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LETTER TO THE EDITOR

Diffusion of objects in superconductors: crossover from classical to quantum behaviour on suppression of infrared couplings

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Abstract. It is shown how the onset of superconductivity in a metal will allow objects moving in the metal to make the entire transition from incoherent diffusion to quantum coherent motion, in an experimentally controllable way, as the gap suppresses the infra-red divergent coupling to electrons. An observable measure of the crossover is the diffusion constant $D(T)$ of the object, which we calculate in detail. This will allow a stringent experimental test of our understanding of this transition.

One of the most fascinating and subtle phenomena occurring in quantum mechanical systems is the crossover to classical behaviour when the system is forced into interaction with the world around it. Such crossovers occur from the very largest scales (as in the hypothesized transition from quantum to classical behaviour of the early universe [1]), right down to microscopic scales, in the motion of foreign objects through solids [2] and liquids [3], (such as defects, extraneous particles, or larger topological objects like vortices). A fundamental problem in the theory is to understand the interplay between infra-red (IR) divergent couplings to the environment (which tend to destroy quantum behaviour) and the kinetic or 'recoil' terms in the system Hamiltonian, which smooth out these divergences, and restore quantum coherence. These IR divergences are now well understood in isolation (they were first noticed in the Kondo problem [4]), but there is still no complete solution to, e.g., the problem of a diffusing particle in a metal (which at low temperature displays some coherent motion, but moves classically at high T).

Unfortunately it has been difficult to test the theory of this crossover on any system, simply because we are not normally at liberty to vary the coupling between the system and its environment (this being fixed by nature). The purpose of this work is to describe how one may surmount this problem, by doing experiments on objects moving in superconductors. We give a theory of the crossover from classical to quantum behaviour, and also briefly analyse possible experiments.

The essential physical argument is simple—one can use the superconducting gap as an IR cut-off, which gradually removes the IR divergences, in an experimentally controllable way; this then allows one to accomplish the complete crossover from classical, incoherent motion of the foreign object to coherent quantum motion.

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We formulate the problem by considering a foreign object, or a 'particle', moving in a superconductor according to the Hamiltonian

$$H = \sum_{p} \varepsilon_p A_p^\dagger A_p + \sum_{p,k,k'} V_{k,k'} c_{k,\sigma}^\dagger c_{k',\sigma} A_{p-k+k'}^\dagger A_p + H_{\mathrm{BCS}} \tag{1}$$

coupling the particle (created by $A_p^\dagger$) to electrons through $V_{k,k'}$. For the superconductor we use the usual BCS Hamiltonian with T-dependent gap $\Delta(T)$ (reducing to the normal state above T_c). To be definite we will assume a one-band model for the particle dispersion of the form

$$\varepsilon_q = 2J(\cos q_x a + \cos q_y a + \cos q_z a) \tag{2}$$

since interband transitions will be negligible at low T.

Now above T_c the full IR coupling is in force, and the particle moves entirely incoherently [5] above a temperature T^*, hopping from one lattice site to another at a rate

$$\nu_N = \frac{J^2}{W}\frac{\cos\pi K_N}{\pi K_N}\Gamma(K_N)\Gamma(1/2 - K_N)\left(\frac{\pi T}{W}\right)^{2K_N-1} \tag{3}$$

where W is is an effective electron bandwidth, and K_N is the dimensionless coupling between the particle and the electrons. In most cases where foreign objects move through solids, the coupling $V_{k,k'}$ is short-ranged, and can often be approximated by the s-wave form $K_N = 2\overline{V_0^2}(1-\sin^2 k_F a/k_F^2 a^2)$, with $\overline{V_0^2}$ being an angular average of $\rho(k_F)^2 V_{kk'}^2$ around the Fermi surface [5]. The temperature T^* is not known exactly (this being part of the crossover problem we are addressing); we shall return to it below.

Now below T_c, the gap $\Delta(T)$ cuts off the IR coupling to electrons and holes at the Fermi energy. Thus we expect a crossover to quantum coherent motion, at least over a distance of several lattice sites, even fairly near T_c. Of course the long-time motion will be diffusive, since the particle will still scatter off quasiparticles at any finite temperature. Now the short-time motion is very difficult to describe theoretically—at the moment the best we have is a very accurate (but approximate) solution to the problem of particle motion between two wells [6]. The complexity of the two-well problem shows what a formidable task the generalization to N wells will be; yet a proper description of the short-time coherent behaviour requires such a generalization.

Nevertheless an experimental test of the crossover does not require such an ambitious undertaking, for in the long-time limit the diffusive particle motion can be parametrized by a diffusion coefficient $D(T)$ which, as we shall see, has a distinctive behaviour [7].

The motion of the particle will be quite generally described by the current–current correlator

$$K_{ij}(q,\omega) = \int \mathrm{d}t \sum_{p} \mathrm{e}^{\mathrm{i}(p\cdot r-\omega t)}\langle J_i(r,t)J_j(0,0)\rangle \tag{4}$$

where we assume $j = \sum_p v_p A_p^\dagger A_p$, $v_q \equiv \partial\varepsilon_q/\partial q$, and $\langle\ldots\rangle = \mathrm{Tr}(\mathrm{e}^{-\beta H}\ldots)/\mathrm{Tr}(\mathrm{e}^{-\beta H})$. The particle diffusion constant is then just $D =$

$(1/3\mathrm{i}\omega)K_{jj}(0,\ \omega)|_{\omega\to 0}$. By standard methods we can then write D in terms of the Green's function $G_p(\omega)$ of the particle as

$$D = \tfrac{1}{3}\mathrm{Re}\int_0^\infty \mathrm{d}t\langle J(t)J(0)\rangle = \tfrac{1}{3}\mathrm{Re}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\sum_p v_p^2 \mathrm{e}^{-\beta(\epsilon_p-\Sigma_p(\epsilon_p))}|G_p(\omega)|^2 \qquad (5)$$

where Re stands for the real part and the Green's function is given as

$$G_p(\omega) = 1/(\omega - \epsilon_p + \Sigma_p(\omega)) = \alpha_p/(\omega - \tilde{\epsilon}_p - \mathrm{i}\gamma_p(\omega)) \qquad (6)$$

where the second form, with renormalized energy $\tilde{\epsilon}_p$, damping γ_p, and wavefunction renormalization α_p, is valid at low energies (the precise conditions are given below).

Now in the normal state the damping $\gamma_p > \tilde{E}_p$ above T^*, leading to the hopping in equation (3). The best present estimate of the crossover temperature T^* in the normal state is provided by the 'dilute-blip' approximation to the spin-boson problem [6], which gives

$$\pi T^* = [\Gamma(1-2K_N)\cos\pi K_N]^{1/(2-2K_N)}(J_0/W)^{K_N/(1-K_N)}(K_N^{-1} - \ln K_N) \qquad (7)$$

for the small value of $K_N \leqslant 0.2$ usually applicable in metals. Usually T^* is pretty small (thus (7) gives $T^* \sim 7$ mK for muons in Cu) and so one only sees incoherent motion in normal systems [8].

However, in the superconducting state the IR cut-off drastically reduces the low-energy value of γ_p; in fact, as we demonstrate below, the self-energy is accurately given, except very close to T_c, by

$$\Sigma_p^{\mathrm{sc}}(z) = \alpha_p^{\mathrm{sc}} V_0^2 \sum_{kk'}\bigg((u_k u_{k'} - v_k v_{k'})^2 \frac{f_k(1-f_{k'})}{z - E_k + E_{k'} - \tilde{\epsilon}_{p-k+k'}} + (u_k v_{k'} + v_k u_{k'})^2 \frac{(1-f_k)(1-f_{k'})}{z - E_k + E_{k'} - \tilde{\epsilon}_{p-k+k'}}\bigg) \qquad (8)$$

where z is a complex frequency; we use symmetric BCS coherence factors, appropriate to spin-symmetric scattering [9], and $E_k^2 = \epsilon_k^2 + \Delta^2$ with ϵ_k the electronic energy measured from ϵ_{F} (the generalization to anisotropic gaps will be given elsewhere). Equation (8) is a second-order (in $V_{kk'}$) perturbation result; and we shall find that the renormalization $\alpha_p^{\mathrm{sc}} \sim 1$.

Now in general one must sum the divergent terms in $\Sigma_p(z)$ to infinite order in $V_{kk'}$, to get a sensible answer [5]; but the gap here acts to cut off these divergences. We see this already from figure 1, which shows the drastic reduction in $\Im\,\Sigma_p(\omega)$ at low ω ($< T$), even quite close to T_c, computed from (8). If one now sums the most divergent graphs for $\Sigma_p^{\mathrm{sc}}(z)$, one finds very accurately

$$G_p(\omega) = (T/W)^{K_{\mathrm{sc}}}/(\omega - (T/W)^{K_{\mathrm{sc}}}\epsilon_p - \mathrm{i}\pi K_{\mathrm{sc}} T) \qquad (9)$$

for $\omega < T$, $\Delta(T)$ and $T < \Delta(T)$, so (9) is valid for $T/T_c < 0.9$; the exponent $K_{\mathrm{sc}} = K_N f(\Delta)$, and for $T/T_c < 0.7$, $K_{\mathrm{sc}} \sim \mathrm{O}(10^{-2})$ or less. If we then compare (9), (8), and figure 1, we see that for $T/T_c < 0.75$ equation (8) is a very good approximation, with $\alpha_p = 1$, and $\tilde{\epsilon}_p = \epsilon_p$. The essential physical reason is

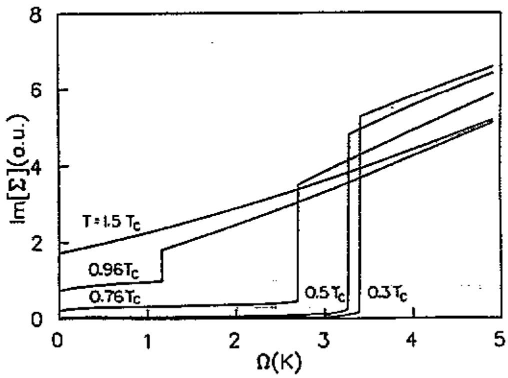

Figure 1. The imaginary part of the self-energy $\Sigma_{\boldsymbol{p}}(\omega)$ as a function of its frequency, for different temperatures below and above T_c. The frequency is measured in units of kelvin; notice that pair-breaking begins at $2\Delta(T)$. This figure is calculated from (8).

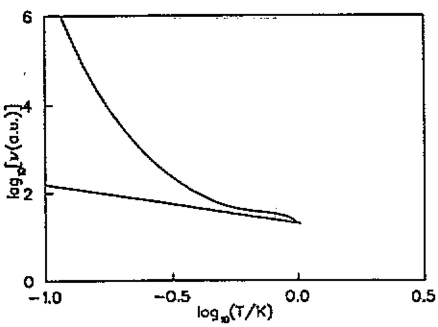

Figure 2. The particle diffusion constant, defined in (5), calculated for $J = 1$ K, $T_c = 1$ K and $K_N = 0.05$. This straight line is the normal-state behaviour, extrapolated below T_c; it describes incoherent motion. The curved line shows the real $D(T)$ in the superconductor. The superconducting curve does not exactly intercept the normal curve at T_c, because (8) is only approximately valid near T_c (see text).

very simple—the gap removes almost all the dissipative couplings up to frequencies $\geqslant 2\Delta(T)$ (the second 'pair-breaking' term in (8)), leaving only a small inelastic term, at low frequencies, coming from thermally excited Bogoliubov quasiparticles.

Now physically what has been accomplished by the transition to superconductivity, and the resulting suppression of the IR coupling to electrons associated with the normal state, is the change from incoherent motion above T_c to almost completely coherent motion below $T/T_c < 0.75$. The implications for the particle diffusion constant $D(T)$ are very interesting. In figure 2 we show an example, computed for $K_N = 0.05$ (this is the value that has been proposed for H in Nb, and also suggested for muons in Al). The procedure used to derive figure 2 was (i) in evaluating the self-energy, we approximated the particle energy by its angular average over the Fermi surface, i.e.

$$\varepsilon_{\boldsymbol{p}-\boldsymbol{k}+\boldsymbol{k}'} \rightarrow \varepsilon(p,\ k_F) = \langle \varepsilon_{\boldsymbol{p}-\boldsymbol{k}+\boldsymbol{k}'}|_{|k|=|k'|=k_F} \rangle. \tag{10}$$

With this approximation (which simply reflects our s-wave scattering approximation), the calculation of $\Sigma_{p}^{sc}(\omega)$ is standard and the the result is $\Sigma^{sc}(\omega - \varepsilon(p,\ k_{F})) = \Sigma(\Omega)$. Then *(ii)* we use this result in (5) to calculate D which is written as

$$D = \tfrac{1}{3}\mathrm{Re}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\sum_{p} v_{p}^{2}\mathrm{e}^{-\beta(\varepsilon_{p}+\Sigma(\varepsilon_{p}-\varepsilon(p,\ k_{F}))}\left|\frac{1}{\omega-\varepsilon_{p}-\Sigma(\Omega)}\right|^{2}. \qquad (11)$$

Now we wish to draw attention to an important feature of figure 2. The diffusion constant, $D(T)$, only gradually starts to rise away from the extrapolation of the normal state value as we lower T through T_c.

This feature has an physical explanation. The important frequency regions of $\Im\Sigma_{p}(\omega,\ T)$ being sampled by $D(T)$ are those where $\omega < \pi T$, and for T in the vicinity of T_c (and for some distance below T_c), $D(T)$ is still picking up pair-breaking contributions; not until $T/T_c \simeq 0.8$ does $D(T)$ begin its fast rise. In figure 2 we have chosen $T_c = 1K$ and $J = 1$ K, which allows a clear separation of T_c and T_0; clearly if $J \gg T_c$, the picture will look rather different [10].

What may we learn from experiments to test our results? As described in the introduction, the physical crossover taking place as we go below T_c is between incoherent classical motion and quantum coherent motion of the particle. Two obvious candidates for particles whose motion can be observed in superconductors are muons and hydrogen atoms. Interestingly, the traditional way in which theorists have analysed such experiments is using the results of the two-well problem [11, 12]. This gives a quite different picture below T_c. While this model may be appropriate to H in, e.g., Nb superconductor (where the H binds to O impurities), we do not believe it to be generally true—the massive reduction in dissipation below T_c must in most systems lead to a complete delocalization of the particle.

Thus an experimental investigation of this crossover to delocalized behaviour would be most interesting (note that it is not a phase transition!). One obvious way would be to try a muon diffusion experiment [13], although it is not clear that we currently have a theory of muon spin relaxation that deals adequately with this delocalized regime [14]. There is also the problem that interaction between the muon and even a very low concentration of impurities can be expected to alter the results seriously if the muon bandwidth is too narrow—this latter feature enters crucially into a very recent interpretation of these experiments by Kagan and Prokofev [15].

It is therefore rather important, in our opinion, that experiments be done on very pure samples, so that impurity effects do not complicate the interpretation. We should mention at this point that one may also vary J/T_c in experiments by applying a magnetic field. This then gives two control parameters (T and J/T_c), both in theory and experiment. The variety of behaviour of $D(T,\ H)$ is actually very rich, and there is no space to describe it here [10]. What is then important is that this gives no leeway to theory in any fits to experiment, and will thus allow a complete and rigorous test of the theory of the entire transition from classical to quantum behaviour of a moving particle. To the best of our knowledge, no such test has ever been possible, on any system, to this date [16]. Such a test would clearly be very important, particularly in view of the extraordinary variety of systems in nature capable of exhibiting such transitions, and whose dynamics are controlled by some IR divergent coupling to their environment.

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[7] A *proof* that the long-time motion can be described by the Einstein–Kubo relation is of course very difficult (although we suspect few physicists would doubt it). In this connection, Chen and Lebowitz have recently proved this for a particle moving in a one-dimensional Bloch potential coupled ohmically to Caldeira–Leggett oscillators:
Chen Y C and Lebowitz J L 1992 *J. Stat. Phys.* at press
It would be interesting to see if their proof could be generalized to the 3D potential, with coupling to Bogoliubov quasiparticles.

[8] It has been *assumed* until now that the coherence is unobservable. However, it is interesting to notice that currently available figures for muon diffusion in normal Al
Kiefl R *et al* *Phys. Rev. Lett.* submitted
yield a $T^* \simeq 4$ K! The crossover to coherent behaviour will in fact be quite slow. We do not address this point further in this paper, since it is not relevant to our superconducting results.

[9] It is possible that time-antisymmetric scattering may play a role in some experiments—we will give the results for this elsewhere.

[10] In fact the different possible curves for $D(T)$ are quite complicated as a function of the independent variables J, T_c and K_N; we will give a thorough analysis in a longer paper (in preparation). If we use a magnetic field to control T_c, almost all of this behaviour becomes accessible experimentally.

[11] Black J L and Fulde P 1979 *Phys. Rev. Lett.* **43** 453

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[13] Previous experiments on quantum diffusion in normal metal, using muons, have only tested theories of incoherent motion (see, e.g.,
Kadono R *et al* 1989 *Phys. Rev.* B **39** 23
and references therein); no observation of any crossover to delocalized motion has yet been claimed (but see [7]).

[14] An interesting recent effort in this direction is by
Gunnarson E and Hedegard P 1992 *Europhys. Lett.* **18** 367

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[16] An experiment similar to the one we suggest was done recently using muons in Al—See
Kadono R *et al* 1990 *Hyperfine Interact.* **64** 737