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LETTER TO THE EDITOR

The anomalous hop rate of localized particles in a marginal Fermi liquid

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Abstract. The hop rate of a localized particle in newly proposed marginal Fermi liquid is examined. It is found that due to the disappearance of the quasi-particle spectral weight at the Fermi surface, the hop rate behaves quite differently from that in all other materials. In particular, the hop rate increases with temperature at finite T, contrary to that in all other known materials. Furthermore, localization can occur at extremely low T. The experimental consequence of this prediction, as well as its connection with muon spin relaxation, is also discussed.

The motion of heavy particles in solids presents an interesting and fundamental problem in condensed matter physics [1–8]. Unlike other studies in solid state physics, (e.g. transport and optical phenomena) where the observables are usually obtained either under sample average or statistical average, the physical properties probed by implanted heavy particles are very closely related to the local properties of the material, such as local interaction strength and local density of states. When the heavy particle moves from one lattice site to the neighbouring one, due to the coupling between the particle and the local environment, the electrons (or phonons) and the elementary excitation associated with them should also rearrange themselves to balance the new position of the particle. The physics related to this phenomena can be best described by the polaron theory [7, 9, 10]. In the case of electron polarons, there exists an infrared divergence in the particle–electron coupling, which is also known as the Fermi surface effect [11, 12]. The diffusion properties of a heavy particle in various materials have been extensively investigated by various authors [1–10]. In all these different materials, the diffusion rate ν always decreases with increasing temperature for $T < \frac{1}{2}\theta$, where θ is the Debye temperature in solids. For example, $\nu \sim T^{-\alpha}$ in normal metals, semiconductors and insulators and $\nu \sim T^{-\alpha}\exp(\Delta_s/T)$ for conventional superconductors (where Δ_s is the superconducting gap).

In this letter, we shall study the diffusion properties of heavy particles in the so-called marginal Fermi liquid (MFL) [13, 14], a newly proposed concept that can explain quite well several unusual normal state properties of Cu–O superconductors. We find that heavy particles move in a rather strange manner in these systems as far as temperature dependence is concerned. In contrast to the known diffusion properties in all other materials mentioned above, the rate in these exotic materials is an increasing function of temperature, quite contrary to that of other known materials. The purpose of work is twofold: (i) to propose a further investigation of the MFL; (ii) to predict some surprising features in the diffusions rate in the MFL.

We consider the process where a heavy particle hops from site 1 ($\boldsymbol{R}_1$) to site 2 ($\boldsymbol{R}_2$) within the MFL. The particle–excitation (boson field) interaction can be described by a Hamiltonian $H_{\rm int}(\boldsymbol{R}_s)$ ($s = 1, 2$). The total Hamiltonian of the system can be written as

$$H(\boldsymbol{R}_s) = H_{\rm p} + H_{\rm B} + H_{\rm int}(\boldsymbol{R}_s) \tag{1}$$

where $H_{\rm p} = \Delta(C_1^\dagger C_2 + C_2^\dagger C_1)$ is the Hamiltonian for the particle with Δ the intersite tunnelling band width (on-site energy has been set to zero), and $C_s^\dagger$ and C_s are the creation and destruction operators for a particle at site s. The term $H_{\rm B}$ represents the Hamiltonian for the MFL. The interaction term can be written as

$$H_{\rm int}(\boldsymbol{R}_s) = \int \mathrm{d}\boldsymbol{x}\, \varphi^\dagger(\boldsymbol{x})\varphi(\boldsymbol{x})V(\boldsymbol{x} - \boldsymbol{R}_s) = \sum_q \eta_q V_q\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}}. \tag{2}$$

Here $\varphi(x)$ is the field operator for the electrons, $V(\boldsymbol{x} - \boldsymbol{R}_s)$ is the particle–electron interaction,

$$\eta_q = \int \mathrm{d}\boldsymbol{x}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\varphi^\dagger(\boldsymbol{x})\varphi(\boldsymbol{x})$$

is the electron density operator, and

$$V_q = \int \mathrm{d}\boldsymbol{x}\, V(\boldsymbol{x} - \boldsymbol{R}) \exp[-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{x} - \boldsymbol{R})].$$

We now consider the hop rate ν of the particle from $\boldsymbol{R}_1$ to $\boldsymbol{R}_2$. To the lowest order in tunnelling matrix Δ, it can be written as [1]

$$\nu = 2\pi \sum_{\rm f} |\langle{\rm f}|H_{\rm p}|{\rm i}\rangle|^2\, \delta(E_{\rm f} - E_{\rm i}) = 2\Delta^2 \int_{-\infty}^{\infty} \mathrm{d}t\, \langle \mathrm{e}^{\mathrm{i}H(\boldsymbol{R}_1)t}\, \mathrm{e}^{-\mathrm{i}H(\boldsymbol{R}_2)t}\rangle. \tag{3}$$

Here we have assumed that the energy level for the particle is the same at site 1 and 2. The average appearing in (3) is performed over all possible initial states,

$$\langle O\rangle = \mathrm{Tr}[\mathrm{e}^{-\beta H(\boldsymbol{R}_1)}O]/\mathrm{Tr}[\mathrm{e}^{-\beta H(\boldsymbol{R}_1)}]. \tag{4}$$

In the interaction representation

$$\phi(t) = \langle \mathrm{e}^{\mathrm{i}H(\boldsymbol{R}_1)t}\, \mathrm{e}^{-\mathrm{i}H(\boldsymbol{R}_2)t}\rangle = \left\langle \hat{T}\exp\left(\mathrm{i}\int_0^t \mathrm{d}\tau\, \hat{V}(\tau)\right)\right\rangle \tag{5}$$

where $\hat{T}$ is the time ordering operator, $\hat{V}(\tau) = \mathrm{e}^{\mathrm{i}H(\boldsymbol{R}_1)\tau}\hat{V}\,\mathrm{e}^{-\mathrm{i}H(\boldsymbol{R}_1)\tau}$ and $\hat{V}$ is defined as

$$\hat{V} = H(\boldsymbol{R}_2) - H(\boldsymbol{R}_1) = \sum_q \eta_q V_q\,(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_2} - \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_1}) = \sum_q \eta_q \tilde{V}_q. \tag{6}$$

With the use of the linked-cluster expansion, we obtain

$$\begin{aligned}\phi(t) &= \exp\left[\sum_l F_l(t)\right]\\ F_l(t) &= (-\mathrm{i})^l \int_{t>t_1>t_2\ldots} \mathrm{d}t_1\, \mathrm{d}t_2 \ldots \langle \hat{V}(t_1)\hat{V}(t_2)\ldots\rangle_{\rm connected}.\end{aligned} \tag{7}$$

The lowest-order contribution is $F_2(t)$:

$$F_2(t) = -\int_{t>t_1>t_2} \mathrm{d}t_1\, \mathrm{d}t_2\, \langle \hat{V}(t_1)\hat{V}(t_2)\rangle = -\int_{t>t_1>t_2} \mathrm{d}t_1\, \mathrm{d}t_2 \sum_{qq'} \hat{V}_q \hat{V}_{q'} \langle \eta_q(t_1)\eta_{q'}(t_2)\rangle. \quad (8)$$

The density–density correlation function can be directly related to the electronic polarizability $P_{q\omega}$ and the screening function $\varepsilon_{q\omega} = 1 - U_q P_{q\omega}$, by the fluctuation-dissipation theorem. We obtain

$$F_2(t) = \int \frac{\mathrm{d}\omega}{\omega^2} \frac{1 - \mathrm{e}^{-\mathrm{i}\omega t}}{1 - \mathrm{e}^{-\beta\omega}} \sum_q \left| \frac{|\tilde{V}_q|^2}{|\varepsilon^2_{q\omega}} \right| \operatorname{Im} P_{q\omega}. \quad (9)$$

Now the dominant contribution to the ω-integration comes from the excitations having energy $\omega \sim 0$. We can therefore use the static screening approximation $\varepsilon_{q\omega} \simeq \varepsilon_q$. As for the electronic polarizability in MFL $P_{q\omega}$, there is no microscopic calculation. Varma *et al* [2] had proposed a phenomenological form for the imaginary part of $P_{q\omega}$. It was further generalized by Peltzer [3] to include the real part as well. The full *ansatz* can be written as

$$P(\omega) = -(2/\pi)N(0)\{\psi[\tfrac{1}{2} + (\omega_c/2\pi T)] - \psi[\tfrac{1}{2} - (\mathrm{i}\omega/2\pi T)]\}/[1 + (\omega/\omega_c)^2] \quad (10)$$

where $\psi(x)$ is the psi function and $N(0)$ is the unnormalized quasi-particle density of states. This *ansatz*, although it can explain a number of unusual normal state properties of the new exotic superconducting materials, does contain a problem when the f-sum rule is considered. An implicit assumption was made in this *ansatz*, i.e., the q-dependence of $P_{q\omega}$ can be factorized out as $P_{q\omega} = g(q)\, P(\omega)$. Then the f-sum rule for $P_{q\omega}$ requires $g(q) \sim q^2$ which is obviously incorrect. This clearly indicates the q-dependence of $P_{q\omega}$ cannot be factorized out. One possible way to remedy this difficulty is to assume that $P_{q\omega}$ contains two terms,

$$P_{q\omega} = D_{q\omega} + P(\omega) \quad (11)$$

where the first term on the right-hand side is the contribution from the bound state caused by the vanishing of single-particle weight and the second term is given by (10). A consistent formalism of $D_{q\omega}$ is currently under investigation and will be presented elsewhere. It turns out that the bound-state term does not contribute to the present problem because its resonant frequency is usually higher. Therefore it is sufficient to use $P(\omega)$ in (9). The imaginary part of $P(\omega)$ is given as

$$\operatorname{Im}\{P(\omega)\} = -[2N(0)/\pi]\tanh(\beta\omega/2)\,(1 + (\omega/\omega_c)^2)^{-1}. \quad (12)$$

In what follows, we shall show that this form of $\operatorname{Im}\{P(\omega)\}$ will lead to some very interesting and unexpected behaviour of the motion of heavy particles.

Now $F(t)$ can be written as

$$F(t) = -K \int \frac{\mathrm{d}\omega}{\omega^2} \frac{1 - \mathrm{e}^{-\mathrm{i}\omega t}}{1 - \mathrm{e}^{-\beta\omega}} \frac{\tanh(\beta\omega/2)}{1 + (\omega/\omega_c)^2} \quad (13)$$

where K is the coupling parameter having energy units,

$$K = \frac{2N(0)}{\pi} \sum_q \left| \frac{\tilde{V}_q}{\varepsilon_q} \right|^2.$$

We may also replace the integral limits by cut-off ω_c. Now the real part of $F(t)$, after some manipulation, becomes

$$F^{\mathrm{R}}(t) = -K \int_0^{\omega_c} \frac{\mathrm{d}\omega}{\omega^2} [1 - \cos(\omega t)] = -t \arctan(\omega_c t) + \frac{1}{2\omega_c} \ln(1 + \omega_c^2 t^2). \quad (14)$$

Very surprisingly, it does not depend on T. We note that this quantity $F^{\mathrm{R}}(t)$ has strong

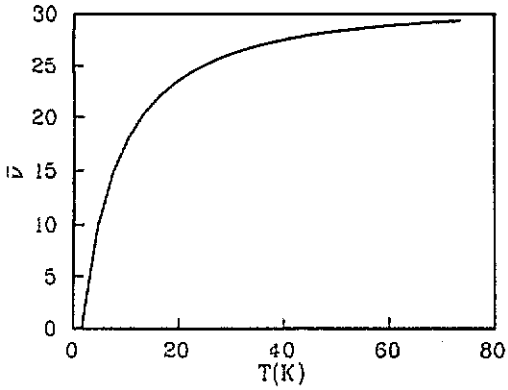

Figure 1. Plot of the normalized hop rate $\bar{\nu} = \nu\omega_c/4\Delta^2$ as a function of temperature for $\omega_c = 1500$ K and $K/\omega_c = 0.01$.

T-dependence in almost all other materials, including metals, semiconductors, insulators and conventional superconductors.

Similarly, the imaginary part of $F(t)$ can be written as

$$F^{\mathrm{I}}(t) = -2K \int_0^{\omega_c} \frac{\mathrm{d}\omega}{\omega^2} \sin(\omega t) \tanh\left(\frac{\beta\omega}{2}\right). \tag{15}$$

Equally surprisingly, while this quantity in other materials is usually T-independent, it does depend on T in the MFL. Making use of (14) and (15) in (3), we obtain the hop rate

$$\nu = 2\Delta^2 \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{F^{\mathrm{R}}(t)}\, \mathrm{e}^{\mathrm{i}F^{\mathrm{I}}(t)} \tag{16a}$$

$$\nu = 4\Delta^2 \int_0^{\infty} \mathrm{d}t\, \mathrm{e}^{F^{\mathrm{R}}}(t) \cos(F^{\mathrm{I}}(t)) \tag{16b}$$

where use has been made of the fact that F^{R} is even and F^{I} is odd to obtain (16*b*). Since the t-integration in (16*b*) is dominated by the contribution from the large-t region, we obtain the following approximate result.

$$\nu \simeq (\Delta^2/K)(8/\pi)(\omega_c/K)^{K/\omega_c}\,\Gamma(1 + K/\omega_c)\cos[F^{\mathrm{I}}(t \to \infty)]. \tag{17}$$

The only temperature dependence of ν is contained in $F^{\mathrm{I}}(t)|_{t\to\infty}$. By using (15) $F^{\mathrm{I}}(t)$ can be calculated. The numerical result of $F^{\mathrm{I}}(t)|_{t\to\infty} = F^{\mathrm{I}}$ reveals some surprising features of ν. At high temperatures (where T is still less than $\frac{1}{2}\theta$), F^{I} is much less than $\pi/2$ and decreases with T. This indicates that ν increases with T, which is quite contrary to the hopping behaviour of heavy particles in all other materials. It should be noted that (17) is only valid when $F^{\mathrm{I}} < \pi/2$ and is not applicable in the extremely low-T region where $F^{\mathrm{I}}(t)$ is very large and $\cos(F^{\mathrm{I}})$ becomes fast oscillating. In this case one must use (16) to calculate ν. It turns out the integral in (16) is very small at low T and approaches zero as the integrand oscillates faster. Therefore we conclude that the particle becomes localized at very low T. A typical result is shown in figure 1. Please note that the absolute value of the hop rate is very small because ω_c/Δ is usually of the order of 10^3–10^4.

Such anomalous T-dependence of ν is rather surprising. It is well known that the hop rate of heavy particles in any other material always decreases with T for T lower than $T^* \sim \frac{1}{2}\theta$, e.g. $\nu \sim T^{-\alpha}$ for normal metals, semiconductors and insulators with α ranging from $\sim$0.5 to 9. Even for conventional superconductors, $\nu \sim T^{-\alpha}\exp[\Delta_s/T]$. In all these materials, hop rate can only increase with T when one takes into account the effect of acoustic phonons and for $T > \frac{1}{5}\theta$. The result (17) indicates that disappearance of the quasi-particle spectral weight at the Fermi surface has some rather strange consequences when the particle motion is concerned: the usual scattering rate, which is proportional to the product of excitation density of states Im $P_{q\omega}$ and allowed phase space $(1 - e^{-\beta\omega})^{-1}$, becomes temperature independent for small ω because in MFL Im $P_{q\omega} \sim \omega/T$ at lower T. In any other systems, this rate is usually about T. The wavefunction overlap or bandwidth renormalization factor is still an increasing function of T at finite T. However, it vanishes in the very-low-temperature region, which leads to complete localization of the heavy particle. Although localization can occur in any system, it is rather surprising that in the MFL, it occurs at low T. The origin of this behaviour is probably the interplay of two competing effects: while a high T creates a larger phase space, it also reduces the excitation density because Im $P_{q\omega}$ is weighted by the inverse temperature.

The results predicted here can be studied experimentally with the use of any heavy particle implanted in the material. The μ-meson (muon) is probably the best candidate for such a quantum diffusion experiment due to its having the lightest mass of any heavy particle ($\frac{1}{9}$ of the proton mass). A typical spin relaxation measurement can yield direct information about ν. In other words, the observed spin relaxation function (zero field or longitudinal field) should also exhibit such anomalous temperature dependence.

In conclusion, the motion of heavy particles in the MFL is examined and some anomalous T-dependence in the hop rate is predicted.

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References

[1] Kondo J 1976 *Physica* B & C **84B** 40; 1984 *Physica* B & C **123B** 175; 1984 *Physica* B & C **124B** 25
[2] Yamada K, Sakurai A and Miyazima S 1980 *Prog. Theor. Phys.* **73** 1342
[3] Yamada K 1984 *Prog. Theor. Phys.* **72** 192
[4] Kadono R *et al* 1989 *Phys. Rev.* B **39** 23
[5] Zhang C, Gumbs G and Tzoar N 1991 *Phys. Rev.* B **43** 1463
[6] Stamp P C E and Zhang C 1991 *Phys. Rev. Lett.* **66** 1902
[7] Kagan Yu and Prokofev N V 1986 *Zh. Eksp. Teor. Fiz.* **90** 2176 (Engl. Transl. 1986 *Sov. Phys.-JETP* **63** 1276)
[8] Zhang C 1990 *Phys. Lett.* **148A** 193
[9] Flynn C P and Stoneham A 1970 *Phys. Rev.* **B 1** 3966
[10] Holstein T 1959 *Ann. Phys., NY* **8** 343
[11] Anderson P W 1967 *Phys. Rev. Lett.* **18** 1049
[12] Mahan G D 1981 *Many-Particle Physics* (New York: Plenum)
[13] Varma C M *et al* 1989 *Phys. Rev. Lett.* **63** 1996
[14] Pelzer F 1991 *Phys. Rev.* B **44** 293
[15] Nozières P and de Dominicis C T 1969 *Phys. Rev.* **178** 1097