_\alpha)$, where E_α are the eigenvalues of $\mathcal{H}$, for samples of size $L \times L$. Our numerical calculations were performed on systems with $L \leq 45$, and real periodic and antiperiodic boundary conditions.

Random site energy vs binary alloy models.—We begin by discussing the NSC models used in the vast majority of earlier work. In field theoretical approaches it is common to assume a Gaussian distribution $P(U) = (\sigma\sqrt{2\pi})^{-1}\exp(-U^2/2\sigma^2)$ for the disorder potential at each site. For technical reasons it is more convenient to consider a uniform "box" distribution $P(U) = 1/(2W)$, $|U| < W$. We have checked that results with the box distribution are similar to the Gaussian, with the mapping $W \simeq \sqrt{3}\,\sigma$. Disorder is thus characterized by a single parameter, in contrast to the binary alloy model, where chemical impurities or vacancies are characterized not only by their individual scattering strength U_0, but also by their concentration n_i. In the normal metal, a correspondence between W and (n_i, U_0) can always be found such that the random site energy and binary alloy models yield similar results. This is no longer true in the superconducting state, because the frequency dependence of the superconducting Green's function can lead to midgap resonances [13], found only in the binary alloy case and observed in experiment [14,15].

Figure 1 shows the DOS of a d-wave superconductor at low energies in the presence of box disorder at different W. When W is small, the self-consistent Born limit reproduces the exact calculation for the box distribution quantitatively. For larger W, the exact calculation shows the formation of a "disorder induced pseudogap" (DIP) over an energy interval $|E| < E_1$, where E_1 grows rapidly with W. The physics of the DIP is clearly not captured by the Born limit approximation for the box distribution, which predicts a finite residual DOS $\rho_{\rm mf}$. In Fig. 2, we study the DIP in more detail. With $v_F = v_\Delta$, and large disorder, we can identify a second, much smaller energy scale E_2 over which $\rho(E) \sim |E|$. This regime disappears quickly, however, as v_Δ is decreased, and we contrast this behavior with the relatively slow scaling of E_1 with v_Δ. Earlier field theoretical studies [3] made predictions for a linear DOS over an energy scale $\sim 1/\rho_{\rm mf}\xi_L^2$. The rapid scaling

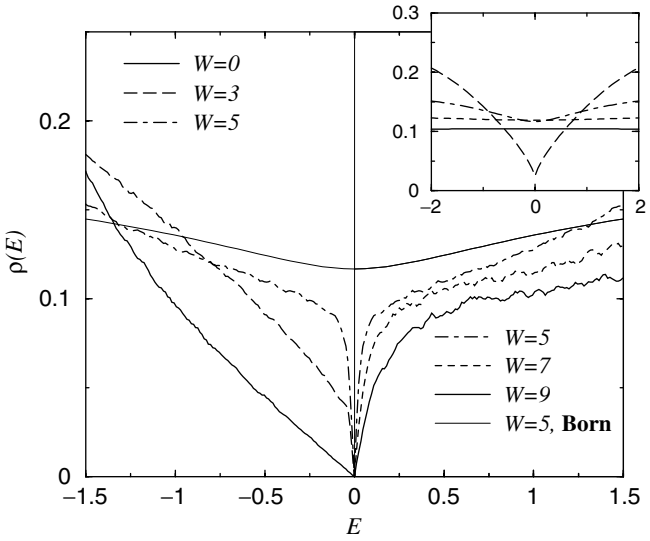

FIG. 1. Density of states for box distributed disorder. Main figure: Exact NSC solution of the BdG equations for different W. For comparison, the Born approximation for $W = 5$ is also shown. Inset: Born approximation for different W. Line types refer to same values of W as in main figure ($W = 0$ not shown). $\Delta_0 = 2$ and $\mu = 1.2$.

of E_2 in Fig. 2 is consistent with the predicted exponential dependence of ξ_L on v_F/v_Δ. It is also tempting to make the connection between the DIP edge E_1 and the much larger predicted scale for weak localization corrections to the DOS [5,16]. In this case, E_1 is expected to scale as $\Delta_0\rho_{\rm mf}$ for small disorder, and it is clear from Fig. 2 that the scaling with Δ_0 holds even for large disorder.

Unitary limit.—There is considerable evidence that simple defects in the CuO_2 planes give rise to local scattering centers close to the unitarity limit, indeed that simple defects in all unconventional superconductors scatter with phase shifts close to $\pi/2$, for reasons which

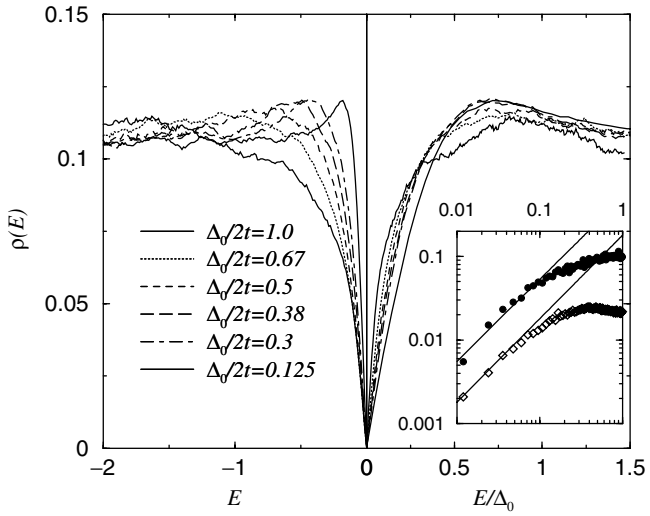

FIG. 2. Scaling of the DOS with Δ_0 for $\mu = 1.2$ and $W = 9$. Inset: Logarithmic plots for $\Delta_0/2t = 1$ (circles) and $\Delta_0/2t = 0.3$ (diamonds; data rescaled for clarity). Lines are guides to the eye indicating linearity.

are not completely understood. For isolated impurities, the signature of unitarity is a resonance in the local DOS at $E = 0$; resonances close to $E = 0$ have been observed in recent scanning tunneling microscopy experiments [14,15] for both "native defects" and Zn atoms substituting on the planar copper sites in BaSrCaCuO-2212. A point which has not been widely appreciated is the fact that the value of the impurity potential U_0 which produces a unitary resonance is dependent on the band structure; for a perfectly symmetric band the unitary limit corresponds to $U_0 \to \pm\infty$ [13], while for an asymmetric band, U_0 is a finite value dependent on the degree of asymmetry [17–19]. There is a fundamental distinction between the two cases, with the first exhibiting perfect particle-hole symmetry on all energy scales [4], and the second exhibiting particle-hole symmetry on energies $|E| < \Delta_0$. Most analytical treatments of the disorder problem do not distinguish between the two, using Δ_0 as a high energy cutoff. We show below that in the many-impurity problem erroneous conclusions may be drawn as a result.

In the unitary limit, the SCTMA predicts that a plateau forms in the DOS over an energy interval $|E| < \gamma$. Recent nonperturbative calculations by Pépin and Lee [4] found that unitary scatterers produce a divergent DOS $\rho(E) \sim 1/|E| \ln^2(|E|/\Delta_0)$ as $|E| \to 0$. This feature was not found in recent numerical work by some of the current authors [9], who considered only tight-binding bands with $\mu \neq 0$. In Fig. 3, we show that a divergent DOS occurs only in models with particle-hole symmetry at all energy scales, for $\mu = 0$ and $U_0^{-1} = 0$ in our case. The effects of breaking particle-hole symmetry are illustrated in Fig. 3. For $\mu = 0$ and $U_0^{-1} \neq 0$, the divergent peak splits, and moves away from $E = 0$ as $|U_0^{-1}|$ grows. This is qualitatively similar to what happens in the single impurity limit [13], although the peak splitting occurs more rapidly in the bulk disordered case. An alternative means of breaking particle-hole symmetry is to let $\mu \neq 0$, in which case the peak structure rapidly disappears (inset, Fig. 3). This differs from the single impurity limit where there always exists some finite U_0 at which a zero energy divergence occurs. A remnant of the isolated impurity resonance remains, however, as a broad accumulation of states at low energies. The extra spectral weight is not reproduced by SCTMA calculations, and it gradually vanishes as we move farther away from perfect symmetry. Evidently the low-energy effective action is unstable both to deviations from unitarity and to deviations from full band particle-hole symmetry.

Local order parameter suppression.—In the above discussion, we have concentrated on the artificial case in which the order parameter was not allowed to vary spatially, with the purpose of understanding a set of disparate theoretical results obtained under this assumption. As discussed in Ref. [9], allowing Δ_{ij} to respond self-consistently to the impurity potential introduces a new source of scattering in the off-diagonal channel, which ultimately leads to a suppression of the DOS at low energy. This effect highlights the complex nature of multi-impurity scattering resonances, and is opposite to the expectations of the naive "Swiss cheese" picture, in which the impurity simply produces a small region of normal metal. In Fig. 4 we show the effect of self-consistency in the unitary limit. In the case of a symmetric band, self-consistency moves the resonance towards the Fermi level (consistent with what is seen in the single impurity case [19,20]), and suppresses the DOS at low energy on roughly the same scale. This kind of DOS suppression is also seen in SC solutions with box distributed disorder [Fig. 4(b)]. In the

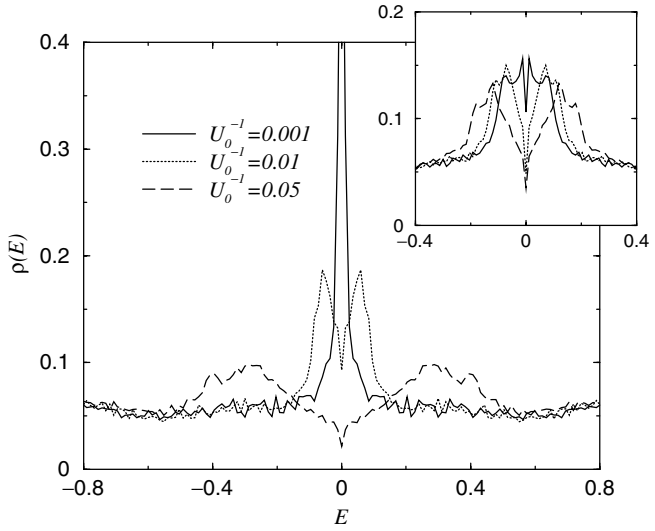

FIG. 3. NSC calculation of DOS near the unitary limit for $\Delta_0 = 2$ and $n_i = 0.05$. Main figure: $\mu = 0$. Inset: $\mu = 0.2$ with $U_0^{-1} = 0.001$ (solid line), 0.01 (dotted line), and 0.02 (dashed line).

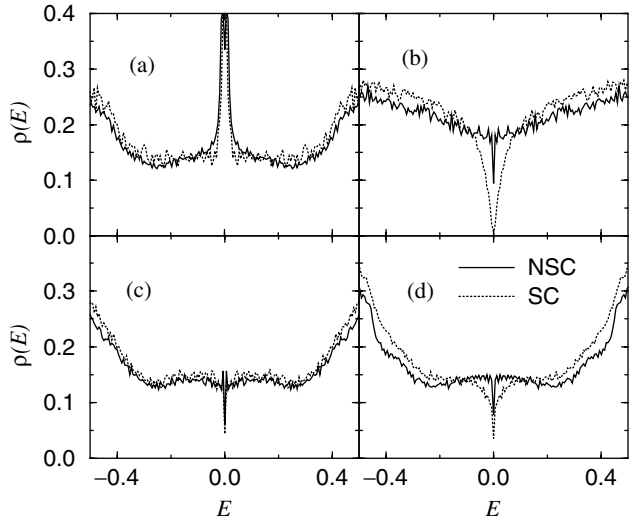

FIG. 4. Exact solutions of BdG equations with (SC) and without (NSC) order parameter self-consistency, for $\Delta_0 = 0.39$: (a) Binary alloy, symmetric band, near unitarity, $U_0 = 100$, $n_i = 0.05$, and $\mu = 0$. (b) Box distribution, $W = 2$, $\mu = 1.2$. (c) Realistic binary alloy model, $U_0 = 5$, $n_i = 0.04$, $\mu = 0.6$. (d) As in (c) but with $\mu = 1.2$.

binary alloy model, however, it is possible to make an empirical connection between the energy scale for DOS suppression and the energy of the single impurity resonance. The energy scales are not equal, but clearly scale together [9]. One interesting implication is that for scatterers sufficiently close to the unitary limit, the DIP will be unobservable, as illustrated in Fig. 4(c), but that the same impurity doped into a different host may cause the DIP to open [Fig. 4(d)]. We speculate that this may be the case with Zn, which is clearly a unitary scatterer in BSCCO [14], but appears to produce a depression in the DOS at small energies in LSCO, as seen in recent specific heat experiments [21].

Conclusions.—We have shown that a number of different approaches to the d-wave disorder problem which produce apparently contradictory results can be understood within a single framework when the appropriate symmetries of the Hamiltonian, and, in particular, of the particular realization of disorder, are accounted for. The most important question we hope to settle here is which of the preceding results, if any, are of relevance to experiment. We remind the reader that experiments which probe the DOS most directly are consistent with the existence of a constant DOS at the Fermi energy [22]. We have shown that a true constant DOS *cannot* be understood in 2D d-wave superconductors with any of the disorder models discussed here [23], and we suggest several possible reasons for the discrepancy. The first possibility is that experiments are unable to access the DIP regime in the optimally doped materials because of native near-unitarity defects [14]. In this case, the only effects of weak localization on the DOS would be the weak nonmonotonicity shown in Figs. 4(c) and 4(d), which is reminiscent of effects seen in the specific heat [24]. The second possibility is that weak coupling to the third dimension destroys the DOS anomalies described above; we expect on general grounds that the influence of the crossed diagrams identified by Nersesyan *et al.* [1] will become negligible in the dilute limit in 3D, and the validity of the SCTMA will be restored. In this context we note that almost all the experiments indicating finite residual DOS in the cuprates have been performed on YBCO, the most 3D of the cuprate materials. We hope our work will serve as an incentive to examine the low-energy properties of disordered 2D materials like BSCCO-2212. Finally, we mention the possibility that many-body effects beyond the BCS approximation play an important role at low energies. There is some speculation that this might be the case in the underdoped cuprates, and the formulation of a relevant theory is an interesting but difficult problem which must be left to future research.

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Note added.—In the final stages of preparation of this manuscript, we received a preprint from Zhu *et al.* [25] in which similar results for the unitarity limit of the symmetric band were obtained.

[1] A. A. Nersesyan, A. M. Tsvelik, and F. Wenger, Nucl. Phys. **B438**, 561 (1995); Phys. Rev. Lett. **72**, 2628 (1994).
[2] K. Ziegler, M. H. Hettler, and P. J. Hirschfeld, Phys. Rev. Lett. **77**, 3013 (1996); Phys. Rev. B **57**, 10 825 (1998).
[3] T. Senthil, Matthew P. A. Fisher, Leon Balents, and Chetan Nayak, Phys. Rev. Lett. **81**, 4704 (1998); T. Senthil and Matthew P. A. Fisher, Phys. Rev. B **60**, 6893 (1999).
[4] C. Pépin and P. A. Lee, cond-mat/0002227; Phys. Rev. Lett. **81**, 2779 (1998).
[5] M. Bocquet, D. Serban, and M. R. Zirnbauer, cond-mat/9910480.
[6] L. P. Gor'kov and P. A. Kalugin, JETP Lett. **41**, 253 (1985).
[7] S. Schmitt-Rink, K. Miyake, and C. M. Varma, Phys. Rev. Lett. **57**, 2575 (1986).
[8] P. J. Hirschfeld, D. Vollhardt, and P. Wölfle, Solid State Commun. **59**, 111 (1986).
[9] W. A. Atkinson, P. J. Hirschfeld, and A. H. MacDonald, preceding Letter, Phys. Rev. Lett. **85**, 3926 (2000).
[10] T. Xiang and J. M. Wheatley, Phys. Rev. B **51**, 11 721 (1995).
[11] M. Franz, C. Kallin, A. J. Berlinsky, and M. I. Salkola, Phys. Rev. B **56**, 7882 (1997).
[12] Amit Ghosal, Mohit Randeria, and Nandini Trivedi, cond-mat/0004481.
[13] A. V. Balatsky, M. I. Salkola, and A. Rosengren, Phys. Rev. B **51**, 15 547 (1995); A. V. Balatsky and M. I. Salkola, Phys. Rev. Lett. **76**, 2386 (1996).
[14] E. W. Hudson, S. H. Pan, A. K. Gupta, K.-W. Ng, and J. C. Davis, Science **285**, 88 (1999); S. H. Pan, E. W. Hudson, K. M. Lang, H. Eisaki, S. Uchida, and J. C. Davis, Nature (London) **403**, 746 (2000).
[15] Ali Yazdani, C. M. Howald, C. P. Lutz, A. Kapitulnik, and D. M. Eigler, Phys. Rev. Lett. **83**, 176 (1999).
[16] P. A. Lee, Phys. Rev. Lett. **71**, 1887 (1993).
[17] R. Fehrenbacher, Phys. Rev. Lett. **77**, 1849 (1996); R. Fehrenbacher and M. R. Norman, Phys. Rev. B **50**, R3495 (1994); R. Fehrenbacher, Phys. Rev. B **54**, 6632 (1996).
[18] R. Joynt, J. Low Temp. Phys. **109**, 811 (1997).
[19] W. A. Atkinson, P. J. Hirschfeld, and A. H. MacDonald, cond-mat/9912158.
[20] Alexander Shnirman, İnanc Adagideli, Paul M. Goldbart, and Ali Yazdani, Phys. Rev. B **60**, 7517 (1999).
[21] C. F. Chang, J.-Y. Lin, and H. D. Yand, Phys. Rev. Lett. **84**, 5612 (2000).
[22] See, e.g., D. J. Scalapino, Phys. Rep. **250**, 329 (1995).
[23] Our numerical calculation for the model proposed by Ziegler *et al.* [2] shows that while the result of nonzero DOS claimed is indeed correct, it depends on the particular choice of band, which we believe to be nongeneric.
[24] D. L. Sisson *et al.,* cond-mat/9904131.
[25] Jian-Xin Zhu, D. N. Sheng, and C. S. Ting, cond-mat/0005266.