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Impurity scattering in d-wave superconductivity. Unitarity limit versus Born limit

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Abstract. As is well known, Zn-substitution of Cu in the Cu-O_2 plane in the hole-doped high T_c cuprates provides a semi-quantitative test of underlying d-wave superconductivity. Here we complement this with a parallel study of Ni-substitution, which gives rise to weak scattering described with the Born approximation.

PACS. 74.72.-h High-Tc compounds – 74.25.Bt Thermodynamic properties – 74.25.Fy Transport properties (electric and thermal conductivity, thermoelectric effect, etc.)

It is well established that superconductivity in hole-doped high T_c cuprates is d-wave [1,2] with the puzzling exception that in electron doped cuprates it is s-wave [3,4]. Here we shall not enumerate the different experiments leading to this general consensus though they can usually be classified into 3 groups: 1) detecting the presence of nodes (or lines of zeros) in the order parameter, 2) phase sensitive experiments, which detect the sign change in $\Delta(\mathbf{k})$ by going around from $\mathbf{k}\|\mathbf{a}$ to $\mathbf{k}\|\mathbf{b}$ and 3) showing that $\Delta(\mathbf{k}+\mathbf{Q}) \cong -\Delta(\mathbf{k})$ where $\mathbf{Q} = (\pi,\pi)$. In this perspective impurity scattering provides the fourth test. In particular, a small amount of Zn-substitution gives rise to dramatic effects [5]: 1) a rapid suppression of the superconducting transition temperature T_c, 2) a dramatic increase of the residual density of states $N(0)$, and 3) a rapid decrease in the superfluid density. These suggest that the scattering due to Zn-impurities can be considered as being in the unitarity limit [5]. Such an analysis within a weak-coupling theory has been confirmed experimentally semi-quantitatively from the Knight shift in NMR [6], low temperature T-linear term in the specific heat [7], and the superfluid density, determined from muon spin rotation [8]. Also the superfluid density of Pr-substituted YBCO [9] appears to be well described within the same model. Here we shall study a parallel analysis of the effect of impurity scattering in the Born limit. This model may apply to Ni-substituted hole-doped high T_c cuprates. Of course similar work has been done previously. In [10] the superfluid density has been obtained both in the unitarity limit and in the Born limit, though we include this for completeness. Also some aspects of the density of states are discussed in [11], though they did not calculate the density of states for the variety of impurity concentration shown in Figure 6. On the other hand, the facts that the simple relation between the spin susceptibility and the superfluid density $\rho_s(T)$ ($\chi_s(T)/\chi_N = 1-\rho_s(T)$) will be broken in the presence of impurities, and that another simple relation exists at $T = 0$ K, $\chi_s(0)/\chi_N = N(0)/N_0$, where $N(0)$ is the electronic density of states at $E = 0$, are established in [5]. We will exploit these relations to calculate the corresponding quantities in the Born limit as well. Also, to our knowledge, the jump in the specific heat in the Born limit has not been discussed previously. A wealth of experimental data of the superfluid density and the optical conductivity from YBCO in the presence of impurities have been reported in [12]. Although a theoretical analysis on this subject has already appeared in the literature [13], the impurity effect on the microwave conductivity has not been studied systematically. Unfortunately this is beyond the scope of the present paper, since we consider mostly the thermodynamic properties of d-wave superconductors in the presence of impurities.

In the presence of the impurity scattering in the Born limit the renormalized Matsubara frequency $\tilde{\omega}$ is given by

$$\begin{aligned}\tilde{\omega} &= \omega + \Gamma\left\langle \frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2+\Delta^2 f^2}}\right\rangle \\ &= \omega + \frac{2}{\pi}\Gamma\frac{\tilde{x}}{\sqrt{1+\tilde{x}^2}}\,K\!\left(\frac{1}{\sqrt{1+\tilde{x}^2}}\right),\end{aligned} \tag{1}$$

where $f = \cos 2\phi$, $\tilde{x} = \tilde{\omega}/\Delta$, $K(z)$ is the complete elliptic integral and $\langle\cdots\rangle$ means the average over ϕ. In the weak-coupling model [14] the gap equation is given by

$$\lambda^{-1} = 2\pi T {\sum_n}' \left\langle \frac{2f^2}{\sqrt{\tilde{\omega}^2+\Delta^2 f^2}}\right\rangle, \tag{2}$$

where λ is the dimensionless coupling constant and ${\sum}'$ means that the ω sum is cut off at $\omega_n = E_c$. In the limit

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$\Delta \to 0$ equation (2) gives

$$-\ln\left(\frac{T_c}{T_{c0}}\right) = \psi\left(\frac{1}{2} + \frac{\Gamma}{2\pi T_c}\right) - \psi\left(\frac{1}{2}\right), \qquad (3)$$

where T_c (T_{c0}) is the superconducting transition temperature in the presence (absence) of impurity and ψ is the di-gamma function. Equation (3) is the same as the well-known Abrikosov-Gor'kov formula for an s-wave superconductor with magnetic impurities [15,16], though here Γ is the scattering rate due to the nonmagnetic impurities. Indeed, this similarity generated a lot of confusion in the early days of high T_c cuprates [17]. We note that $T_c = 0$ for $\Gamma = \Gamma_c = 0.8819 T_{c0}$. On the other hand at $T = 0$ K equation (2) is rewritten as

$$-\ln\left(\frac{\Delta(0,\Gamma)}{\Delta_{00}}\right) = 2\langle f^2 \mathrm{arcsinh}(C_0/f)\rangle + 2\left(\frac{2}{\pi}\right)^2 \times \frac{\Gamma}{\Delta}\int_{C_0}^{\infty} d\tilde{x}(K-E)\left(E - \frac{\tilde{x}^2}{1+\tilde{x}^2}K\right), \qquad (4)$$

where $\Delta(0,\Gamma)$ (Δ_{00}) is the order parameter at $T = 0$ K in the presence (absence) of impurities and $K = K(1/\sqrt{1+\tilde{x}^2})$ and $E = E(1/\sqrt{1+\tilde{x}^2})$ are the complete elliptic integrals. Here C_0 is determined from

$$\sqrt{1+C_0^2} = \frac{2}{\pi}\frac{\Gamma}{\Delta}K\left(\frac{1}{\sqrt{1+C_0^2}}\right). \qquad (5)$$

Also the residual density of states (*i.e.* the quasi-particle density of states at $E = 0$) is given by

$$\frac{N(0)}{N_0} = \frac{2}{\pi}\frac{C_0}{\sqrt{1+C_0^2}}K\left(\frac{1}{\sqrt{1+C_0^2}}\right), \qquad (6)$$

where N_0 is the density of states in the normal state. In Figure 1 we show T_c/T_{c0}, $\Delta(0,\Gamma)/\Delta_{00}$, and $N(0)/N_0$ as functions of Γ/Γ_c. Compared with those in the unitarity limit [5], although the T_c behavior is the same, $\Delta(0,\Gamma)$ decreases much more slowly with Γ, and $N(0)/N_0$ is almost zero until $\Gamma/\Gamma_c \geq 0.4$. Therefore $N(0)/N_0$, as measured by the Knight shift in NMR [6] or by the T-linear term in the specific heat [7], can clearly discriminate the two limiting behaviors of impurities.

Another quantity of interest is the superfluid density $\rho_s(T,\Gamma)$, which is given by

$$\rho_s(T,\Gamma) = 2\pi T\sum_n \left\langle \frac{f^2\Delta^2}{(\tilde{\omega}^2 + \Delta^2 f^2)^{3/2}}\right\rangle. \qquad (7)$$

At $T = 0$ K, this reduces to

$$\rho_s(0,\Gamma) = 1 - \frac{N(0)}{N_0} - \left(\frac{2}{\pi}\right)^2 \frac{\Gamma}{\Delta}\int_{C_0}^{\infty} d\tilde{x}\frac{(K-E)^2}{1+\tilde{x}^2}, \qquad (8)$$

where the argument of K and E is the same as in equation (4). We note that in the Born limit $\rho_s(0,\Gamma) \leq \rho_{s,spin}(0,\Gamma) = 1 - N(0)/N_0$, while in the unitarity limit $\rho_s(0,\Gamma) > \rho_{s,spin}(0,\Gamma)$. In Figures 2-5 we show: T_c/T_{c0} *versus* $N(0)/N_0$ for the Born limit and the unitarity limit (Fig. 2), T_c/T_{c0} *versus* $\Delta(0,\Gamma)/\Delta_{00}$ for both limits (Fig. 3), T_c/T_{c0} *versus* $\rho_s(0,\Gamma)$ for both limits (Fig. 4) and $\Delta C/\Delta C_0$ *versus* T_c/T_{c0} for both limits (Fig. 5), where ΔC is the jump in the specific heat at $T = T_c$. By expanding the gap equation in powers of Δ and keeping up

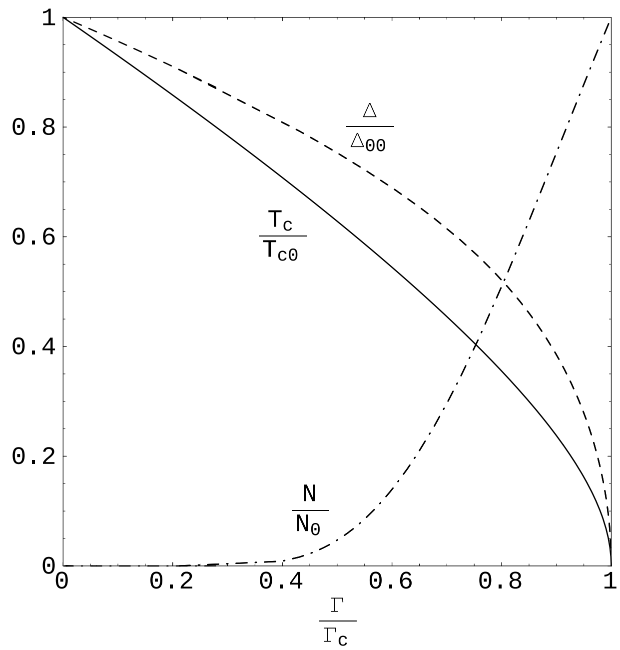

Fig. 1. The Born limit: $\Delta(0,\Gamma)/\Delta_{00}$ $(\cdots\cdots)$, T_c/T_{c0} (———) and the residual density of states $N(0)/N_0$ $(-\cdot-\cdot-)$ are shown as functions of Γ/Γ_c , where $\Gamma_c = 0.4122\Delta_{00}$.

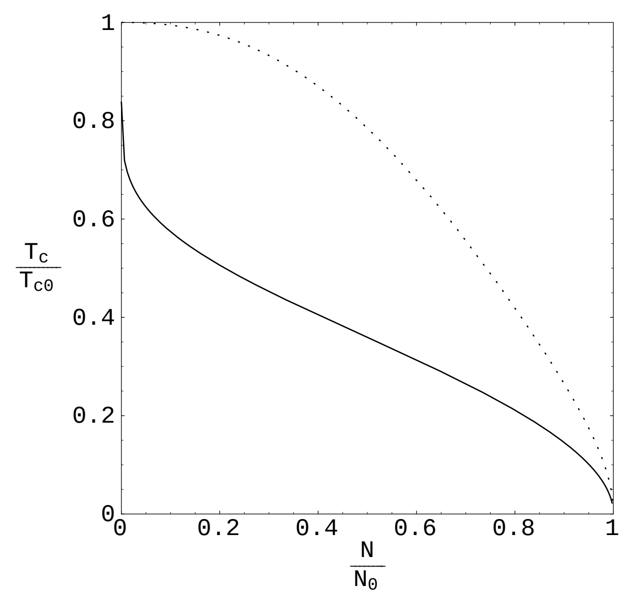

Fig. 2. The normalized transition temperature T_c/T_{c0} is shown as a function of the residual density of states $N(0)/N_0$ for the Born limit (———) and the unitarity limit $(\cdots\cdots)$.

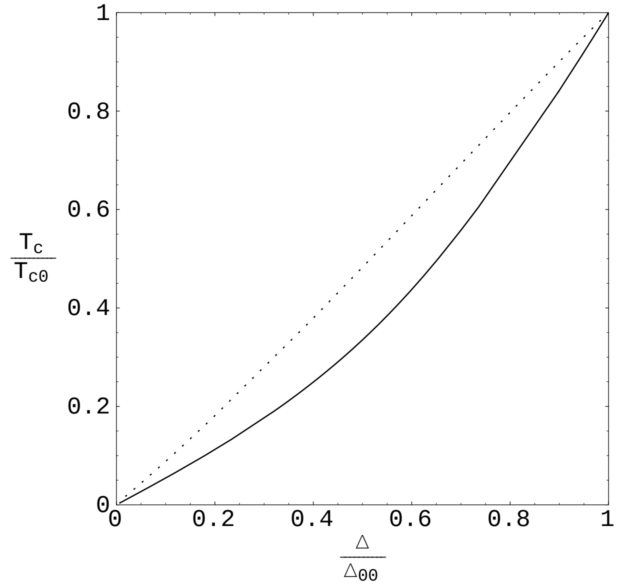

Fig. 3. T_c/T_{c0} is shown as a function of the normalized order parameter $\Delta(0,\Gamma)/\Delta_{00}$ at $T = 0$ K for the Born limit (———) and the unitarity limit (······).

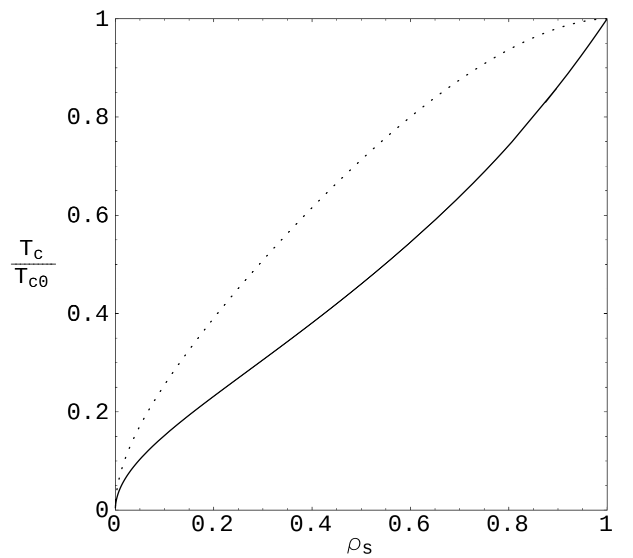

Fig. 4. T_c/T_{c0} is shown as a function of the superfluid density $\rho_s(0,\Gamma)$ for the Born limit (———) and the unitarity limit (······).

to the term of Δ^2, we obtain

$$\frac{\Delta C}{\Delta C_0} = \frac{21}{8}\zeta(3)\left(1-\rho\psi^{(1)}\left(\frac{1}{2}+\rho\right)\right)^2 \times\left[-\frac{3}{16}\psi^{(2)}\left(\frac{1}{2}+\rho\right)\pm\frac{1}{24}\rho\psi^{(3)}\left(\frac{1}{2}+\rho\right)\right]^{-1}, \quad (9)$$

where $\rho = \Gamma/2\pi T_c$, $\zeta(z)$ is the Riemann zeta-function, $\psi^{(1)}(z)$, $\psi^{(2)}(z)$ and $\psi^{(3)}(z)$ are the poly-gamma functions and the $\pm$ sign corresponds to the unitarity limit and the Born limit respectively. In Figure 4, $\rho_s(0,\Gamma)$ in the unitarity limit corrects an erroneous curve published in recent papers [17]. In general, for the same reduction of T_c the impurity in the unitarity limit affects the superconductivity much more strongly.

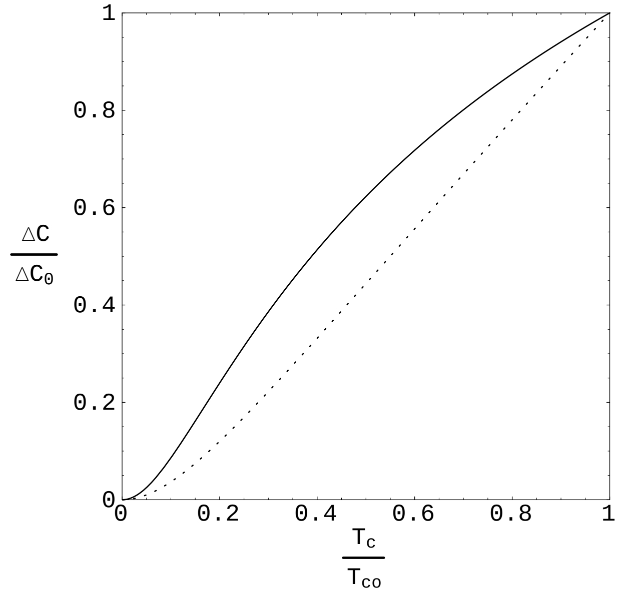

Fig. 5. The normalized jump in the specific heat at $T = T_c$, $\Delta C/\Delta C_0$ is shown as a function of T_c/T_{c0} for the Born limit (———) and the unitarity limit (······).

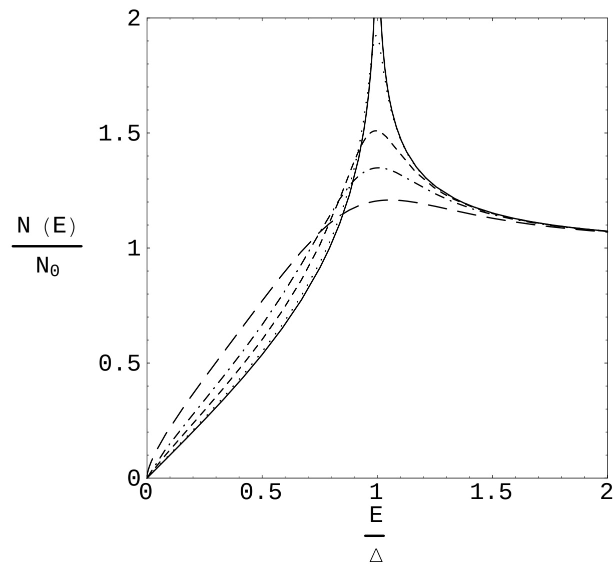

Fig. 6. The density of states in the Born limit for $\Gamma/\Delta = 0$ (———), 0.01 (······), 0.05 (- - - - -), 0.1 (– · – · –), and 0.2 (— — —) is shown as a function of E/Δ.

In Figure 6 we show the quasi-particle density of states

$$\frac{N(E)}{N_0} = \mathrm{Re}\left\langle\frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2+\Delta^2 f^2}}\right\rangle \quad (10)$$

for different Γ/Δ as functions of E/Δ. Here $\tilde{\omega}$ is determined from equation (1), but $\omega = -iE$. The curves are quite different from those in the unitarity limit [18].

In particular, the absence of the conspicuous peak (at $E = 0$) should be a clear sign of the Born limit.

Very recently the tunneling density of states is observed in partially Zn-substituted Bi2212 and the Ni-substituted one [19]. In the Zn-substituted Bi2212 the zero bias density of states increases very rapidly, whereas nothing happens to $N(0)$ in the Ni-substituted Bi2212, which is consistent with the present analysis. On the other hand it appears that the order parameter Δ increases in the Ni-substituted Bi2212, which is not described within the present model.

We can discuss the thermal conductivity in the Born limit as well. At low temperature (say, $T < 0.1\,T_c$), the thermal conductivity of monocrystals is mostly electronic and proportional to T, the temperature [5,20]

$$\kappa = \frac{2\pi}{3} T \frac{n}{m\Delta(0,\Gamma)} \frac{1}{\sqrt{1+C_0^2}}\, E\left(\frac{1}{\sqrt{1+C_0^2}}\right). \qquad (11)$$

In the Born limit, since C_0 is very small and the Γ-dependence of $\Delta(0,\Gamma)$ is small, the impurity will provide a beautiful test case of Lee's universality [21]. Also, as in the case of the unitarity limit, the Wiedemann-Franz law is obeyed between the real part of the electric conductivity and the thermal conductivity.

In summary, we have studied a few physical properties of d-wave superconductivity in the presence of impurities in the Born limit. Though the effect of impurities on the superconducting transition temperature is the same as in the unitarity limit, there are many different features. Experimental studies of these features in Ni-substituted hole-doped cuprates will provide another test of d-wave superconductivity.

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