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Delocalization of quasiparticles in quasi-two-dimensional disordered superconductors with s-wave pairing

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Abstract. We investigate localization behavior of quasiparticles in disordered multi-plane superconductors with s-wave pairing. By introducing disorder with random site energies, the spatial fluctuations of Bogoliubov-de Gennes pairing potential are self-consistently determined. The size dependence of rescaled localization length for a long bar is calculated by using the transfer-matrix method. From the finite-size scaling analysis we show that there exists a critical point of the disorder strength W_c which separates the extended and localized quasiparticle states in such quasi-two-dimensional systems. The associated critical behavior is studied and the relationship of the results to the number of planes is discussed.

PACS. 72.15.Rn Localization effects (Anderson or weak localization) – 73.20.Jc Delocalization processes – 72.80.Ng Disordered solids – 74.78.-w Superconducting films and low-dimensional structures

1 Introduction

There are two important types of phase transition in the condensed matter physics: the transition to superconductivity due to the attractive interaction of electrons and the metal-insulator transition caused by localization from disorder. They are essentially different phenomena in nature related to the quantum effects. The transition to the superconductivity is owing to the Cooper instability of the Fermi liquid in the presence of the effective attraction among electrons. On the other hand, the Anderson localization which causes the metal-insulator transition in the presence of disorder is originated from the quantum interference among randomly scattered waves. The Anderson theorem guarantees that the nature of the transition from a Fermi liquid to an s-wave superconductor is unchanged by the presence of nonmagnetic impurities or disorder provided that the system remains being metal in the normal state [1]. However, if the disorder is strong enough in three dimensions (3D), or is present in 1D or 2D, the electron systems will become insulating in the normal state due to the localization [2]. Thus, it becomes interesting to know what happens when the Cooper instability occurs in systems where electron states are localized due to the disorder.

The properties of electron systems in the coexistence of disorder and attractive interaction have been investigated for a long time [3–5]. In fact, in the coexistence of the superconducting pairing and disorder, a complicated situation may appear in 2D. The ground state of the system may be an insulator, a metal, or a superconductor, determined by an infinite-wavelength and zero-frequency current-current correlation function as a criteria discussed in reference [6]. The self-consistent calculations based on the Bogoliubov-de-Gennes (BdG) framework for systems with strong disorder show that although the spectral gap persists, the local pairing amplitude develops broad spatial fluctuations and off-diagonal correlations exhibit a substantial reduction [7–9]. It is shown by a finite-size scaling analysis that a d-wave component of the pairing potential is necessary for the delocalization of quasiparticle states in a 2D disordered system [10]. For dirty films, the critical conductance g_c below which the superconductivity vanishes was obtained by Finkelstein by including the inter-electron interaction [11], and re-derived in Keldysh formalism by Feigemanl'man et al. [12]. Experimentally, the effects of the disorder on 2D or quasi-2D s-wave superconductors have also been investigated [13].

In the present paper, we consider a multilayered quasi-2D disordered model with the s-wave pairing to investigate the combined effect of disorder and pairing symmetry on diffusion properties of quasiparticles. By introducing disorder with random site energies, the spatial fluctuations of Bogoliubov-de Gennes pairing potential are self-consistently determined. A transition from localized to extended states has been exhibited in a finite-size scaling analysis. The results are different from those obtained in one-plane pure 2D systems where the quasiparticles are always localized. The associated critical behavior is studied and the relationship of the results to the number of planes is discussed.

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The paper is organized as follows: In the next section we describe the basic formalism in our calculations. In Section 3 we present the main results and discuss the related physical implication. The last section is devoted to brief summary of conclusions.

2 The basic formalism

We consider a quasi-2D square lattice with on-site disorder and on-site attractive interaction:

$$H = \sum_{i,j,k;\sigma} (\epsilon_{ijk} c^{\dagger}_{ijk,\sigma} c_{ijk,\sigma}) + \sum_{\langle ijk,i'j'k' \rangle;\sigma} (t_0 c^{\dagger}_{ijk,\sigma} c_{i'j'k';\sigma} + \text{h.c.}) - V \sum_{i,j,k} (c^{\dagger}_{ijk;\uparrow} c^{\dagger}_{ijk;\downarrow} c_{ijk;\downarrow} c_{i'j'k';\uparrow}), \quad (1)$$

where $c_{ijk,\sigma}$ is annihilation operator for electron on site (i,j,k) with spin σ, i, j and k label the positions of sites in the x, y and z directions, ϵ_{ijk} and t_0 denote the site energy and hopping integral, respectively, and V is the strength of on-site attractive interaction. Here, we assume that the Fermi level is at the band center and set as the energy zero. The z-direction is along the normal of the quasi-2D system, so $k = 1, 2, \ldots, N$ with N being the number of atomic planes. We only consider the nearest-neighbor (NN) hopping and set it as energy units ($t_0 = 1$). The on-site energies are uniformly distributed between $-W/2$ and $W/2$ with W being the measure of disorder. As we only consider s-wave pairing, the BdG pairing potential is written as

$$\lambda_{ijk} = -V \langle c^{\dagger}_{ijk;\uparrow} c^{\dagger}_{ijk;\downarrow} \rangle, \quad (2)$$

where $\langle \ldots \rangle$ stands for the statistical averaging. From this mean-field treatment the Hamiltonian becomes

$$H = \sum_{i,j,k;\sigma} (\epsilon_{ijk} c^{\dagger}_{ijk,\sigma} c_{ijk,\sigma}) + \sum_{\langle ijk,i'j'k' \rangle;\sigma} (t_0 c^{\dagger}_{ijk,\sigma} c_{i'j'k';\sigma} + \text{h.c.}) + \sum_{i,j,k} (\lambda_{ijk} c_{ijk,\downarrow} c_{ijk,\uparrow} + \text{h.c.}). \quad (3)$$

In order to calculate the localization length within the scheme of finite-size scaling, we investigate an $M \times L \times N$ bar with M and L being the width in the x-direction and the length in the y-direction of the strip, respectively. In the site representation a quasiparticle wavefunction can be written as a linear superposition

$$|\Psi\rangle = \sum_{i=1}^{M} \sum_{j=1}^{L} \sum_{k=1}^{N} (a_{ijk} c^{\dagger}_{ijk,\,\sigma} + b_{ijk} c_{ijk,\,-\sigma}) |F\rangle, \quad (4)$$

where $|F\rangle$ denotes the Fermi sea in the normal state. By applying the Hamiltonian on this superposition, one can obtain the BdG equations for the coefficients. For a system with cross section $M \times N$, the BdG equations can be rewritten as relations between coefficients of adjacent sections in the form of the transfer matrix

$$\begin{pmatrix} \vec{a}_{j+1} \\ \vec{b}_{j+1} \\ \vec{a}_j \\ \vec{b}_j \end{pmatrix} = \hat{T}_j \begin{pmatrix} \vec{a}_j \\ \vec{b}_j \\ \vec{a}_{j-1} \\ \vec{b}_{j-1} \end{pmatrix}, \quad (5)$$

where vector $\vec{a}_j$ ($\vec{b}_j$) has MN components a_{ijk} (b_{ijk}) with $i = 1, 2, \ldots, M$ and $k = 1, 2, \ldots, N$, and $\hat{T}_j$ is a $4MN \times 4MN$ transfer matrix. From BdG equations $\hat{T}_j$ can be written as

$$\hat{T}_j = \begin{pmatrix} \hat{u}_1 & \hat{v} & -\hat{1} & \hat{0} \\ \hat{v}^{\dagger} & \hat{u}_2 & \hat{0} & -\hat{1} \\ \hat{0} & \hat{0} & \hat{1} & \hat{0} \\ \hat{0} & \hat{0} & \hat{0} & \hat{1} \end{pmatrix}, \quad (6)$$

where the symbols with hat are $M \times M$ matrices and their elements are

$$\{\hat{u}_1\}_{ii';kk'} = \delta_{i,i'} \delta_{k,k'} \frac{\varepsilon - \epsilon_{ijk}}{t_0} - \delta_{i,i'-1} - \delta_{i,i'+1} - \delta_{k,k'-1} - \delta_{k,k'+1}, \quad (7)$$

$$\{\hat{u}_2\}_{ii';kk'} = -\delta_{i,i'} \delta_{k,k'} \frac{\varepsilon + \epsilon_{ijk}}{t_0} - \delta_{i,i'-1} - \delta_{i,i'+1} - \delta_{k,k'-1} - \delta_{k,k'+1}, \quad (8)$$

$$\{\hat{v}\}_{ii';kk'} = -\delta_{i,i'} \delta_{k,k'} \frac{\lambda^*_{ijk}}{t_0}. \quad (9)$$

Here, ε is energy of the quasiparticle.

For a strip with length L, the coefficients at one end are related to the coefficients at the other end with the transfer matrices

$$\begin{pmatrix} \vec{a}_L \\ \vec{b}_L \\ \vec{a}_{L-1} \\ \vec{b}_{L-1} \end{pmatrix} = \left(\prod_{j=1}^{L-1} \hat{T}_{L-j} \right) \begin{pmatrix} \vec{a}_1 \\ \vec{b}_1 \\ \vec{a}_0 \\ \vec{b}_0 \end{pmatrix}. \quad (10)$$

The Lyapunov exponents of quasiparticle states can be calculated by using the transfer-matrix method, in which the orthonormalization procedure is adopted [14]. The Lyapunov exponents are the logarithms of eigenvalues of the transfer matrix. In the present case there are $4MN$ eigenvalues for the transfer matrix, corresponding to MN spatial transverse channels, two particle-hole channels, and two propagating directions (forward and backward). The logarithms of eigenvalues for the forward and backward waves have opposite signs, and we only keep the $2MN$ positive ones, whose inverses, $\xi_l(\varepsilon, M)$ with $l = 1, 2, \ldots, 2MN$, are the localization lengths of the corresponding channels. According to reference [15], the rescaled localization length is defined as

$$\Lambda_l(\varepsilon, M) = \xi_l(\varepsilon, M)/M. \tag{11}$$

The properties of the system, such as the superconductivity and the conductance in the normal state, are related to the localization behavior of quasiparticles. We consider a quasi-2D square system of size $MN \times MN$. From reference [16], the off-diagonal long-range order (ODLRO) is defined as the probability of finding a Cooper pair at the right edge after it being injected from the left edge. If the Cooper pair is injected into the lth channel of the left edge, the probability of finding it at the right edge is related to the rescaled localization length as

$$P_l(\varepsilon, M) = \sum_{i=1}^{M}\sum_{k=1}^{N} |a_{l;i0k} b_{l;i0k}|^2 \exp[-2/\Lambda_l(\varepsilon, M)], \tag{12}$$

where $a_{l;i0k}$ and $b_{l;i0k}$ are the components of the lth eigenvector of the transfer matrix. It can be seen that besides the prefactor $\sum_{i=1}^{M}\sum_{k=1}^{N} |a_{l;i0k} b_{l;i0k}|^2$, that represents the strength of pairing in this channel, the ODLRO has the same scaling behavior as the rescaled localization length. Thus, from the M dependence of the largest $\Lambda_l(\varepsilon, M)$, we can determine whether the ODLRO in one channel vanishes or not in the thermodynamical limit. In some cases the properties are determined by the total contribution from all the channels, so it is also interesting to investigate the M dependence of the following dimensionless quantity

$$g(\varepsilon, M) = \sum_{l=1}^{2MN} \frac{1}{\pi}\left[\frac{\tau_l(\varepsilon, M)}{1-\tau_l(\varepsilon, M)}\right], \tag{13}$$

where $\tau_l(\varepsilon, M)$ is the transmission coefficient of the lth channel

$$\tau_l(\varepsilon, M) = \exp[-2/\Lambda_l(\varepsilon, M)].$$

$g(\varepsilon, M)$ can be regarded as the probability that a quasiparticle can travel through the system from the left to the right, no matter what channel is taken.

3 Numerical results

The transfer-matrix calculations and the scaling analysis on a quasi-2D system with N atomic planes are performed on a very long strip of length $L = 5 \times 10^4$ in the y direction and with a varying width M in the x direction, for which the periodic boundary conditions are applied. For a given energy ε, the $4MN \times 4MN$ transfer matrix maps the amplitudes of a quasiparticle wave function at the left end of the strip to those at the right end. The propagation of quasiparticles along the strip is determined by the Lyapunov exponents and the rescaled localization lengths of the transfer matrix obtained from the orthonormalization procedure. In this procedure, the self averaging over the randomness is achieved by the large length of the strip.

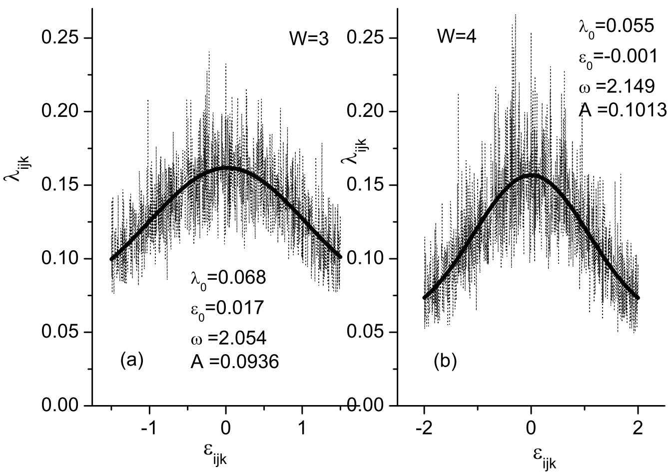

Fig. 1. Dependence of the self-consistent pairing potential λ_{ijk} on the on-site energy ϵ_{ijk} for one realization of random ϵ_{ijk} with given distribution width W. Dashed curves are the results from the solutions of the BdG equations in a $20 \times 20 \times 3$ quasi-2D square lattice, and the solid curves are the fitting ones. The attractive interaction $V = 1.8t_0$. Energy unites are set to be the hopping integral t_0.

Since the attractive interaction V in the Hamiltonian is a constant and the spatial fluctuations of pairing potential λ_{ijk} are caused by the randomness of site energies ϵ_{ijk}, we should first determine the dependence of $\{\lambda_{ijk}\}$ on $\{\epsilon_{ijk}\}$ with self-consistent calculations on an $MN \times MN$ square system. The result is shown in Figure 1. It can be seen that the local order parameter averagely has a dependence on the local site energy. The fluctuations around the average curve correspond to the long-range dependence which will be neglected in the transfer-matrix calculation because the long-strip geometry with varying width will distort the long-range correlation and produce unexpected errors. This approximation can reflect the main features of the dependence of the local order parameter on the randomness of the site energies, and allow the transfer-matrix calculation to be carried out. The average curves are of the Gaussian type, i.e., $\bar{\lambda}_{ijk} = \lambda_0 + A \exp\left[-2\left(\frac{(\epsilon_{ijk}-\epsilon_0)}{\omega}\right)^2\right]$, and the corresponding parameters are given in the figure. This dependence provides a way for determining the values of λ_{ijk} in the transfer-matrix calculations of the long strip.

Figure 2 shows the largest rescaled localization length $\Lambda(M)/M$ as a function of width M for various values of disorder strength W in the case of $\varepsilon = -0.5t_0$ and $N = 3$. Despite the statistical fluctuations seen in the figure, there exists a $W_c \sim 4$, and the size dependence of the rescaled localization length is different between $W < W_c$ and $W > W_c$. For $W > W_c$, the rescaled localization length is decreased with increasing width M, implying the localization behavior of the quasiparticles. For $W < W_c$, the rescaled localization length is slightly increased with increasing W. This difference in scaling behavior suggests a transition from localized to extended quasiparticle states in such a quasi-2D system. This is different from the

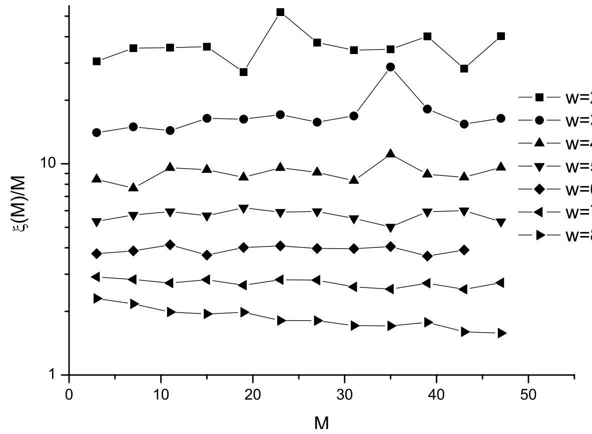

Fig. 2. Largest rescaled localization length as a function of width M. The energy $\varepsilon = -0.5t_0$ and the average pairing potential $\bar{\lambda} = 0.2t_0$. The thickness of the quasi-2D system is $N = 3$.

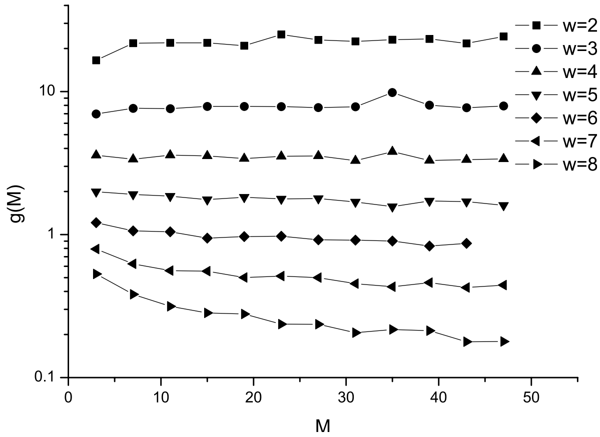

Fig. 3. Dimensionless quantity g as a function of width M for different values of M. Other parameters are the same as those in Figure 2.

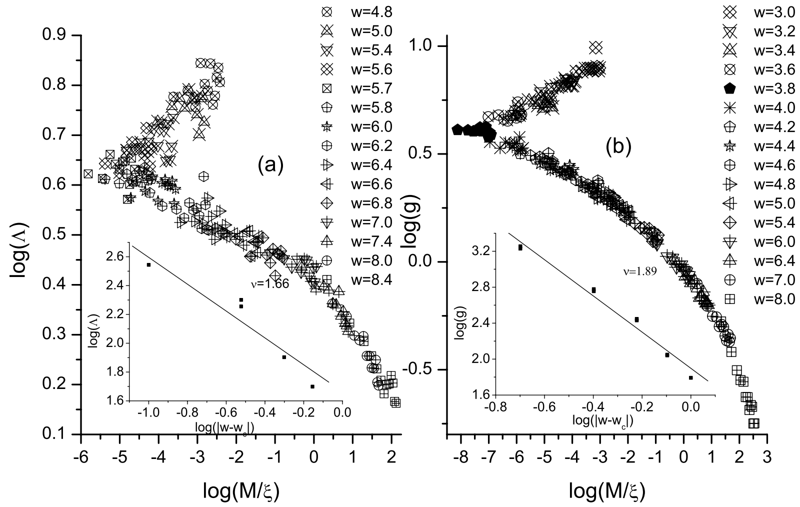

Fig. 4. Scaling function of (a) the rescaled localization length (b) the dimensionless quantity g for quasi-2D system. Insets: the log-log plot of (a) the rescaled localization length (b) the dimensionless quantity g as a function of $\mid W - W_c \mid$, where the symbols represent values from the data and the straight line is the fitting function $\zeta \propto |W - W_c|^{-\nu}$ with the shown value of ν. Other parameters are the same as those in Figure 3.

situation of pure-2D system with the s-wave pairing where all the quasiparticle states exhibit the behavior of localization [10,17]. The same transfer-matrix calculation has been done for a pure-2D system with the s-wave pairing and the curves shown in Figure 2b of reference [10] indicate the decrease of the rescaled localization length with increasing the width for all investigated parameters. In the present case the increase of $\xi(M)/M$ with M in the range $W < W_c$ is very weak, implying that the trend of transition to extended states is still limited by the dimensionality.

The rescaled localization length shown in Figure 2 reflect the localization behavior of quasiparticle in every channel. This corresponds to the properties which rely on the transport in one or a few channels. If the contributions from all possible channels are considered, we can calculate the dimensionless quantity g in equation (13). Figure 3 shows the M dependence of g for different values of disorder strength W. It shows a scaling behavior similar to that of Figure 2, except for less statistical fluctuations due to the summation of all channels. The transition point is $W_c \sim 4$, the same as determined from Figure 2. This means that in the present case the scaling behavior is the same for the largest rescaled localization length and the summation of contributions from all channels.

The rescaled localization length and the dimensionless quantity g for a finite $MN \times MN$ square system near the critical point can be expressed with a scaling function by using the finite-size scaling ansatz [14,15]. We make a further assumption that this scaling function varies as $|W - W_c|^{-\nu}$ in the vicinity of the critical point. In Figure 4, we display the scaling function for the rescaled localization length and the dimensionless quantity g. We also determine the corresponding values of ν from the fitting procedure. $\nu = 1.66$ and $\nu = 1.89$ as determined from the rescaled localization length and from g, respectively.

4 Conclusion and discussion

We have investigated the diffusion behavior of quasiparticles in quasi-2D superconductors with on-site energy disorder and s-wave pairing symmetry. By applying the transfer-matrix method and the finite size-scaling analysis, it is found that the quasiparticle states undergo a transition from localized to extended states by varying the W. This is originated from the combined effects of the disorder, the pairing potential, and the quasi-two-dimensionality. This conclusion is different from the situation of the 2D one-plane systems with s-wave pairing where all the quasiparticle states will be localized by small amount of disorder. As the realistic systems are always quasi-2D ones, they can be superconducting if the disorder is not strong. The critical conductance g_c, below which the superconductivity vanishes, can be estimated from Figure 3 as $g_c \sim 3.5$ in units of $e^2/\hbar$, in consistence with that obtained with the Feigemanl'man's formula [11,12]. The results are also consistent with related experiments [13].

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