Effects of Electron Correlations, Dynamical Screening and Plasmon Excitations on Muon Diffusion in Metals

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Abstract

An investigation is made of the effects of electron-electron interaction on muon diffusion in metals. It is shown that electron-electron correlation plays an important role in the motion of muons. The equation-of-motion method is used to calculate the correlation function. It is shown that electron correlations effectively reduce the muon hopping rate at low temperatures. It is also shown that the effect of dynamic screening increases the hopping rate. We found that due to plasmon excitation, the hopping rate is reduced by a factor which can be as large as one to two orders of magnitude.

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Ever since the pioneering work of Kondo[1] was carried out, it has become well known that the electron cloud screening a charged particle plays an important role in the motion of charged particles in metals[1-5]. When a heavy charged particle hops from one lattice site to a neighboring one, the electronic wavefunction must be rearranged so that it is centered around the new site. Kondo has shown that due to electron-charged particle interactions the bare tunneling matrix Δ is renormalized by a factor which is essentially the overlap integral between an electron wavefunction with a muon at a nearest-neighbor lattice site. The overlap integral is proportional to T^{2K} at low temperatures. By assuming a model electron muon interaction V_0 and a constant density of states ρ of width D for conduction electrons, one obtains $K = V_0^2 \rho^2 (1 - \sin^2 k_F a / (k_F a)^2)$. Here k_F is the Fermi wavevector and a is the nearest neighbor hopping distance. This result is a consequence of the "Anderson orthogonality catastrophe"[6].

Our objective in this paper is to study the effect of electron-electron interactions on quantum diffusion at low temperatures. We investigate the role played by these interactions on the T^{2K} behavior. We calculate K when the electron-muon interactions are included as well as when the electron-electron interaction is screened. The two-particle Green's function is calculated via the equation-of-motion method and electron-electron screening is treated selfconsistently in the Hartree-Fock approximation. The contributions to hopping rate ν due to plasmon excitations and particle-hole modes are obtained.

The transition probability of a muon in eigenstate $|i\rangle$ hopping from lattice site 1 to a lattice site 2 in eigenstate $|f\rangle$ within a metal is given by[2,12]

$$\nu = 2\Delta^2 \int_0^\infty dt \langle e^{iH_0 t} e^{-iH_I t} \rangle, \quad (1)$$

For convenience of notation, we set $\hbar = 1$. The average appearing in Eq. (1) is carried out over all possible initial states. The initial Hamiltonian H_i is given by (assuming spin degeneracy)

$$H_i = \sum_k \epsilon_k a_k^\dagger a_k + \sum_{k,k',q} v_q a_{k+q}^\dagger a_{k'-q}^\dagger a_k a_k + V_1, \quad (2)$$

where $a_k^\dagger$ and a_k are creation and destruction operators for an electron with wavevector k and energy ϵ_k , $v_q = 4\pi e^2 / q^2$ is the Fourier transform of the Coulomb interaction and V_1 denotes the electron-muon interaction for a muon at lattice site 1 and is given by

$$V_1 = \sum_{k,q} \frac{4\pi e^2}{q^2} a_{k+q}^\dagger a_k e^{iq \cdot R_1}$$

In the following, we take $R_1 = 0$ and denote the lattice vector joining nearest-neighbor lattice sites by a . In the interaction representation

$$\phi(t) \equiv \langle e^{iH_0 t} e^{-iH_I t} \rangle = \langle \hat{T} \exp[i \int_0^t d\tau V(\tau)] \rangle \quad (3)$$

where $\hat{T}$ is the time-ordering operator, $V(t) \equiv e^{iH_0 t} V e^{-iH_0 t}$ and V is defined as

$$V = H_f - H_i = \sum_{k,q} V_q a_{k+q}^\dagger a_k$$

where $V_q = \frac{4\pi e^2}{q^2} (e^{iqa} - 1)$. Expanding $\phi(t)$, keeping only connected diagrams, we obtain

$$\phi(t) = \exp \left[\sum_{l=1}^{\infty} F_l(t) \right], \quad (4)$$

where

$$F_l(t) = (-i)^l \int_{t_1 > t_2 > \dots > t_l} dt_1 \dots dt_l (V(t_1) \dots V(t_l))_{\text{connected}} \quad (5)$$

In our calculations, we keep terms up to order V^2 . Therefore, the average in $F_2(t)$ can be replaced by the average over $H_0 = H_i - V_i$. The average in $F_l(t)$ is still taken with respect to H_i . It can be shown that $F'(t)$ always cancels a term linear in t from $F_2(t)$. In a straightforward way, we obtain the lowest order term

$$\langle V(t) V(t') \rangle = \sum_{q,q'} V_q V_{q'}^* \sum_{k,k'} \Phi(k, q, k', q'; t, t'), \quad (6)$$

where $\Phi(k, q, k', q'; t_1, t_2) = \langle a_{k+q}^\dagger(t_1) a_k(t_1) a_{k'-q'}^\dagger(t_2) a_{k'}(t_2) \rangle$. In the absence of electron-electron interactions, the average over the four electron operators can be paired into two sets, resulting in a product of two single particle Green's functions. To evaluate the average in Eq. (6) we consider the retarded Green's function defined by

$$G_r(t_1, t_2) = -i\theta(t_2 - t_1) \langle [a_{k'-q'}^\dagger(t_2) a_{k'}(t_2), a_{k+q}^\dagger(t_1) a_k(t_1)] \rangle, \quad (7)$$

where $\theta(t)$ is the Heaviside step function. The advanced Green's function, $G_a(t_1, t_2)$ is obtained by replacing $-i\theta(t)$ by $i\theta(-t)$ in Eq.(7). The advantage of working with Green's functions is that their value at $t_1 = t_2$ is obtained by evaluating the commutation relation and the single-particle probability function. In thermal equilibrium, there is a direct relation between the Green's functions and the corresponding correlation function

$$\Phi(k, q, k', q'; \omega) = i[\tilde{G}_r(k, q, k', q'; \omega) - \tilde{G}_a(k, q, k', q'; \omega)] [e^{\beta\omega} - 1]^{-1} \quad (8)$$

where $\beta = T^{-1}$. The function $\tilde{G}(t)$ is the Fourier transform of $G(t)$.

To calculate G_r and G_a , we use the equation-of-motion method. In a straightforward way, it can be shown that G_r satisfies the equation

$$\left[\frac{\partial}{\partial t_2} + \epsilon_{k'-q'} - \epsilon_{k'} \right] G_r(k, q, k', q'; t_1 - t_2) = (f_{k'} - f_{k'-q'}) \delta(k + q - k') \delta(q - q') \delta(t_1 - t_2) \\ - i\theta(t_2 - t_1) \sum_{l,q''} v_{q''} \langle [a_{k'-q'}^\dagger(t_2) a_{l-q''}^\dagger(t_2) a_l(t_2) a_{k'-q''}(t_2), a_{k+q}^\dagger(t_1) a_k(t_1)] \rangle \\ + i\theta(t_2 - t_1) \sum_{l,q''} v_{q''} \langle [a_{k'-q'}^\dagger(t_2) a_{l-q''}^\dagger(t_2) a_l(t_2) a_{k'}(t_2), a_{k+q}^\dagger(t_1) a_k(t_1)] \rangle \quad (9)$$

where $f_k = [e^{\beta(\epsilon_k - \mu)} + 1]^{-1}$ is the Fermi-Dirac function. So far, no approximations have been applied in obtaining Eq. (9). To proceed further with our calculations, we use a decoupling procedure. In the mean-field approximation, the three-particle

Green's function on the right-hand side of Eq. (9) is replaced by a product of three two-particle Green's functions. This is a reasonably good approximation when the electron coupling is assumed weak. We keep only those terms in the linearization which arise from direct Coulomb interaction—that is, terms from the summation in Eq.(9) that contain a factor $\delta(q' - q'')$. These introduce a factor $4\pi e^2/q'^2$ into Eq.(9) that is highly divergent in the limit $q' \rightarrow 0$. Thus such terms can be large even if the electron-electron interaction is very weak. This approximation (essentially RPA) may not be enough when large momentum scattering is involved and short-range correlations must be included. It has been shown[3,14] that short-range correlation effects can be included by replacing the bare Coulomb interaction v_q by an effective interaction u_q , with $u_q = v_q(1 - W_q)$, where the local field correction W_q is defined as

$$W_q = \int dq' \frac{q \cdot q'}{q'^2} [S(q - q') - 1];$$

the structure factor is defined as $S(q) \equiv \frac{1}{v_q} \int d\omega \Im \epsilon_q(\omega)$. Here $\Im(x)$ stands for the imaginary part and $\epsilon_q(\omega)$ is a nonlocal dielectric function which is calculated below. The integral equation for $\tilde{G}_r(k, q, k', q'; \omega)$ is

$$[\omega + i\delta + \epsilon_{k'-q'} - \epsilon_{k'}] \tilde{G}_r(k, q, k', q'; \omega) - u_{q'} [f_{k'-q'} - f_{k'}] \sum_l \tilde{G}_r(k, q, l, q'; \omega) \\ = (2\pi)^{-1} [f_{k+q} - f_k] \delta(k + q - k') \delta(q - q') \quad (10)$$

whose solution can be easily obtained. The advanced Green's function $\tilde{G}_a$ is obtained from $\tilde{G}_r$ by replacing δ by $-\delta$.

Substituting $\tilde{G}_r$ and $\tilde{G}_a$ into Eq.(8), summing over k and k' , and then taking Fourier transforms, we obtain

$$\sum_{k,k'} \Phi(k, q, k', t_1 - t_2) = \int_{-\infty}^{\infty} d\omega e^{-i\omega(t_1 - t_2)} \frac{\delta(q - q')}{e^{\beta\omega} - 1} \frac{1}{v_q} \Im \frac{1}{\epsilon_q(\omega)}, \quad (11)$$

where the dielectric function is defined as

$$\epsilon_q(\omega) = 1 - \frac{v_q \Pi_q^0(\omega)}{1 + W_q v_q \Pi_q^0(\omega)}. \quad (12)$$

and the single-particle density-density response function is

$$\Pi_q^0(\omega) = \sum_k \frac{f_{k+q} - f_k}{\epsilon_{k+q} - \epsilon_k - \omega - i\delta}. \quad (13)$$

Of course, when $W_q = 0$ we obtain the RPA dielectric response function. Substituting Eq.(11) in Eq.(5) for $F_2(t)$ and integrating over t_2 and t_1 , the term linear in t cancels exactly $F_1(t)$. We obtain

$$F(t) \approx 2 \sum_q |V_q|^2 \int d\omega \frac{1 - e^{-i\omega t}}{\omega^2 [e^{\beta\omega} - 1]} \frac{1}{v_q} \left(\Im \epsilon_q(\omega) + \pi \delta(\Re \epsilon_q(\omega)) \right). \quad (14)$$

In the low temperature limit, $T/E_F \ll 1$, we use zero temperature value for ε . In eq.(14) we separate the particle-hole (ph) from the plasmon (p) contributions by writing $F(t) = F_{ph}(t) + F_p(t)$. The particle-hole term we obtain is a generalization of Kondo's result¹ to include dynamical screening. Since electrons having energy close to the Fermi energy dominate, the main contribution to the integral in Eq.(14) comes from $\omega \sim 0$, in which case we can approximate the dielectric function by its value in the static limit and obtain

$$F_{ph}(t) = \frac{m^2}{2\pi} \int_0^{2k_F} dq q \left(\frac{4\pi e^2}{q^2 \varepsilon_q(0)} \right)^2 \left(1 - \frac{\sin qa}{qa} \right) \times \left[\ln \left\{ \frac{\sinh \pi T t}{\pi T t} \sqrt{1 + \xi_q^2 t^2} \right\} + i \tan^{-1} \xi_q t \right], \quad (15)$$

where $\xi_q = qv_F - q^2/2m$ is the cutoff which determines the range over which $\Im \varepsilon(\omega) \sim \omega$ is valid. For large t , we obtain

$$\phi_{ph}(t) \approx (T/E_F)^{2K} e^{-B} \exp(-2\pi K T |t|) \exp(-i\pi K \operatorname{sgn}(t)). \quad (16)$$

The parameter K is defined as

$$K \equiv \frac{4}{\pi^2} \left(\frac{4}{9\pi} \right)^{2/3} r_s^2 \int_0^2 \frac{dz}{z^3} \frac{1}{\varepsilon_z(0)} \left[1 - \frac{\sin z k_F a}{z k_F a} \right]$$

and B is given by

$$B \equiv \frac{8}{\pi^2} \left(\frac{4}{9\pi} \right)^{2/3} r_s^2 \int_0^2 \frac{dz}{z^3} \frac{1}{\varepsilon_z(0)} \left(1 - \frac{\sin z k_F a}{z k_F a} \right) \ln \xi_z.$$

where the dimensionless variable $z = q/2k_F$ and $r_s = (9\pi/4)^{1/3} (m e^2 / k_F)$ is the plasma parameter. We have calculated K by using the RPA limit ($W_q = 0$) as well as when short-range correlations are included. Our calculations show a significant difference for these two approximations. In Fig. 1, the function K for both cases are plotted vs the plasma parameter r_s . As r_s increases, short-range electron correlations reduce the density of screening clouds and effective electron-muon interaction becomes stronger. As a result, the K is larger and increases faster with r_s in the correlated case than in the RPA case. We have also calculated $\phi(t)$ for the case of dynamical screening. In the large- t region, we found that $\phi^{dyn}(t) \sim \exp(-2\pi K^{dyn} T t)$ with $K^{dyn} < K^{sta}$. The temperature-dependence of K^{dyn} is rather weak.

We now turn to the contribution to $F(t)$ due to plasmon excitations. In the long wavelength limit, our calculations show that

$$F_p(t) = 2r_s \left(1 - \frac{\tan^{-1}(k_c a)}{(k_c a)^2} \right) \left(\frac{1 - e^{-i\omega_p t}}{1 - e^{-\beta\omega_p}} \right), \quad (17)$$

where ω_p is the local plasmon frequency $k_c = \omega_p/v_F$ is the cutoff wavenumber. The oscillatory term $e^{-i\omega_p t}$ has no contribution to the t -integration. Therefore, F_p is independent of time. In addition to the factor T^{2K} , the hopping rate involves another

factor $\exp(-F_p)$ which is weakly temperature dependent at low temperature. For Cu $F_p \approx 4.6$. Our calculations show that the hopping rate is given by

$$\nu = (\Delta^2/E_F) e^{-F_p} e^{-B} \frac{\cos \pi K}{\pi K} \left[\frac{T}{E_F} \right]^{2K-1} \quad (18)$$

for the static case. When both the electron-muon and electron-electron interactions are dynamically screened we find that K is weakly temperature-dependent. Kondo's result Eq.(1) corresponds to $\xi_q = D$, $4\pi e^2/q^2 \varepsilon_q(\omega) = V_0$ and $F_p = 0$. In Fig.2. we have plotted $w = \nu E_F/\Delta^2$ as a function of temperature for both dynamic and static screening case. Our result shows that hopping rate is larger in the dynamical case. We may say that orthogonality is softened by dynamic process.

In conclusion, we have shown that the overlap integral of two electronic wavefunctions with a muon at different lattice sites is modified by electron-electron interactions in two ways: short-range correlations reduce this integral while dynamical screening increases this integral. We also found that there is a further reduction in the tunneling matrix due to plasmon excitations. Without any assumption for electron-muon interaction and the density of states of conduction electrons, our result for K is in good agreement with the recent experiment findings.⁸

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Figure Captions

Fig.1. Plot of K vs r_s in the static approximation, solid lines: correlated case, and broken lines: RPA case, from top to bottom, $k_F a = 5.0, 3.0, 2.0$.

Fig.2. Plot of w vs temperature in correlated case, where $r_s = 2.7$ and $k_F a = 3.0$, upper curve: dynamic screening, and lower curve: static screening.

Fig. 1

Fig. 2