Quasiparticle Localization in Disordered d-Wave Superconductors

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An extensive numerical study is reported on the disorder effect in two-dimensional d-wave superconductors with random impurities in the unitary limit. It is found that a sharp resonant peak shows up in the density of states at zero energy and correspondingly the finite-size spin conductance is strongly enhanced which results in a nonuniversal feature in one-parameter scaling. However, all quasiparticle states remain localized, indicating that the resonant density peak alone is not sufficient to induce delocalization. In the weak disorder limit, the localization length is so long that the spin conductance at small sample size is close to the universal value predicted by Lee [Phys. Rev. Lett. **71**, 1887 (1993)].

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Since the discovery of the d-wave pairing symmetry in high-T_c cuprates, there has been increased interest in low-energy quasiparticle properties in unconventional superconductors. In such a d-wave superconductor, quasiparticles are gapless along the four nodal directions on the essentially cylindrical Fermi surface, in contrast to the conventional s-wave superconductors, where quasiparticles are gapped everywhere. The issues of how the disorder affects the low-energy quasiparticle excitations and whether these quasiparticles are localized remain unresolved. Some perturbative self-consistent T-matrix calculations [1–8] and a nonperturbative one [9] predicted a nonzero constant density of states (DOS) in the low-energy region in the presence of weak disorder. However, most nonperturbative calculations [10,11] and one numerical study [12] showed that the DOS at zero energy vanishes. With this constant or even vanishing DOS, some groups [4,13] suggested that all quasiparticle states are localized. On the other hand, it has been shown [14] that a single unitary scattering impurity produces a zero-energy quasiparticle resonant state while the long-range overlap between these impurity states [15] may lead to an extended quasiparticle band near zero energy. More recently, a singularity in the DOS at zero energy was obtained by the nonperturbative T-matrix method [16] for the random distributed unitary impurities. It is noteworthy that in one dimension, there is a direct relation between the localization length and the DOS [17]; thus a singularity in zero-energy DOS signals the delocalization in the system. However, in two dimensions, this theorem does not hold generally [16]. For example, in two-dimensional integer quantum Hall systems, it has been shown that the delocalization property at the quantum critical point is not changed by the changing of the DOS due to strong electron-electron interaction [18]. Therefore, the localization of quasiparticles in a d-wave superconductor in the presence of nonmagnetic unitary impurities is still an open question.

In this Letter, we numerically examine the disorder effect in d-wave superconductors with nonmagnetic impurities in the unitary limit. The quasiparticle DOS is calculated by exact diagonalization and the spin conductance is computed by the transfer matrix method. It is found that, depending on the particle-hole symmetry of the Hamiltonian, a sharp DOS peak can occur at zero energy and correspondingly the spin conductance is strongly enhanced at finite sample size. However, using one parameter scaling analysis we show that all the quasiparticle states are always localized regardless of the existence of the zero-energy peak in the DOS. In weak disorder limit, the localization length is so long that the spin conductance at small sample size remains close to the universal value $2\xi_0/a$ (ξ_0 is the coherence length of the superconductor and a is the lattice constant) in agreement with the theoretical prediction by Lee [4]. A nonuniversal feature in one-parameter scaling of conductance related to the resonant DOS peak is also discussed.

We begin with a lattice Hamiltonian for the d-wave superconductor [19]

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

where $\langle ij\rangle$ refers to the two nearest neighboring sites with the hopping integral taken as the unit, μ is the chemical potential, and U_i is the impurity potential. We mainly consider the unitary limit where U_i takes a nonzero value U_0 only at a fraction n_i of the sites which are randomly distributed in space. The d-wave symmetry is imposed by choosing order parameters: $\Delta_{i,i\pm\hat{x}} = -\Delta_{i,i\pm\hat{y}} = \Delta_d$, which yields the excitation spectrum $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$, with $\epsilon_k = -2(\cos k_x + \cos k_y) - \mu$ and $\Delta_k = 2\Delta_d(\cos k_x - \cos k_y)$. Therefore, gapless quasiparticle states exist along the direction $|k_x| = |k_y|$ in the momentum space. Unless otherwise stated, $\mu = 0$, $\Delta_d = 0.1$, and $U_0 = 100$ are taken throughout the work. In the presence of a single impurity in the unitary scattering

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limit, an earlier study has shown [20] that the order parameter is strongly suppressed near the impurity site on a scale of a few lattice constants. To take into account this effect, the order parameters on bonds connecting with the strong impurity sites are taken as zero. By exactly diagonalizing the Hamiltonian (1), one can calculate the quasiparticle DOS, which is defined as [12,21]

$$\rho(E) = \frac{1}{N_L} \sum_n \delta(E - E_n), \qquad (2)$$

where $N_L = L \times L$ with L the linear dimension of the system in units of lattice constant ($a = 1$). In Fig. 1(a), the DOS is plotted as a function of quasiparticle energy E with impurity density $n_i = 0.1$ ($\mu = 0$ and $\Delta_d = 0.1$) at $N_L = 90 \times 90$. In the calculation the periodic boundary condition is used and it has been checked that the results do not depend on the boundary condition for large L considered here. As shown in Fig. 1(a), we find that a sharp zero-energy peak shows up in the DOS, which can be fitted by the analytical form $c_0 n_i/2|E|(\ln^2|E/E_g| + \pi^2/4)$ from Ref. [16] with $c_0 = 0.66$ (the superconducting gap $E_g \sim 4 \times \Delta_d$) as shown in the inset of Fig. 1(a). The fitting breaks down at an energy scale close to $1/N_L$ [22]. The strength of the zero-energy peak is reduced when n_i is changed to 0.04 as shown in the $E < 0$ part of Fig. 1(b). The overall shape of the peak is sample size independent (from $N_L = 25 \times 25$ to 120×120, as well as a strip system 30×300) with the DOS value at the peak position increasing with N_L very slowly. Note that in the presence of disorder, the order parameter Δ_{ij} is in principle subject to the self-consistency condition: $\Delta_{ij} = -g_{ij}\langle c_{j\downarrow} c_{i\uparrow}\rangle$, where $g_{ij} = g_0$ is the attracting interaction for d-wave pairing. We have also calculated the DOS by diagonalizing the Hamiltonian Eq. (1) self-consistently for each disorder configuration with $N_L = 25 \times 25$. The obtained DOS is also shown in Fig. 1(b) ($E > 0$ part), which is averaged over 50 impurity configurations and 8×8 wave vectors in the supercell Brillouin zone. As can be seen, the DOS value at E_g is reduced due to the suppression of Δ_{ij} around each impurity site. However, all other features remain essentially unchanged [compared to the $E < 0$ part of Fig. 1(b)].

The presence of a zero-energy peak in the DOS crucially depends on the symmetry of the Hamiltonian. Since a repulsive or attractive impurity center with infinite strength (i.e., unitary limit) is equivalent to the exclusion of a lattice site, both the local and global particle-hole symmetry remain if the chemical potential $\mu = 0$, which then produces a resonant peak at $E = 0$ [16]. This feature was not exhibited in earlier works because of either the breaking of local particle-hole symmetry by the soft impurity scattering [10,11,13] or the breaking of the band particle-hole symmetry by considering $\mu \neq 0$ [12], which indicates the importance of the realization of the disorder model. In Fig. 1(c), the DOS is presented for random on-site disorders with U_i uniformly distributed between $[-1, 1]$ with a homogeneous order parameter at all sites. Because of the

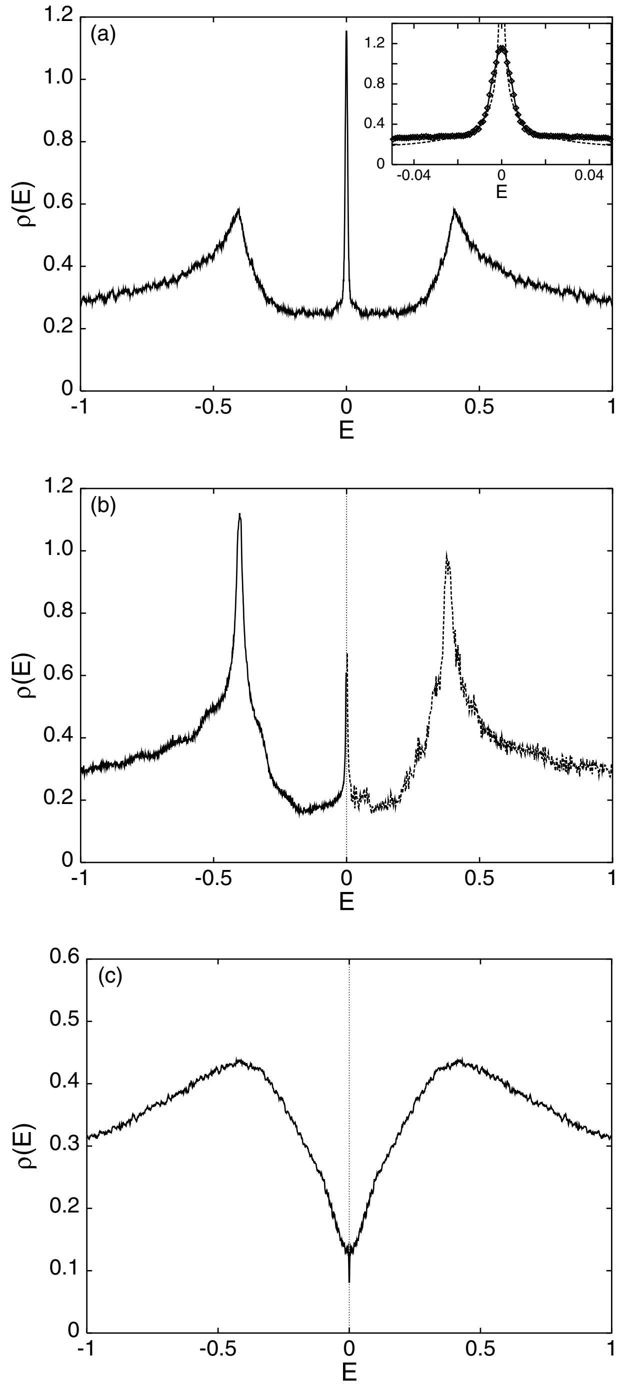

FIG. 1. (a) Density of states $\rho(E)$ in a d-wave superconductor (sample size 90×90) with a fraction $n_i = 0.1$ of the randomly distributed impurities in the unitary scattering limit $U_0 = 100$. Inset of (a): the DOS peak is fitted using the analytical form $c_0 n_i/2|E|(\ln^2|E/\Delta_g| + \pi^2/4)$ ($E_g = 4 \times \Delta_d$) from Ref. [16] with $c_0 = 0.66$. (b) Comparison of $\rho(E)$ ($E < 0$ part) at $N_L = 90 \times 90$ for $n_i = 0.04$ with the self-consistent result ($E > 0$ part) at $N_L = 25 \times 25$ (averaged over 8×8 supercells). (c) $\rho(E)$ at $N_L = 90 \times 90$ with on-site random disorders distributed between $[-1, 1]$.

absence of the local particle-hole symmetry in this case, $\rho(E)$ has a finite value at the low-energy region down to a mesoscopic scale $E \sim 1/N_L$, below which it shows a zero-energy dip, in agreement with those of the nonperturbative calculations [10,11,13]. We have also relaxed the unitary scattering limit by taking $U_0 = 10$ (comparable to the band width) or (and) broken the band particle-hole symmetry by taking $\mu = -1$ and found that the DOS at $E = 0$ is always strongly suppressed, which is similar to the results obtained in Ref. [12]. There is a smooth crossover from the zero-energy peak to dip in the DOS with the varying of model parameters as long as the Hamiltonian is driven away from the perfect particle-hole symmetry. Therefore, our numerical result indicates that different realizations of disorder give rise to different profiles of the DOS as the energy approaches the Fermi level.

In the absence of the zero-energy resonant peak in DOS due to the breaking of band particle-hole symmetry by $\mu \neq 0$, Franz *et al.* [23] have studied a similar problem by examining the sensitivity of the wave function to the boundary conditions and by analyzing the finite-size dependence of inverse participation ratios and presented strong evidence for the localization of low-energy quasiparticles. Here we are concerned with the question of quasiparticle localization or delocalization in the disordered d-wave superconductor when the zero-energy peak appears in the DOS. We employ the transfer-matrix method to calculate the finite-size localization length and the longitudinal conductance. We consider the quasi-one-dimensional strip sample with the length $L \geq 10^5$ and width M. The quasiparticle wave function amplitudes in the ixth and $(ix + 1)$th slices satisfy the following equation:

$$\begin{pmatrix} \hat{\phi}_{ix+1} \\ \hat{\phi}_{ix} \end{pmatrix} = T_{ix} \begin{pmatrix} \hat{\phi}_{ix} \\ \hat{\phi}_{ix-1} \end{pmatrix}, \tag{3}$$

where $\hat{\phi}_{ix}$ is a $2M$-component vector of the Bogoliubov amplitudes for quasiparticle states, and T_{ix} is a $4M \times 4M$ transfer matrix. The transfer matrix through the whole system, $P_L = \prod_{ix=1}^{L} T_{ix}$, has a set of $2M$ pairs of Lyapunov exponents, which determine the inverse of length λ_i $(i = 1, 2, \ldots, 2M)$. The usual orthonormalization procedure is taken [24] in our calculation. Correspondingly, the longitudinal conductance g_s extrapolated for a square sample with width M is given by [25]

$$g_s(M, n_i) = \sum_{j=1}^{2M} \cosh^{-2}\Lambda_j\,, \tag{4}$$

where $\Lambda_j = \lambda_j/M$. Note that g_s corresponds to the spin conductance as the spin carried by the quasiparticle is conserved [13]. As shown in Fig. 2(a), g_s as a function of M monotonically decreases with the increase of M at $E = 0$ for each selected impurity density from $n_i = 0.01$ to 0.16, consistent with localization in the large M limit. All the data between $M = 32$ and $M = 120$ at different n_i can be collapsed onto a single curve:

$$g_s(M, n_i) = f\left(\frac{\xi(n_i)}{M}\right), \tag{5}$$

as shown in Fig. 2(b) in accordance with the one-parameter scaling law. Here $\xi(n_i)$ is the thermodynamic

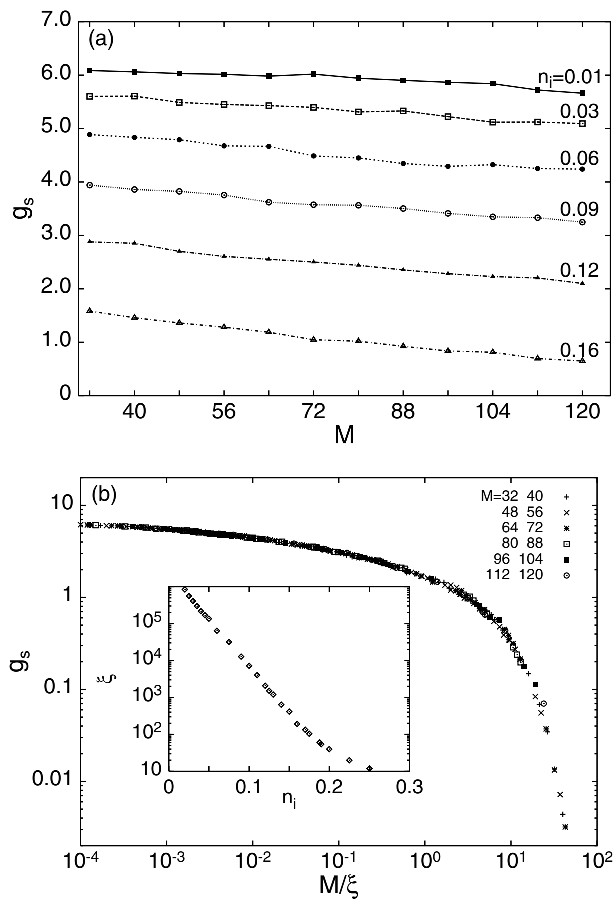

FIG. 2. (a) Spin conductance g_s as a function of the strip width M for different impurity density n_i at $E = 0$. (b) Double logarithmic plot of g_s as a scaling function of M/ξ at $E = 0$ for all the data with $0.01 \leq n_i \leq 0.275$. Inset of (b): the scaling parameter ξ as a function of n_i at $E = 0$. The other parameters are $\mu = 0$, $\Delta_d = 0.1$, and $U_0 = 100$.

localization length which depends only on n_i as shown in the inset of Fig. 2(b), and it remains finite for all the disorder density n_i, suggesting that all the states are localized even in the unitary limit with the presence of the zero-energy resonant peak. In addition, we display in Fig. 3 the conductance g_s as a function of quasiparticle energy E at sample width $M = 48$ and 96 with $n_i = 0.1$. It is found that g_s is strongly enhanced as $E \rightarrow 0$ in the region $E \sim 0.01$ corresponding to the width of the DOS peak while away from this region g_s generally increases with the increase of E. For quasiparticle at low energy with $E < 0.1$, it has been found that g_s always decreases with the increase of M and all the states are localized in the large M limit. However, the scaling curve $g_s(M, n_i) = f(\frac{\xi(n_i)}{M})$ found at E away from the DOS peak $(E > 0.01)$ is different from that for $E = 0$ at the peak of the DOS, indicating the breaking down of the universal one-parameter scaling law due to the presence of the resonant peak in the DOS. In addition, for all values of Δ_d, g_s decreases with M, implying localization in all the parameter region. At fixed M, g_s always decreases monotonically with the increasing Δ_d, in agreement with

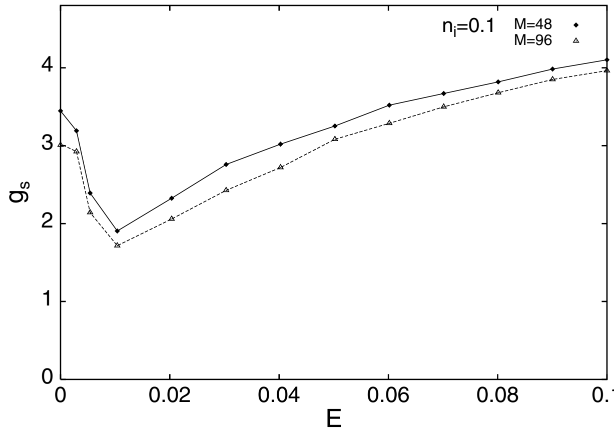

FIG. 3. g_s as a function of quasiparticle energy E at $M = 48$ and 96 for $n_i = 0.1$. All the other parameters are the same as in Fig. 2.

the general argument that quasiparticle states in a superconducting phase are always more localized [4] than the corresponding normal state. Given the localization of the quasiparticle states, the spin conductance at the longest length scales must vanish. However, in the weak disorder (the impurity density $n_i \leq 4\%$), i.e., the Born limit, we found that the localization length is so long that at small sample size $M \sim 32$, the spin conductance g_s^0 follows the universal form [4] $g_s^0 = 2\xi_0/a$ as the coherence length ξ_0 is changed from 1.6 to 6.4 by changing Δ_d between 0.05 and 0.20. For the strong disorder, the conductance is generally smaller than the Born limit value due to the onset of the localization effect.

In conclusion, we have studied the quasiparticle states in 2D d-wave superconductors with randomly distributed strong impurities in the unitary scattering limit. As the particle-hole symmetry holds, a very sharp DOS peak is obtained at zero energy. Such a DOS peak enhances the finite-size conductance. However, using one-parameter scaling analysis we have shown that all the quasiparticle states at low energy are still localized and the localization effect is generally enhanced with the increase of the superconducting order parameter.

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Note added.—After the submission of this paper, we received a preprint from Atkinson *et al.* [26] where similar results for the DOS in the unitary limit of the symmetric band were obtained.

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