Quasiparticle delocalization induced by novel quantum interference in disordered \textit{d}-wave superconductors

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(accepted in final form 25 April 2003)

PACS. 74.25.Fy – Transport properties (electric and thermal conductivity, thermoelectric effects, etc.).
PACS. 73.20.Fz – Weak or Anderson localization.
PACS. 74.20.-z – Theories and models of superconducting state.

Abstract. – The diagrammatic approach is applied to study quasiparticle transport properties in two-dimensional \textit{d}-wave superconductors with dilute, substitutional nonmagnetic impurities both in Born and in unitary limits. It is found that a novel quantum interference process gives rise to a weak-antilocalization correction to the spin conductivity, indicating the existence of extended low-energy quasiparticle states. When coming close to unitarity and nesting, this correction is suppressed and eventually vanishes due to the global particle-hole symmetry.

In recent years, there has been increasing interest in the understanding of low-energy quasiparticle (QP) states in disordered two-dimensional (2D) \textit{d}-wave superconductors [1]. The \textit{d}_{x^2-y^2}-wave pairing state is characterized by an anisotropic energy gap, which vanishes along four nodal directions. There exist Dirac-type QP excitations near the gap nodes. In contrast to the \textit{s}-wave superconductors, even nonmagnetic impurities can drastically change the behavior of the low-energy QP states in \textit{d}-wave superconductors. A central issue, not only experimentally relevant but also theoretically intricate, is whether these QP states are localized and how disorder affects the QP transport properties. Over the last decade, a variety of conceptually and methodologically different approaches to the problem have been developed, many of their predictions contradicting each other. Based on the self-consistent treatments [2], a nonlinear-sigma model [3], or numerical studies [4,5], some groups suggested that all the QP states are localized. On the other hand, Balatsky and Salkola have shown that the long-range overlaps between the impurity states yield an extended QP band [6]. The singularity in the density of states (DOS) at zero energy obtained recently by the nonperturbative \textit{T}-matrix method signals the QP delocalization as well [7]. The possible appearances of critical states [8] and localization-delocalization transitions [9] in random Dirac fermions have also been discussed. As a result, the problem of QP localization in disordered \textit{d}-wave superconductors still remains controversial and deserves further scrutiny.
Since the QP spin is conserved in the singlet superconductors, to study the spin conductivity is an important approach to the issue of QP localization [3, 4]. It is well known that the quantum interference (QI) effects, resulting from the cooperon and diffuson in the diagrammatic language, play an important role in the QP transport in disordered $d$-wave superconductors [3,10,11]. Unlike in a normal metal, every cooperon or diffuson mode in the retarded-advanced (RA) channel entails a corresponding mode in the retarded-retarded (RR) or advanced-advanced (AA) channel due to the local particle-hole symmetry (LPHS) in the superconducting state [12]. In the unitary limit and nesting case, each of these 0-mode (RR) or advanced-advanced (AA) channel due to the local particle-hole symmetry (LPHS) in the retarded-advanced (RA) channel entails a corresponding mode in the retarded-retarded superconductors [3,10,11]. Unlike in a normal metal, every cooperon or diffuson mode in 2D $d$-wave superconductors with dilute, substitutional nonmagnetic impurities both in Born and in unitary limits. The disorder model considered here is a binary alloy, which is different from the random-site-energy model studied in ref. [3]. At the one-loop level, we find a new impurity-scattering polarization diagram related to the LPHS, which has never been considered previously. This novel QI process is found to have a profound effect on the spin conductivity. It is shown that, in general, the spin conductivity is subject to a weak-antilocalization correction, while the electrical conductivity has a weak-localization one. Such a weak-antilocalization effect indicates the existence of extended low-energy QP states. When coming close to unitarity and nesting, the corrections of both spin and electrical conductivities are suppressed, and eventually vanish due to the GPHS. A semiclassical picture involving interfering trajectories of the novel QI process is also present.

Let us start from a most extensively studied model for a 2D $d_{x^2-y^2}$-wave superconductor, in which the normal-state dispersion and energy gap are given, respectively, by $\xi_k = -t(\cos k_x a + \cos k_y a) - \mu$ and $\Delta_k = \Delta_0(\cos k_x a - \cos k_y a)$, with $t$ the nearest-neighbor hopping integral, $a$ the lattice constant, and $\mu$ the chemical potential. In the vicinity of the four gap nodes $k_n = (\pm k_F, \pm k_F)/\sqrt{2}$, the QP spectrum $\epsilon_k = (\xi^2_k + \Delta^2_0)/2$ can be linearized as $\epsilon_k \approx [(v_f \tilde{k})^2 + (v_g \tilde{k})^2]^{1/2}$, where $v_f = (\partial \xi_k/\partial k)_{k_n}$, $v_g = (\partial \Delta_k/\partial k)_{k_n}$, and $\tilde{k}$ is the momentum measured from the node $k_n$. Consider pointlike nonmagnetic impurities to be randomly substituted for the host atoms, then the time-reversal and spin-rotational invariances are preserved (symmetry class CI in the classification of ref. [12]). The impurities are assumed to have a low concentration $n_i$ and an identical potential strength $V$. The Hamiltonian for the impurity scattering is given by $H_{\text{imp}} = V \sum_{j=1}^{N_i} \sum_{\sigma} C^\dagger_{j\sigma} C_{j\sigma} = V \sum_{j=1}^{N_i} \sum_{kk'\sigma} C^\dagger_{j\sigma} C_{k\sigma} e^{i(k-k') \cdot R_j}$, where $N_i$ is the total number of impurities, $R_j$ is the position of the impurity on site $j$, $C_{j\sigma}$ and $C_{k\sigma}$ denote, respectively, the annihilation operators of electrons in lattice and momentum representations. After averaging over impurity positions, the Green’s functions are characterized by the momentum conservation. In the self-consistent $T$-matrix approximation, the QP self-energy can be expressed in the Nambu spinor representation as [13] $\Sigma^{(R)}(\epsilon) = n_i T^{(R)}(\epsilon) = (\lambda e + i\gamma)\tau_0 + \eta \gamma \tau_3$ for $|\epsilon| \ll \gamma$. Here $\lambda$ is the mass renormalization factor, $\gamma$ is the impurity-induced relaxation rate, $\eta$ is a dimensionless parameter, $\tau_0$ and $\tau_i$ ($i = 1, 2, 3$) stand for the $2 \times 2$ unity and Pauli matrices, respectively. A use of Dyson’s equation yields the impurity-averaged one-particle Green’s functions as

$$G_k^{(R)}(\epsilon) = \frac{[(1 - \lambda)\epsilon \pm i\gamma]\tau_0 + \Delta k \tau_1 + \xi k \tau_3}{[(1 - \lambda)\epsilon \pm i\gamma]^2 - \xi^2_k}. \quad (1)$$
The impurity-induced DOS at zero energy is calculated as \( \rho_0 = -(1/\pi) \text{Im} \sum_k \text{Tr} G_k^R(0) = 4l\gamma/\pi^2 v_f v_g \), where \( l = \ln(\Gamma/\gamma) > 1 \) with \( \Gamma \sim \sqrt{v_f v_g}/a \). The parameters \( \gamma \), \( \lambda \), and \( \eta \) can be evaluated consistently via the self-consistent \( T \)-matrix equation [13], yielding

\[
\gamma = 2n_i/\pi \rho_0 (1 + \eta^2), \quad \lambda = (1 - \eta^2)(l - 1)/(\eta^2 + 2l - 1), \quad \text{and} \quad \eta = 2/\pi \rho_0 U with U^{-1} = V^{-1} + \sum_k \xi_k (\epsilon_k^2 + \gamma^2)^{-1}. 
\]

The Born and unitary limits correspond to \( \eta^2 \gg 2l \) and \( \eta \to 0 \), respectively.

As in the study of disordered interacting electron systems [14], all the leading polarization diagrams responsible for the QI effects (fig. 1) can be generated from the lowest-order self-energy corrections (figs. 1(c) and (d) in ref. [13]). Figure 1(b) denotes a sum of the well-known maximally-crossed diagrams. Figure 1(a) was first proposed by Altland and Zirnbauer in the random-matrix theory of mesoscopic normal/superconducting systems [12], its physical effects have also been studied in ref. [3], as well as in the mixed superconducting state [10]. Figure 1(c) is a new polarization diagram, which has not been considered previously. Although diagram 1(c) contains two cooperons, it is a one-loop diagram as the two cooperons have the same total momentum \( q \). Therefore, the contribution of fig. 1(c) is of the same order as those of figs. 1(a) and (b). A similar situation occurs in the lowest-order interaction correction to the conductivity in disordered electron systems [14]. In addition, it can be shown that fig. 1(d), as well as all the one-loop diagrams with 0-mode diffuson, has a vanishing contribution. The nonvanishing contributions of both diagrams 1(a) and (c) stem from the existence of the cooperon in RR channel. We wish to emphasize here that diagram 1(c) describes a novel QI effects.
process in $d$-wave superconductors. As will be shown below, it is the existence of diagram 1(c) that leads to a weak-antilocalization correction to the spin conductivity.

The Kubo formula is used to calculate the QP transport coefficients. For the spin conductivity, each vertex of the diagrams in fig. 1 contains a vector $[15] \Lambda_\mathbf{k} = \frac{1}{2} [\mathbf{v}_g(\mathbf{k}) \tau_1 + \mathbf{v}_f(\mathbf{k}) \tau_3]$. The contributions of these diagrams to the spin conductivity can be expressed by $\sigma^s = (1/2\pi) \text{Re} (\Pi^\text{RA} - \Pi^\text{RR})$ ($\chi = a, b, c$), where $\Pi^\text{RA}$ and $\Pi^\text{RR}$ stand for the corresponding zero-frequency spin current-current correlation functions in RA and RR channels, respectively. According to Feynman’s rule, we have

$$\Pi^\text{RA} = \frac{1}{2} \sum_{qk} \sum_i C(q)_{ii}^\text{RR} \text{Tr} (\Lambda_\mathbf{k} G^\text{R}_\mathbf{k} \tau_i G^\text{R}_{-\mathbf{k}} \tau_i G^\text{R}_{-\mathbf{k}} \Lambda_\mathbf{k} G^\text{A}_\mathbf{k}),$$

$$\Pi^\text{RA} = \frac{1}{2} \sum_{qk} \sum_i C(q)_{ii}^\text{RA} \text{Tr} (\Lambda_\mathbf{k} G^\text{R}_\mathbf{k} \tau_i G^\text{R}_{-\mathbf{k}} \Lambda_\mathbf{k} G^\text{A}_\mathbf{k} G^\text{A}_\mathbf{k}),$$

$$\Pi^\text{RA} = \frac{1}{2} \sum_{qk} \sum_i C(q)_{ii}^\text{RR} C(q)_{jj}^\text{RA} \text{Tr} \left( \Lambda_\mathbf{k} G^\text{R}_\mathbf{k} \tau_i G^\text{R}_{-\mathbf{k}} \tau_j G^\text{R}_{-\mathbf{k}} \tau_j G^\text{R}_{-\mathbf{k}} \Lambda_\mathbf{k} G^\text{A}_\mathbf{k} G^\text{A}_\mathbf{k} \right),$$

with $G^\text{R}(\mathbf{k}) = G^\text{R}(\mathbf{k}) (0)$ and $C(q)^\text{RR}(\mathbf{k}) = C(q; 0; 0)^\text{RR}(\mathbf{k})$. The expressions of $\Pi^\text{RR}$ are easily obtained by replacing all “A” by “R” in those of $\Pi^\text{RA}$. As an example, we shall calculate $\Pi^\text{RR}$. Assuming that $A, A', B,$ and $B'$ are arbitrary linear superimpositions of $\tau_1$ ($i = 0, 1, 2, 3$), one can easily show that $\frac{1}{2} \sum_{ij} C_{ii} C_{jj} \text{Tr} (\tau_i A \tau_j A' \tau_j B B') = \sum_i (\mathbf{C} M^\prime)_{ii}$, where $\mathbf{C} = \sum_i C_{ii} \tau_i \otimes \tau_i, \mathbf{C}' = \sum_j C_{jj} \tau_j \otimes \tau_j, M = A \otimes B,$ and $M' = A' \otimes B'$. Using this formula, we can re-express $\Pi^\text{RR}$ as

$$\Pi^\text{RR} = \sum_q \sum_i [C(q)^\text{RR} \mathbf{M}_q \cdot C(q)^\text{RR} \mathbf{M}_q]_{ii},$$

with $\mathbf{M}_q = \sum_k G^\text{R}(q-k) \otimes (G^\text{R}(\Lambda \mathbf{k}) G^\text{R}(\mathbf{k}))$, where the summation over $\mathbf{k}$ is restricted near the four gap nodes. Since $C(q)^\text{RR}$ contains the diffusion pole, we need only the expression of $\mathbf{M}_q$ for small $q$. Noting that $\mathbf{M}_{q=0} = 0$ due to $\Lambda(q) = -\Lambda(q)$, we get $\mathbf{M}_q \approx -\sum_k (q \cdot \nabla G^\text{R}(\mathbf{k})) \otimes (G^\text{R}(\Lambda \mathbf{k}) G^\text{R}(\mathbf{k}))$. Substituting eq. (1) into this expression, we show that

$$\mathbf{M}_q = \frac{1}{12\pi^2 \gamma^2} \left\{ q \left[ 2 \alpha \tau_0 \otimes \tau_0 - (2 \alpha - \beta) \tau_1 \otimes \tau_1 - (2 \alpha + \beta) \tau_3 \otimes \tau_3 \right] - \hat{q} (\tau_1 \otimes \tau_3 + \tau_3 \otimes \tau_1) \right\},$$

where $\alpha = (v_f^2 + v_g^2)/2 v_f v_g, \beta = (v_f^2 - v_g^2)/2 v_f v_g$, and $\hat{q} = (q \cdot f) g + (q \cdot g) f$ with $f$ and $g$ the unity vectors parallel, respectively, to $\mathbf{v}_f$ and $\mathbf{v}_g$ at one of the four nodes. The upper and lower cutoffs of $|q|$ are set to be $1/l_e$ and $1/L$, respectively, with $l_e = \sqrt{D/2\gamma}$ the elastic mean free path, and $L$ the sample size. Substituting eqs. (2) and (4) into eq. (3), we obtain $\Pi^\text{RR} = -(-4/\pi) \ln (L/l_e)$. Similarly, one can show that $\Pi^\text{RA} = 0$. As a result, we get the contribution of diagram 1(c) as $\sigma^s = (2/\pi^2) \ln (L/l_e)$. Using the formula $\frac{1}{2} \sum_i C_{ii} \text{Tr} (\tau_i A \tau_i B) = \sum_i (\mathbf{C} M)_{ii}$, one can similarly show that $\sigma^s = \sigma^s / 2 = -(-1/2\pi^2) \ln (L/l_e)$. The total correction to the spin conductivity is given by $\delta \sigma^s = 2 \sigma^s + \sigma^s + 2 \sigma^s_e$, yielding a weak-antilocalization correction as

$$\delta \sigma^s / \sigma^s = (4/\alpha) \ln (L/l_e),$$

where $\sigma^s_0 = (v_f^2 + v_g^2)/4\pi^2 v_f v_g$ is the universal spin conductivity [15], which satisfies the Einstein relation $\sigma^s_0 = \rho_0 D/4$. For the electrical conductivity, each vertex vector in the diagrams
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Fig. 2 – Semiclassical scattering paths of QPs corresponding to figs. 1(a)-(c).

equals \[ -e v_f(k) \tau_0 \], from which we can show that \( \sigma_b = \sigma_c = 0 \). Then the total correction to the electrical conductivity is given by \( \delta \sigma = 2 \sigma_a \), yielding a weak-localization correction as 

\[ \delta \sigma / \sigma_0 = -2(2/\alpha) \ln(L/l_e), \]

with \( \sigma_0 = e^2 v_f / \pi^2 v_g \) the universal electrical conductivity [2,15].

In the unitary limit (\( \eta \to 0 \)) and at perfect nesting (\( \mu \to 0 \)), there exist the \( \pi \)-mode cooperon and diffuson [13,15]. Owing to the GPHS we have 

\[ \tau^2_G R(A) k(\epsilon) = \tau^2 G R(A) Q + k(\epsilon) \]

with \( Q = (\pm \pi/a, \pm \pi/a) \) the nesting vector. Any small deviation either from the unitary limit or from the perfect nesting makes the \( \pi \)-mode cooperon and diffuson gapped. They are given by 

\[ D_{\pi}(q; \epsilon, \epsilon') = C_{\pi}(q; \epsilon, \epsilon')_{RR(A)} = \sum_i C_{\pi}(q; \epsilon, \epsilon')_{ii} \tau_i \otimes \tau_i, \]

where 

\[ C_{\pi}(q; \epsilon, \epsilon')_{ii} = d_{RR}^{\pi}/[Dq^2 - i(\epsilon \pm \epsilon') + 2\delta], \]

with \( \delta = 2\eta^2 \gamma + \mu^2/\ell \gamma \ll \gamma \) and 

\[ -d_{0}^{\pi} = d_{1}^{\pi} = d_{2}^{\pi} = d_{3}^{\pi} = -4\gamma^2/\pi \rho_0. \]

To the lowest order, besides the 0-mode cooperon, the \( \pi \)-mode cooperon also contributes to the QI effects; the corresponding diagrams can be obtained by replacing \( q \) by \( Q + q \) in all the diagrams in fig. 1. By summing up all the contributions of the 0-mode and \( \pi \)-mode cooperons, we obtain 

\[ \delta \sigma^s / \sigma_0^s = -2 \delta \sigma / \sigma = 2 \alpha \ln \left( 1 + \frac{\delta L^2}{\gamma l_e^2} \right). \]

At finite \( L \), both corrections given by eq. (6) are suppressed by decreasing \( \delta / \gamma \) and vanish at \( \delta = 0 \), indicating that \( \sigma^s \to \sigma_0^s \) and \( \sigma \to \sigma_0 \). This result agrees with the numerical studies for \( \sigma^s \) in the weak-disorder limit [4]. Here we show that the physical origin is the existence of \( \pi \)-mode cooperon. The contributions of 0-mode and \( \pi \)-mode cooperons have the same magnitude but opposite signs due to the GPHS. As a result, the corrections to the spin (electrical) conductivity coming from the 0-mode and \( \pi \)-mode cooperons just cancel out.

It is instructive to analyze the scattering processes described by the diagrams in fig. 1. While fig. 1(a) yields a suppression of forward scattering of QPs, fig. 1(b) corresponds to an enhancement of back-scattering. Therefore, both figs. 1(a) and (b) give rise to the weak-localization effect on the QP states. Figure 1(c) represents a more complicated scattering process, including an enhancement of forward scattering (\( k \) and \( k' \) located near the same node) and a suppression of back-scattering (\( k \) and \( k' \) located near the antipodal nodes). The total contribution of diagram 1(c) leads to a weak-antilocalization effect on the QP states. As has been seen above, the QP delocalization stems from the fact that the weak-antilocalization effect prevails over the weak-localization one. In order to understand the novel QI process, we depict in fig. 2 the semiclassical paths corresponding to diagrams 1(a)-(c). Figure 2(a) describes a pair of QP scattering paths, in which the closed loop circled twice involves only one of the two paths. Figure 2(b) represents a pair of paths that differ by a sequence of scattering events traversed in opposite directions. The scattering paths in fig. 2(c) look like a composite of figs. 2(a) and (b). All the interference effects in fig. 2 arise from a combination of impurity- and Andreev-scattering processes. In the unitary limit and at perfect nesting, the
contributions of 0-mode and π-mode cooperons cancel each other. This is because the phase differences of coherent paths in fig. 2 for the π-mode cooperon differ by π from those of the 0-mode cooperon, due to the additional GPHS.

The scaling function is defined by \( \beta(g^s) = d \ln g^s / d \ln L \) with \( g^s = \sigma^s / (1/2)^2 \). It is easy to show that both eqs. (5) and (6) can be collapsed into a single universal scaling function as \( \beta(g^s) = 8/\pi^2 g^s \) for \( g^s \rightarrow \infty \). The positive \( \beta(g^s) \) strongly indicates the existence of extended low-energy QP states. This spin metal state is characterized by the absence of charge diffusion. The observation that \( \beta(g^s) \) decreases with \( g^s \) implies that these extended low-energy QP states are different in character with the usual extended bands. We argue that this novel phenomenon is related to the strong anisotropy of energy gap in \( d \)-wave superconductors, as the wave vectors of all extended low-energy QP states are nearly along the four nodal directions. It is worthy to mention that the extended QP states have been predicted by Balatsky et al. [6] from the novel network of delocalized impurity states in the unitary limit. However, the physical mechanisms for the formation of extended states are different from each other in ref. [6] and in the present theory. On the other hand, the nonlinear-sigma-model calculations in ref. [3] predicted a QP localization effect for the random-site-energy model of \( d \)-wave superconductors. We note that the weak-localization calculations in ref. [3] do not include the contribution of fig. 1(c). Therefore, there are two possibilities accounting for the disagreement between the predictions in the present work and in ref. [3]. The first one is that fig. 1(c) has a vanishing contribution in the random-site-energy model, implying that different disorder models may lead to various theoretical predictions for the QP transport coefficients. A similar situation occurs in the QP DOS [1]. The numerical studies [16] have shown that the binary-alloy and random-site-energy models yield qualitatively different predictions for the low-energy DOS in the \( d \)-wave superconductor. The other possibility is that fig. 1(c) does contribute to the QI effect in the random-site-energy model, and thus the theory of ref. [3] is to be further developed to include the contribution of fig. 1(c). The novel QI process is expected to exist in superconductors that belong to symmetry classes C and D. We note that RR-cooperons are not influenced by the time-reversal breaking [1,3,10]. How a magnetic field (or dilute magnetic impurities) affects the QP delocalization effect is another interesting and open problem.

Since the QP energy is also conserved, the electronic thermal conductivity \( K \) should obey the Wiedemann-Franz law \( K / T \sigma^s = 4\pi^2 k_B^2 / 3 \). Here the temperature dependence of the QI correction \( \delta \sigma^s(T) \) results from the dephasing time \( \tau_\phi(T) \), the latter may be obtained by considering the interactions between QPs [11]. Since the self-consistent \( T \)-matrix approximation is valid only for the case of dilute impurities [13], we do not rule out the possibility of localized QP states at higher impurity concentrations. Should it appear, there might exist a quantum transition from spin metal to spin insulator in 2D disordered \( d \)-wave superconductors, which is expected to be observed in a low-temperature thermal transport experiment. By increasing the impurity concentration, the temperature dependence of \( K \) would change from metallic to insulating behavior.

In conclusion, we find a new, one-loop diagram in the binary-alloy model for disordered 2D \( d \)-wave superconductors, which qualitatively modifies the usual weak-localization results. The QI process described by this diagram is shown to produce extended low-energy QP states in weak-disorder cases.

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We acknowledge the support of the National Natural Science Foundation of China under Grants No. 10274008 and No. 10174011. This work was also supported by Grants No. BK2002050, No. BK2001002, No. G19980614, and No. NSC 91-2816-M-029-0001-6.
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