Quasiparticle Transport and Localization in High-T_c Superconductors

T. Senthil, Matthew P. A. Fisher, Leon Balents,* and Chetan Nayak†

Institute for Theoretical Physics, University of California, Santa Barbara, California 93106-4030

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We present a theory of the effects of impurity scattering in $d_{x^2-y^2}$ superconductors and their quantum disordered counterparts, based on a nonlinear-sigma-model formulation. We show the existence, in a quasi-two-dimensional system, of a novel spin-metal phase with a nonzero spin diffusion constant at zero temperature. With decreasing interlayer coupling, the system undergoes a quantum phase transition (in a new universality class) to a localized spin insulator. Experimental implications for spin and thermal transport in the high-temperature superconductors are discussed. [S0031-9007(98)07710-2]

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Over the last few years, experiments [1] have convincingly established that the superconducting state of the hole-doped cuprate materials is characterized by spin singlet $d_{x^2-y^2}$ pairing. In such a superconductor, the gap vanishes at four points on the (two-dimensional) Fermi surface. The quasiparticle excitations at these "nodes" have a linear dispersion, and an associated density of states that vanishes linearly on approaching the Fermi surface. This leads to power law dependences of various physical quantities on temperature. Impurity scattering is expected to strongly modify these properties. Experimentally, the power law temperature dependences are rounded off, apparently approaching constant, temperature-independent behavior at the lowest temperatures. This fact is well reproduced by approximate, self-consistent treatments of impurity scattering which show that a constant finite density of states is generated at the Fermi energy for any arbitrarily weak impurity strength [2,3]. Quasiparticle transport properties have also been investigated [4,5] theoretically with such self-consistent approximations with some phenomenological success. Going further, Lee [2] has suggested, on the basis of calculations of the zero frequency microwave conductivity, that the quasiparticle eigenstates are strongly localized.

In this paper, we reconsider the effects of disorder on the low energy quasiparticles in the $d_{x^2-y^2}$ superconductor. We point out that the problem of quasiparticle transport and localization in a superconductor is conceptually very different from the more familiar situation of noninteracting electrons in a random potential. This is because, unlike in a normal metal, the charge of the quasiparticles in the superconductor is not a conserved quantity. This immediately implies that the quasiparticle charge in the superconductor cannot be transported through diffusion. Indeed, the quasiparticle charge density is *not* a hydrodynamic mode in the superconductor. However, in a singlet superconductor (and in particular in the high-T_c superconductors), the condensate does not carry any spin, and consequently the spin of the quasiparticles is a good quantum number and is conserved. The quasiparticle energy is also conserved. Thus, there is the possibility of having spin and energy diffusion without charge diffusion. These differences in symmetry lead to interesting differences between the localization properties of quasiparticles in the superconductor, and in the normal metal. Such differences have been pointed out before [6] in the context of the random matrix theory of mesoscopic normal/superconducting systems.

We address quasiparticle transport using a replica field theoretic formulation. As expected, the field theory is different from that describing Anderson localization in a normal metal. The properties of the theory are determined by a single coupling constant, which is the dimensionless *spin* conductance. This is the physically correct quantity whose behavior as a function of system size enables construction of a scaling theory of localization. By analyzing the properties of the field theory, we show the existence of a logarithmic "weak localization" correction in two dimensions suggesting localization at the largest length scales. This correction persists, in part, in the presence of an orbital magnetic field (unlike usual Anderson localization) or a Zeeman field, but is suppressed when both are present. In all cases, however, the quasiparticles are generically ultimately localized in two dimensions. Upon inclusion of interlayer coupling, there is the interesting possibility of a quantum phase transition between an extended *spin metal* and a localized *spin insulator*. The spin metal has diffusive spin correlations, a finite spin susceptibility, and an associated finite spin conductivity all *at zero temperature*. We are not aware of the existence of such a spin phase in any insulating Heisenberg spin model with or without randomness.

The spin insulator is expected to exhibit local moments and spin-glass or random-singlet behavior at very low temperatures. The transition between these two phases is described by the critical point of the replica field theory (neglecting quasiparticle interactions), and is a new universality class for localization.

Most of these results also go over unmodified to the quantum disordered version of the $d_{x^2-y^2}$ superconductor—the "nodal liquid" phase that has been analyzed recently [7] as a possible low-temperature theory of the pseudogap regime in the cuprate materials.

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We begin our analysis with the lattice quasiparticle Hamiltonian for a singlet superconductor,

$$\mathcal{H} = \sum_{i,j}\left[t_{ij}\sum_{\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} + \Delta_{ij}c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow} + \Delta^{*}_{ij}c_{j\downarrow}c_{i\uparrow}\right], \quad (1)$$

where i, j are site labels. Using Hermiticity combined with spin-rotational and time-reversal invariances, t and Δ may be taken to be real-symmetric matrices. Note that the total number of particles is not conserved by this Hamiltonian while their total spin is. In the presence of impurities, we define $t_{ij} = t^0_{ij} + t^1_{ij}$ and $\Delta_{ij} = \Delta^0_{ij} + \Delta^1_{ij}$, where t^0 and Δ^0 are the Fourier transforms of the kinetic energy ϵ_k (measured from the Fermi energy) and the gap function Δ_k, respectively. In the $d_{x^2-y^2}$ superconductor of primary interest, we may take $\Delta_k = \Delta_0(\cos k_x - \cos k_y)$. We mention in passing that for weak impurities, a continuum limit may be taken, focusing on wave vectors near the d wave nodes. The resulting "dirty Dirac" Hamiltonian is similar to various models in the literature [8], but differs from previously studied variants in that it contains several random *anomalous couplings*. The Hamiltonian above can be regarded as a lattice regularization of this continuum effective field theory for the $d_{x^2-y^2}$ superconductor, hence our results are quite general and not restricted to a BCS approximation.

The effect of weak randomness can be analyzed by perturbative renormalization group calculations [9] which show that the randomness is a (marginally) relevant perturbation. To make progress then, we employ a field-theoretic reformulation of the self-consistent treatment adopted in earlier works on dirty d-wave superconductivity [2]. This begins with the standard coherent-state functional integral formulation, in which the electron operators $c, c^{\dagger}$ are replaced by Grassman fields $c, \overline{c}$ averaged with respect to a statistical weight e^{-S}, where S is an action. As the randomness is independent of time and $\mathcal{H}$ is quadratic, different pairs of frequencies $(\omega, -\omega)$ decouple, and it is sufficient for our purposes to focus simply on $\omega = 0$.

Several notational conventions are convenient. We define four-component fields $\psi_{ia\alpha}$, with $\psi_{i1\alpha} \equiv c_{i\alpha}/\sqrt{2}$ and $\psi_{i2\alpha} \equiv i\sigma^{y}_{\alpha\beta}\overline{c}_{i\beta}/\sqrt{2}$. From this point on we adopt a notation in which $\vec{\tau}$ and $\vec{\sigma}$ matrices act in the particle/hole (a) and spin (α) spaces, respectively. A conjugate field is then defined by $\overline{\psi}_i = (C\psi_i)^T$, where $C = \sigma^y\tau^y$. The action in these variables appears nonanomalous,

$$S = \sum_{ij}\overline{\psi}_i(t_{ij}\tau^z + \Delta_{ij}\tau^x)\psi_j + i\eta\sum_i \overline{\psi}_i\sigma^z\psi_i\,. \quad (2)$$

At this stage we have also included an infinitesimal imaginary Zeeman field η, which acts to generate physical correlation functions.

To compute disorder-averaged quantities, we replicate the fields $\psi \to \psi^{\mu}$, with $\mu = 1 \ldots n$, so that for $n \to 0$ the statistical weight is normalized for each realization of the randomness. Physical quantities can now be simply expressed. In particular, the spin susceptibility is $\chi_0 = -(1/\pi)\,\mathrm{Im}\langle\overline{\psi}^{\mu}_i\sigma^z\psi^{\mu}_i\rangle$ (no sums). Angular brackets denote both field-theoretic (ψ) and disorder averages. The spin diffusion constant, D_s, can also be determined from the "diffusion propagator" P_{ij}, whose Fourier transform is $P(q) = \sum_j P_{ij}\exp[\vec{q}\cdot(\vec{x}_i - \vec{x}_j)] = 8\pi\chi_0/(D_s q^2)$. One has $P_{ij} = -\langle(\overline{\psi}^{\mu}_i\sigma + \psi^{\nu}_i)(\overline{\psi}^{\nu}_j\sigma - \psi^{\mu}_j)\rangle$, with $\sigma^{\pm} = (\sigma^x \pm i\sigma^y)/2$ and no replica sum should be taken.

The ensemble average over t^1, Δ^1 can now be immediately performed, generating a translationally invariant action with nontrivial quartic couplings between different replicas. A more general analysis [9] demonstrates that the essential features are captured by uncorrelated zero-mean local Gaussian fields $t^1_{ij} = t^1_i\delta_{ij}$ and $\Delta^1_{ij} = \Delta^1_i\delta_{ij}$ with covariances $[t^1_i t^1_j]_{\mathrm{ens}} = [\Delta^1_i\Delta^1_j]_{\mathrm{ens}} = u\delta_{ij}$. With this choice, the algebra is particularly simple, and the quartic interactions can in turn be decoupled via two $2n \times 2n$ Hermitian Hubbard-Stratonovich fields, Q and P, acting in the spin and replica spaces (diagonal in the particle/hole space). The effective action becomes

$$S = \sum_i \frac{1}{u}\mathrm{Tr}[[Q(i)]^2 + [P(i)]^2] + 2\sum_{ij}\overline{\psi}_i[[iQ(i) - P(i)\tau^y + i\eta\sigma^z]\delta_{ij} + t^0_{ij}\tau^z + \Delta^0_{ij}\tau^x]\psi_j\,, \quad (3)$$

where we have suppressed spin and replica indices.

A saddle-point (in Q and P) analysis of Eq. (3) recovers the conventional self-consistent approximation. In particular, one finds $Q = 2\pi\chi_0\sigma^z$ and $P = 0$. The constant χ_0 appears as an imaginary self-energy, is (the saddle-point approximation to) the physical spin-susceptibility, and represents a generation of a nonzero "quasiparticle density of states (DOS)" due to disorder. The conclusion that $\chi_0 \neq 0$ is amply supported by experiment, leading us to believe that this saddle-point is a physically correct starting point. The imaginary self-energy also has a complementary interpretation as a finite (inverse) elastic scattering time $1/\tau_e$. For times longer than τ_e, quasiparticles no longer move ballistically, and we expect diffusion *of the conserved energy and spin densities*.

Fluctuations around this saddle-point represent both diffusion and corrections to it. Near two spatial dimensions these fluctuations are captured by a nonlinear-sigma-model (NLσM) treatment. The crucial ingredients are the physical (nonstatistical) symmetry properties of the Hamiltonian, which determine symmetries of the replicated action, Eq. (3). For the SU(2) and time-reversal invariant form chosen, the crucial symmetry group is $\mathrm{Sp}(2n) \times \mathrm{Sp}(2n)$. In particular, consider the transformation $\psi_i \to U\psi_i$, with $U = \frac{1}{2}[U_A(1 + \tau^y) + U_B(1 - \tau^y)]$, with $U_{A,B}$ $2n \times 2n$ unitary matrices in the spin and replica spaces satisfying $U^T_{A,B}\sigma^y U_{A,B} = \sigma^y$. Under this transformation, the other fields rotate according to $Q + iP \to U^{\dagger}_A(Q + iP)U_B$. For $\eta = 0$, all such

rotations leave S invariant, while this is true for nonzero η only when $U_B = \sigma^z U_A \sigma^z$, hence η breaks the symmetry infinitesimally from $\mathrm{Sp}(2n) \times \mathrm{Sp}(2n)$ to $\mathrm{Sp}(2n)$. For a single replica, note that as $\mathrm{Sp}(2) \simeq \mathrm{SU}(2)$, one of these Sp(2) symmetries is just spin rotation invariance. The other Sp(2) symmetry is actually a consequence of time reversal invariance, and can be traced to the reality of the Hamiltonian H.

The NLσM is constructed by considering fluctuating $\mathrm{Sp}(2n) \times \mathrm{Sp}(2n)$ rotations of saddle-point solutions that are slowly varying in space. In general, these can be shown to take the form of an Sp(2n) matrix $\mathrm{U}(\vec{x})$, with $Q(x) + iP(x) = \frac{\pi}{2}\chi_0 \sigma^z \mathrm{U}(\vec{x})$. The form of the action for U is determined entirely on symmetry grounds, and is verified by a direct calculation [9] expanding Q and P and integrating out noncritical massive modes. We find

$$S_{\mathrm{NL}\sigma\mathrm{M}} = \int d^2x \, \frac{1}{2g} \mathrm{Tr}(\nabla U \cdot \nabla U^\dagger) - \eta \, \mathrm{Tr}(U + U^\dagger), \tag{4}$$

where $\mathrm{U}(x) \in \mathrm{Sp}(2n)$. This field theory is known as the "principal chiral Sp(2n) model" in the field theory literature. In contrast to the conventional sigma models used to describe the localization of noninteracting electrons, here the field variables live on a group manifold instead of a coset space. The $\mathrm{Sp}(2n) \times \mathrm{Sp}(2n)$ symmetry acts on U via global left and right multiplication with independent Sp(2n) matrices.

The replica-diagonal self-consistent approximation used in other work corresponds to keeping only the configuration $\mathrm{U}(x) = \mathbf{1}$ in the action. Small quadratic fluctuations around this solution correspond to diffusion, and a direct calculation of P_{ij} in this approximation [9] relates the coupling constant to the spin-conductance σ_s, to wit $\frac{1}{g} = \frac{\pi}{2}\sigma_s$. The derivation of the sigma model provides an estimate for the bare coupling constant: $\frac{1}{g_0} = \frac{1}{4\pi}\frac{v_F^2 + v_\Delta^2}{v_F v_\Delta}$ with v_F, the Fermi velocity, and v_Δ, the slope of the $d_{x^2-y^2}$ gap linearized near the nodes. Note that this is independent of the disorder strength. A similar result for the zero frequency microwave conductance was obtained earlier by Lee [2], in particular $\sigma(\omega = 0^+) = \frac{1}{\pi^2}(v_F/v_\Delta)e^2/h$. The difference in the velocity-dependence of the prefactors is conceptually significant: the spin-conductance obeys an Einstein relation while the microwave conductance cannot. This distinction arises because the quasiparticle charge is not a good quantum number.

Consider separately the orbital and Zeeman couplings to an applied magnetic field. The orbital field breaks time-reversal symmetry but not SU(2), and similar manipulations to those above lead ultimately to a $\mathrm{Sp}(2n)/\mathrm{U}(n)$ NLσM, also distinct from the three conventional universality classes of dirty metals. The Zeeman coupling, by contrast, breaks SU(2) invariance, leaving only a U(1) spin-rotation symmetry around the field axis (say $\hat{\mathbf{z}}$). Using the particle/hole transformation, $c_\downarrow \to c_\downarrow^\dagger$, this U(1) symmetry is easily shown to play the same role as does the charge-conservation U(1) in conventional localization. Consequently, the Zeeman field leads to the usual orthogonal sigma model, and Zeeman and orbital effects together drive the system to the unitary universality class.

All these field theories exhibit diffusion on length scales of order the elastic mean free path ℓ_e. Beyond this scale, quantum interference corrections can play an important role. They are determined by the renormalization group (RG) equation for g, which for the Sp(2n) and $\mathrm{Sp}(2n)/\mathrm{U}(n)$ sigma models can be found in Refs. [10]:

$$\frac{dg}{d\ln L} = -\epsilon g + \frac{\alpha g^2}{4\pi} + O(g^3), \tag{5}$$

where $\epsilon = d - 2$ and we have set $n = 0$. The number $\alpha = 1, \frac{1}{2}$ for the $\mathrm{Sp}(2n), \mathrm{Sp}(2n)/\mathrm{U}(n)$ models, respectively. Equation (5) describes the evolution of the physical coupling (and hence the spin conductance) with length scale L, which could be either the system size or an inelastic thermal cutoff length at finite temperature. Note that in two dimensions ($\epsilon = 0$), g grows logarithmically with L, giving an additive logarithmic reduction of the conductance and signaling a crossover to localized behavior at long distances. Notice that to this order ("one-loop") the leading logarithmic correction is not completely suppressed by an orbital field. This result is in sharp contrast to conventional weak localization, but is in agreement with similar observations made in the context of the random matrix theory of systems with these symmetries [6,11]. Complete suppression of the logarithmic correction occurs only with the introduction of Zeeman coupling and subsequent crossover to the unitary NLσM.

These perturbative results strongly suggest that in two spatial dimensions with weak magnetic fields, the quasiparticles are ultimately always localized. A crude estimate for the localization length may be obtained from the one loop perturbation theory to be $\xi \sim \ell_e e^{4\pi/g_0}$ where ℓ_e is the mean free path and g_0 the bare coupling constant. Using the estimate $\frac{v_F}{v_\Delta} \sim 7$ in high T_c, we get $\xi \approx 1000\ell_e$. We note in passing that since $\Pi_2(\frac{\mathrm{Sp}(2n)}{\mathrm{U}(n)}) = Z$, a nontrivial topological term is allowed for nonzero orbital coupling; this suggests the possibility of isolated extended quasiparticle states for strong magnetic fields [9].

Inclusion of coupling between two-dimensional layers (with spacing d) drives the system three dimensional, making possible an extended phase where the spins diffuse at the longest length scales. Based on the quasi-2d NLσM [9], the boundary between 3d spin-metal and spin-localized phases occurs when the bare z-axis spin conductivity $\sigma_s^{zz} \sim d\ell_e^{-2} e^{-8\pi/g}$ (see Fig. 1). Given this steep curvature of the phase boundary near the origin, even a modest interlayer coupling can drive the system into the spin metal phase. In zero field, or neglecting Zeeman coupling, the transition between the spin metal and the spin insulator is in a new universality class.

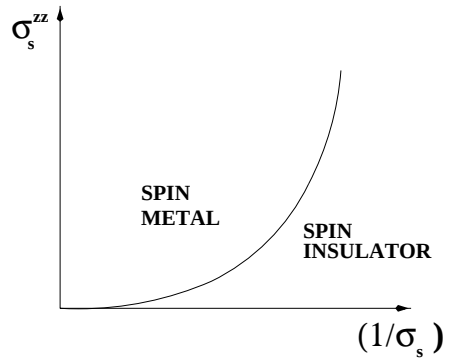

FIG. 1. Schematic phase diagram of the layered dirty $d_{x^2-y^2}$ superconductor.

Quasiparticle interactions, which we have ignored so far, can be shown [9] to lead to the usual Altshuler-Aronov singularities for the tunneling density of states for the diffusive spin metal. Interaction effects are expected to be more crucial in the spin insulator, and ultimately should produce a low density (considerably less than, e.g., the hole doping) of local magnetic moments which may then at low temperature freeze into a spin glass or stay paramagnetic in a random-singlet phase with a diverging spin susceptibility.

An important application of the theory outlined here is to the quantum disordered $d_{x^2-y^2}$ superconductor—a novel zero temperature phase that has been proposed [7] very recently to exist between the antiferromagnetic and superconducting regions of the high-T_c phase diagram. The low-temperature spin and thermal transport properties of the nodal liquid are identical to those of the superconductor, and with (weak) disorder, all the results mentioned above obtain. One quantitative point is worth mentioning: as one moves from the superconductor towards the antiferromagnet through the nodal liquid, the ratio v_F/v_Δ decreases monotonically, thereby decreasing the bare spin conductance. Thus localization effects are expected to become more important on going to the nodal liquid region. It is interesting that it is precisely in this region that experiments find a spin glass phase at low temperature.

We conclude with a few brief suggestions for experiments, leaving a detailed discussion to Ref. [9]. Spin transport can be probed by NMR techniques. It should also be possible to observe the localization physics in thermal transport. Ignoring the weak interaction effects, we predict that the thermal conductivity κ is related to the *spin* conductivity by the Wiedemann-Franz law:

$$\kappa/T\sigma_s = 4\pi^2/3 . \tag{6}$$

Physically, this follows from the equality of spin and thermal diffusion constants, the Einstein relation, and the relation between specific heat and density of states. (The Lorenz number differs by a factor of 4 from the usual one as the charge e in the usual formula is replaced by spin $\frac{1}{2}$ in our case.) Within the self-consistent theory this gives $\kappa = 2k_B^2 T(v_F^2 + v_\Delta^2)/3v_F v_\Delta \hbar$. In contrast, the microwave conductivity does not satisfy an Einstein relation and is, in general, not related to the thermal conductivity by the Weidemann-Franz law (as can be explicitly seen in the self-consistent theory, unless in the limit $v_F \gg v_\Delta$ [5]).

Finally, we expect that *localization* effects should be most pronounced when the nodal anisotropy v_F/v_Δ is minimized, as is expected to occur on reducing the hole concentration within the nodal liquid phase. If signatures of localization can be observed, it may be useful to perturb the system with a Zeeman (i.e., in-plane) field. A large enough Zeeman coupling is theoretically expected to open the d-wave nodes into Fermi pockets [12], dramatically increasing the density of states and the bare conductance, hence potentially probing some of the localization transitions discussed here.

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*Present address: Rm. 1D-368, Lucent Technologies, Bell Labs, 700 Mountain Ave., Murray Hill, NJ 07974.
†Present address: Physics Department, University of California, Los Angeles, CA 90095-1547.

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