Impurities of arbitrary range and strength in d-wave superconductors

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Abstract

The selfconsistent T-matrix approximation (SCTMA) for an alloy model of defects, described by scattering potentials of arbitrary range, is used to calculate quasiparticle lifetime effects as well as the order parameter renormalization in 2D d-wave superconductors. The study has been motivated by measurements of the microwave conductivity at low temperatures of extremely high quality samples of YBCO, the results of which do not really fit into the widely accepted d-wave picture. Poorly screened defects outside the CuO_2-planes could be the cause of the discrepancy. Apart from changing the single particle properties, the finite range of the defects affects the conductivity through vertex corrections, which project out forward scattering.

Key words: cuprates; d-wave pairing; SCTMA; microwave properties

1. Introduction

The description of nonmagnetic impurities in two-dimensional d-wave superconductors has turned out to be far more intricate than in the case of conventional superconductors, with results depending on the model used to describe disorder, the underlying band structure, and the computational methods employed. [1] In most of the published work, the scattering centers are assumed to be short ranged (s-wave scattering). In $YBa_2Cu_3O_{7-\delta}$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$, not intentionally doped with Zn, Ni etc, the disorder is due to oxygen nonstoichiometry and cation disorder. The defects thus reside on lattice sites away from the conducting CuO_2-planes and hence are only poorly screened and consequently long ranged. In order to generalize previous work on the conductivity [2,3], in which the case of coexisting strong and weak s-wave scatterers has also been considered, we want to treat impurities of arbitrary range and strength within the selfconsistent T-matrix approximation, assuming a circular Fermi surface and an infinitely wide band. This latter assumption not only simplifies the calculations, it also avoids artefacts resulting from the weak coupling approximation. [4] A finite range of the defect potentials introduces vertex corrections into the calculation of the electrical conductivity and renders the "universal conductivity" nonuniversal thus improving agreement with experiment. [5] However, it also leads to a selfenergy which renormalizes the d-wave order parameter OP. As can be seen below, the small but finite density of states (DOS) at zero energy found even in the Born limit for s-wave scatterers does not exist for purely forward scattering. If the pairing interaction is modelled such that the OP has the form $\cos 2\phi$, then this form is not changed by the selfenergy. However, the T_c-reduction caused by scattering in unconventional superconductors can be argued away by invoking mostly forward scattering. [6] In view of the large amount of doping related disorder, this could be a very important point. For more complicated pairing interaction, the shape of the gap will be changed by momentum dependent scattering. [7]

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2. Theory and numerical results

For the model outlined above the equations for the components of the T-matrix in an expansion with respect to Pauli matrices read

$$t^0(\varphi,\phi) = \eta \int_0^{2\pi} \frac{d\psi}{2\pi} U(\varphi-\psi) \left[g_0\, t^3(\psi,\phi) - g_1\, t^2(\psi,\phi)\right]$$

$$t^1(\varphi,\phi) = \eta \int_0^{2\pi} \frac{d\psi}{2\pi} U(\varphi-\psi) \left[g_0\, t^2(\psi,\phi) - g_1\, t^3(\psi,\phi)\right]$$

$$t^2(\varphi,\phi) = \eta \int_0^{2\pi} \frac{d\psi}{2\pi} U(\varphi-\psi) \left[g_0\, t^1(\psi,\phi) + g_1\, t^0(\psi,\phi)\right]$$

$$t^3(\varphi,\phi) = U(\varphi-\phi) + \eta \int_0^{2\pi} \frac{d\psi}{2\pi} U(\varphi-\psi) \left[g_0\, t^0(\psi,\phi) + g_1\, t^1(\psi,\phi)\right]$$

$U(\varphi)$ describes the momentum dependence and hence the range of the scattering potential. It is normalized such that $\int d\varphi U^2(\varphi) = 2\pi$. For pure s-wave scattering, $U = 1$, while in the Born approximation the limit $U^2(\varphi) = 2\pi\delta(\varphi)$ could be taken. $\eta = \pi N(0)v$ contains the normal state DOS and the strength of the potential v. $g_0(\psi)$, $g_1(\psi)$ are the energy integrated normal and anomalous Green functions [2],depending on the selfenergies $\Sigma_i(\psi) = n_{\rm imp} v t^i(\psi,\psi),\ i = 0, 1$. For reasons of symmetry, $t^2(\psi,\psi) = 0$ and hence makes no contribution as in the case of s-wave scattering. Due to particle-hole symmetry, $t^3(\psi,\psi)$ drops out when the single particle Green functions are energy integrated, but it does make an important contribution to the conductivity. [2] In general, all four components are required for the calculation of $\Sigma_{0,1}$. The above equations could be transformed to an algebraic system of equations by introducing Fourier expansions. [8] Since the t^i depend on φ and ϕ separately, a double expansion is required. So far, we have solved these equations directly by iteration. The range of angular integrations can be reduced by a factor 16 by exploiting various symmetries. For a sharply peaked $U(\varphi)$ convergence is obtained only for rather small values of η, corresponding to a selfconsistent Born calculation.For U we have used a Gaussian

$$U(\varphi) = I_0^{-1/2}(2\gamma)\, e^{\gamma \cos\varphi}$$

Choosing $\gamma = 5$, which would in the normal state give a transport time twenty times larger than the qp lifetime, we have a FWHM of 0.34π, still comparable with the range of angles in which the OP changes from minimum to maximum. Kee [6] uses a potential which is an order of magnitude narrower. Clearly, a detailed calculation of the potential arising from an out-of-plane defect is highly desirable.

For the rather weak scattering considered so far,

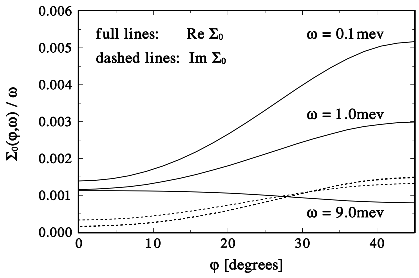

Fig. 1. $\Sigma_0 \equiv \omega Z(\omega) - \omega$ as function of angle. 45° is the nodal direction. $\Delta(T = 9\,\mathrm{K}) = 16.6\,\mathrm{meV}$. $\eta = \pi N(0)v = 0.16$ and $n_{\rm imp}/\pi N(0) = 0.5\,\mathrm{meV}$ have been used in the calculation. This corresponds to a normal state scattering rate of $0.012\,\mathrm{meV}$.

$\mathrm{Re}\Sigma_1(\omega,\varphi) \propto \Delta(T)\cos 2\varphi$ is independent of ω, while $Im\Sigma_1(\omega,\varphi) \propto \omega^2$ shows a more complicated angular dependence. Shown in the figure is $\Sigma_0(\omega,\varphi)$, which is approximately proportional to ω for $\omega << \Delta(T)$ as in the case of s-wave scattering. For this reason we plotted Σ_0/ω. The size of Σ_0 has been increased by more than an order of magnitude by increasing $n_{\rm imp}$ and η, but the significant variation with angle is determined mainly by the width of $U(\varphi)$. This variation, which is largest for small frequencies, should have a profound effect on the microwave surface resistance. Calculations are in progress.

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