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LETTER TO THE EDITOR

Quasiparticle lifetimes in the charged Bose gas and the cuprates

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Abstract

The scattering cross-section of a Coulomb potential screened by a charged Bose gas is calculated both above and below the Bose–Einstein condensation temperature, using the variable-phase method. In contrast with the case for the Bardeen–Cooper–Schrieffer superconductor, the screened scattering potential and quasiparticle lifetime are found to be very different in the superconducting and normal states. We apply the result to explain the appearance of a sharp peak in the angle-resolved photoemission spectra in some cuprates below the superconducting transition.

There is a growing body of evidence that cuprate superconductivity is due to the condensation of bipolarons, local bosonic pairs of carriers bound by the strong electron–phonon interaction [1]. The theory has been applied to explain the upper critical field [2], magnetic susceptibility [3], anisotropy [4], isotope effect on the supercarrier mass [5] and the pseudogap [1, 6, 7]. It provides a parameter-free formula for the superconducting T_c [8] and a parameter-free fit to the electronic specific heat near the transition [9]. The d-wave order parameter and the single-particle tunnelling density of states can be understood in the framework of Bose–Einstein condensation of inter-site bipolarons as well [10, 11]. We have also explained various features of the data from angle-resolved photoemission spectroscopy (ARPES) [12]. We assumed that a single photoexcited hole in the oxygen band is scattered by impurities, while the chemical potential is pinned inside the charge-transfer (optical) gap due to bipolaron formation. The normal-state gap, the spectral shape and the polarization dependence of the angle-resolved photoemission spectra were well described within this approach for a few cuprates. Recently it has been observed at certain points in the Brillouin zone that the ARPES peak in the bismuth cuprates is relatively sharp at low temperatures in the superconducting state, but that it almost disappears into the background above the transition [13, 14].

In our earlier paper [12], we mentioned that the scattering rate may be different above and below the transition in the cuprates due to anomalous screening below T_c in the charged Bose gas. In this letter, we present the results of calculations that justify this assertion. First we calculate the cross-section for scattering of single-particle excitations off a Coulomb scattering centre in the charged Bose gas (CBG), both above and below the Bose–Einstein condensation (BEC) temperature. We then propose that the appearance of a sharp ARPES peak below the transition in the cuprates is caused by a large increase in the quasiparticle lifetime due to condensate screening of scatterers.

First we calculate the scattering cross-section of a charged particle (mass m, charge e) scattered by a static Coulomb potential $V(r)$ screened by the CBG. The general theory of potential scattering in terms of phase shifts was developed in the earliest days of quantum mechanics (see for instance [15].) While in principle this allows scattering cross-sections to be calculated for an arbitrary potential, in practice the equations for the radial part of the wavefunction may only be solved analytically for a few potentials, and in the standard formulation are not in a suitable form for numerical computation. The 'variable-phase' approach [16] solves this problem by making the phase shifts functions of the radial coordinate, and then the Schrödinger equation for each radial component of the wavefunction reduces to a first-order differential equation for the corresponding phase shift. This technique has been used successfully in the study of two-dimensional plasmas in semiconductors [17].

In dimensionless units ($\hbar = 2m = 1$), the Schrödinger equation for the radial part of the angular momentum l component of the wavefunction of a particle with wavevector k undergoing potential scattering is

$$u_l''(r) + \left[k^2 - l(l+1)/r^2 - V(r)\right] u_l(r) = 0. \tag{1}$$

It is necessary in order for the following theory to apply that the restriction that the potential $V(r)$ vanishes faster than r^{-1} as $r \to \infty$. The scattering phase shift δ_l is obtained by comparison with the asymptotic relation

$$u_l(r) \xrightarrow{r\to\infty} \sin(kr - l\pi/2 + \delta_l) \tag{2}$$

and the scattering cross-section is then

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} \sin^2 \delta_l \tag{3}$$

In the variable-phase method [16], we must satisfy the condition that

$$V(r) \xrightarrow{r\to 0} V_0 r^{-n} \tag{4}$$

with $n < 2$. The phase shift for angular momentum l is then

$$\delta_l = \lim_{r\to\infty} \delta_l(r) \tag{5}$$

where the phase function $\delta_l(r)$ satisfies the phase equation

$$\delta_l'(r) = -k^{-1} V(r) \left[\cos \delta_l(r) j_l(kr) - \sin \delta_l(r) n_l(kr)\right]^2 \tag{6}$$

with

$$\delta_l(r) \xrightarrow{r\to 0} -\frac{V_0 r^{-n}}{k^2} \frac{(kr)^{2l+3}}{(2l+3-n)[(2l+1)!!]^2} \tag{7}$$

and $j_l(x)$ and $n_l(x)$ are the Riccati–Bessel functions [16]. In the $l = 0$ case, the phase equation reduces to

$$\delta_0'(r) = -k^{-1} V(r) \sin^2[kr + \delta_0(r)]. \tag{8}$$

In the slow-particle limit, we may also neglect higher-order contributions to the scattering cross-section, so

$$\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0. \tag{9}$$

The effective potential about a point charge in the CBG was calculated by Hore and Frankel [18]. The static dielectric function of the CBG is

$$\epsilon(\vec{q},0) = 1 + \sum_{\vec{p}} \frac{4\pi(e^*)^2}{q^2\Omega}\left(\frac{F_0(\vec{p}) - F_0(\vec{p}-\vec{q})}{-(1/m_b)\vec{p}\cdot\vec{q} + q^2/2m_b}\right) \tag{10}$$

in which $e^* = 2e$ is the boson charge, Ω is the volume of the system and $F_0(\vec{p}) = (\mathrm{e}^{(p^2/2m_b-\mu)/k_BT} - 1)^{-1}$ is the Bose distribution function. It has been shown [19] that equation (10) is valid even beyond the simplest random-phase approximation assumed in reference [18]. Eliminating the chemical potential, for small q the dielectric function for $T < T_c$ is

$$\epsilon(\vec{q},0) = 1 + \frac{4m_b^2\omega_p^2}{q^4}\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right] + \mathrm{O}\left(\frac{1}{q^3}\right) \tag{11}$$

and for $T \to \infty$ it is

$$\epsilon(\vec{q},0) = 1 + \frac{1}{q^2}\frac{m_b\omega_p^2}{k_BT}\left[1 + \frac{\zeta(3/2)}{2^{3/2}}\left(\frac{T_c}{T}\right)^{3/2} + \cdots\right] + \mathrm{O}(q^0) \tag{12}$$

with $\omega_p^2 = 4\pi(e^*)^2\rho/m_b$ and ρ the boson density. If the unscreened scattering potential is the Coulomb potential $V(r) = V_0/r$, then performing the inverse Fourier transforms, one finds that for $T < T_c$ [18]

$$\lim_{r\to\infty} V(r) = \frac{V_0}{r}\exp[-K_sr]\cos[K_sr] \equiv V_s(r) \tag{13}$$

with

$$K_s = \left(m_b^2\omega_p^2\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right]\right)^{1/4} \tag{14}$$

and for $T \to \infty$,

$$\lim_{r\to\infty} V(r) = \frac{V_0}{r}\exp[-K_nr] \equiv V_n(r) \tag{15}$$

with

$$K_n = \left(\frac{m_b\omega_p^2}{k_BT}\right)^{1/2}\left[1 + \frac{\zeta(3/2)}{2^{3/2}}\left(\frac{T_c}{T}\right)^{3/2} + \cdots\right]^{1/2}. \tag{16}$$

The $T < T_c$ result is exact for all r at $T = 0$.

There are two further important analytical results; the first (Levinson's theorem [16]) states that for 'regular' potentials (which include all those which we shall be concerned with), the zero-energy phase shift, δ_l is equal to π multiplied by the number of angular momentum l bound states of the potential. The second is the well known Wigner resonance scattering formula [15], which states that for slow-particle scattering of a particle with energy E off a potential with a shallow bound state of binding energy $\epsilon \lesssim E$, the total scattering cross-section is

$$\sigma = \frac{2\pi}{m}\frac{1}{E + |\epsilon|}. \tag{17}$$

We have used this to check that our calculation method works correctly by comparing our results with equation (17) for various potentials with shallow bound states (figure 1).

The zero-energy scattering cross-sections for the potentials $V_n(r) = -(V_0/r)\mathrm{e}^{-Kr}$ and $V_s(r) = -(V_0/r)\mathrm{e}^{-Kr}\cos(Kr)$ are shown in figure 2(a). These graphs are plotted for $V_0 = 1$;

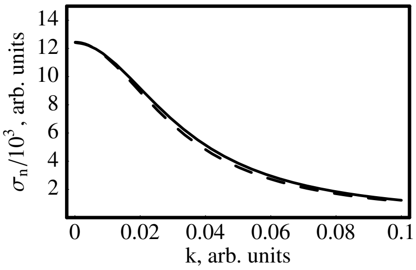

Figure 1. A plot of the scattering cross-section σ_n against the scattered particle momentum k for small k (solid line) and a fit using the Wigner formula (broken line) for the potential $V_n(r) = (-1/r)\exp(-0.55r)$. There is good agreement between the numerical and Wigner results.

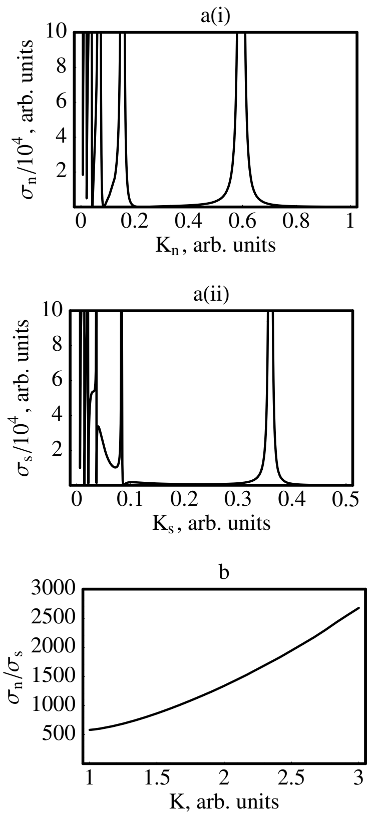

Figure 2. (a) Plots of the zero-energy scattering cross-sections (i) σ_n and (ii) σ_s against the screening wavevector $K = K_n = K_s$ for the potentials (i) $V_n(r) = -(1/r)\mathrm{e}^{-K_n r}$ and (ii) $V_s(r) = -(1/r)\mathrm{e}^{-K_s r}\cos(K_s r)$. (b) A plot of σ_n/σ_s for a range of $K = K_n = K_s$ in which neither potential has any bound states. In each case the units are those used to derive the phase equation.

in each case, the equivalent graph for arbitrary V_0 may be found by rescaling σ and K. According to the Wigner formula (equation (17)), as K is decreased, when a new bound state appears there should be a peak in the cross-section, as there will then be a minimum in the binding energy of the shallowest bound state. This is the origin of the peaks in figure 2(a), which may be checked using Levinson's Theorem. It can also be seen that as $K = K_n = K_s$ is decreased, the first few bound states appear at higher K in the ordinary Yukawa potential; this agrees with the intuitive conclusion that the bound states should in general be deeper in the non-oscillatory potential. Another intuitive expectation which is also borne out is that for a given V_0 and $K = K_n = K_s$, the non-oscillatory potential should be the stronger scatterer; in figure 2(b) it may be seen that this is the case when K is large enough for neither potential to have bound states (the difference in cross-sections is then in fact about three orders of magnitude.)

Now we address the possible application of our results to the ARPES linewidth for the cuprates. According to [12], the ARPES peak is related to photoexcited holes with small group velocity near the top of the oxygen band. The quantities necessary in order to calculate the scattering cross-section of impurities (the dopants) in the cuprates are the static dielectric constant, the effective mass of the bipolaronic carriers, the charge on the scattering centres and the bipolaron density. The situation is however complicated by the anisotropy of the effective-mass tensor. The value of the effective mass of the bipolarons in the cuprates is readily found from the penetration depth [8]. In BSCCO the in-plane bipolaron mass m_b is about 5–6 m_e. The dopants in $Bi_2Sr_2CaCu_2O_{8+\delta}$ are O^{2-} ions, and thus the Coulomb potential between a scattering centre and a hole is $V(r) = -2e^2/(\epsilon_0 r)$. The issue of the dielectric constant is more contentious: measurements suggest that it may be as high as 1000 [20]. The variable-phase method has only been derived for the isotropic problem, so we cannot apply our theory to reach a quantitative conclusion about the quasiparticle lifetime at different temperatures in the cuprates. However, we can provide an important general conclusion about the relative value of the cross-sections in the normal and superconducting states.

At zero temperature, the screening wavevector is $K_0 = (m_b\omega_p)^{1/2}$, and at a temperature αT_c well above the transition, it is $K_{\alpha T_c} = (m_b\omega_p^2/k_B\alpha T_c)^{1/2}$. Substituting ω_p and $k_B T_c = 3.3n^{2/3}/m_b$, we obtain

$$\frac{K_{\alpha T_c}}{K_0} = \left(\frac{2.1em_b^{1/2}}{\epsilon_0^{1/2}\rho^{1/6}\alpha}\right)^{1/2}. \tag{18}$$

From this, we see that the ratio is only marginally dependent on the boson density, so substituting for $\rho = 10^{21}$ cm^{-3}, e and m_e, we obtain

$$\frac{K_{\alpha T_c}}{K_0} = 3.0\left(\frac{(m_b/m_e)^{1/2}}{\epsilon_0^{1/2}\alpha}\right)^{1/2}. \tag{19}$$

With realistic boson masses and dielectric constants, $K_{\alpha T_c}$ and K_0, while different, are of the same order of magnitude. In the isotropic model, if the screening wavevectors are such that neither the normal-state nor the condensate impurity potentials have bound states, with these parameters it would then follow that the quasiparticle lifetime is much greater in the superconducting state; see figure 2(b). We propose that this effect also occurs in the realistic non-isotropic model, and could then explain the appearance of a sharp ARPES peak in the superconducting state of BSCCO. With doping, the screening radius decreases both in the normal, equation (16), and superconducting states, equation (14). This explains another fascinating experimental observation, namely the strange doping dependence of the ARPES linewidth. Optimally and overdoped cuprates, due to the higher carrier density, have shorter-range scattering potentials with smaller cross-sections compared with the underdoped cuprates. In addition, some cuprates, particularly overdoped samples, may be in the BCS–BEC crossover regime, which has been studied in detail by a number of authors, e.g. [22]. It is the presence of bosons, irrespective of whether fermions are also present, which causes the unusual screening below T_c, so our theory may be applied in these circumstances as well.

In summary, we have calculated the scattering cross-section of a Coulomb scattering centre in the charged Bose gas both above and below the condensation temperature. In contrast to the case for the BCS superconductor, the scattering potential in the CBG is different in the normal and superconducting states. This is because the coherence length in the CBG is the same (at $T = 0$) as the screening radius [21], while in the BCS superconductor it is a few orders of magnitude larger. We find that for the realistic parameters, the scattering cross-section above T_c in the bismuth cuprates might be around three orders of magnitude larger than at $T = 0$. We propose that the appearance of a sharp peak in the angle-resolved photoemission spectra of BSCCO below the superconducting transition and its doping dependence are due to the condensate screening of the scattering potential.

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