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Consistent model for the screening of slow muons in metals

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By using a sum rule for scattering phase shifts at the Fermi level, a consistent screened potential of a slow positive muon in an electron gas is constructed. This consistent model potential is applied in the theoretical characterizations of the overlap parameter in muon quantum diffusion, the retarding force of the electron gas, and the Knight shift. Comparisons with available experimental results are made, and a good agreement is found. [S0163-1829(99)50542-0]

The motion of light particles in metals is a topic of fundamental interest since it involves the interaction of simple, singly charged units (positive muons: μ^+), with electrons and nuclei belonging to the metals. The goal of the theoretical investigation to be described here is to provide a consistent model for the screening of μ^+ which is the basic input in the following three (i–iii) important areas of the topic.

i. At low temperatures, where these light particles ($m_\mu \simeq m_p/9$ in proton mass) may still be mobile, their diffusion is dominated by quantum tunneling between lattice sites.[1] Specifically, copper and aluminum fcc metals are well suited for detection of muon diffusion because of the large nuclear moments of target atoms, which give rise to strong depolarization effects when the muons move slowly enough.[2] In 1984, Kondo recognized the crucial role of conduction electrons in the diffusion process.[3] It turns out that one should take into account the overlap of two many-body ground states with the same local, screened potential at different sites (characterized by a distance a) of μ^+ in the electron gas.[4–6] The overlap parameter $[K(a)]$ is related to the scattering phase shifts (δ_l) of electrons, caused by this screened potential, at the Fermi energy $p_F^2/2$ (we use atomic units $e^2=m_e=\hbar=1$ throughout). The small-distance ($p_F a \ll 1$) behavior is expressed as[5,6]

$$K(a)=\frac{1}{3}\left(\frac{p_F a}{\pi}\right)^2\frac{p_F^2}{4\pi}\sigma_{tr}(p_F). \tag{1}$$

The long-distance ($p_F a \gg 1$) behavior (denoted as K_∞) is expressed directly in terms of the scattering phase shifts[4,6]

$$K_\infty=\frac{2}{\pi^2}\sum_l (2l+1)[\tan^{-1}(\tan\delta_l)]^2. \tag{2}$$

In Eq. (1) $\sigma_{tr}(p_F)$ is the usual transport cross section:

$$\sigma_{tr}(p_F)=\frac{4\pi}{p_F^2}\sum_l (l+1)\sin^2[\delta_l(p_F)-\delta_{l+1}(p_F)], \tag{3}$$

thus $K(p_F a \ll 1)$ is related to the dissipative behavior of the electron gas as we shall discuss below.

ii. A charged particle with mass $m \gg m_e$, moving slowly with a given velocity v in the electron system, experiences a longitudinal force (F) arising from the response of the system:

$$F=v\,n_0\,p_F\,\sigma_{tr}(p_F), \tag{4}$$

in which $n_0=p_F^3/(3\pi^2)$ is the electron density.[7] The energy dissipation is due to electron-hole excitations at the Fermi level. This so-called stopping power[8] (energy loss per unit path length) is a measurable quantity by standard transmission and backscattering methods for normal particles, i.e., for protons. Very recently, a muon spin resonance (μSR) method for directly imaging the implantation depth of positive muons in metals was presented.[9] Application of this method for epithermal muon beams[10] with tunable kinetic energies ($10-10^4$ eV) provides a source of experimental facilities to be used in condensed matter physics. Clearly, the knowledge of theoretical stopping powers of low-energy muons should have relevance in detailed studies of solid-state excitations.

iii. The third important area is the measurement of Knight shifts in metals. The electron spins are polarized under the action of a magnetic field (H). The polarization generates an extra field which acts on the spin of the muon. This effect leads to a shift of the magnetic resonance frequency of the ''nucleus.'' The extra (ΔH) magnetic field is given as[11,12]

$$\Delta H=\frac{8\pi}{3}H\chi_P E(p_F), \tag{5}$$

TABLE I. In this table we present theoretical results obtained for the screening parameter λ [see Eq. (6)], for the transport cross section $\sigma_{tr}(p_F)$ [see Eq. (3)], for the long-distance overlap parameter K_∞ [see Eq. (2)], for the reduced enchancement factor of a scattered wave at the impurity position $E^*(p_F)$ [see Eq. (8), and the text after it], and for the susceptibility enchancement $E_P(p_F)$, as a function of the density parameter r_s of the electron system.

r_s	λ	$\sigma_{tr}(p_F)$	K_∞	$E^*(p_F)$	$E_P(p_F)$
1	2.51	0.78	0.103	0.984	1.15
2	1.71	9.43	0.291	1.054	1.31
3	1.23	33.13	0.487	1.038	1.46
4	0.97	63.82	0.301	0.947	1.62
5	0.82	95.31	0.221	0.901	1.79

in an electron system with spin (Pauli) susceptibility χ_P. This form is due to the dominant contact interaction. In Eq. (5), $E(p_F)$ is the enchancement factor for *s*-wave ($l=0$) scattering of electrons on the Fermi surface at a μ^+ site. We note at this point that experiments designed[13] to look for bound electron states around a positive muon have been unsuccesful (see, also Ref. 14; for muoniums in insulators, see Ref. 2).

After these clarifications of the topic we satisfy the main physical requirement that must be satisfied in our problem, i.e., that the charge be completely shielded, in the following way. Within the framework of an electron-gas description of a real solid we shall use a physically motivated one-parametric (λ) model potential[15]

$$V(r)=-Z\frac{\lambda}{e^{\lambda r}-1}, \tag{6}$$

in order to represent the screening of (slow) muons ($Z=1$). To achieve an internal *consistency* [the measurable quantities in Eqs. (1)–(5) are tied to the Fermi momenta] we fix the screening parameter (λ) via a nontrivial constraint published recently by Zwerger.[16]

Around a slowly moving massive impurity there is a backflow in the electron system. For a charged impurity (with charge Z) the dipolar backflow identically cancels the longitudinal part of the impurity current due to the perfect shielding. Using this dynamical requirement Zwerger extended the well-known linear response result[17] and thus obtained the following sum rule:

$$Z=\frac{1}{\pi}\sum_l (2l+1)\sin 2\delta_l+\frac{4}{\pi}\sum_1 (l+1)^2 \times\sin\delta_l\sin\delta_{l+1}\sin(\delta_l-\delta_{l+1}). \tag{7}$$

Note, that the derivation of this rule needed scattering characteristics *solely* at the Fermi level [$\delta_l(p_F)$].

We have determined the phase-shift values from the numerical solutions of the Schrödinger equation with $p_F^2/2$ scattering energy using $V(r)$ of Eq. (6). By forcing this to satisfy the sum rule of Eq. (7) we obtained the consistent screening parameters as a function of the density parameter r_s. These results are given in Table I for the important (metallic) range of our problem $r_s\in[1,5]$. The consistently determined phase shifts are used to calculate the long-distance overlap parameter K_∞ of Eq. (2) and $\sigma_{tr}(p_F)$ of Eqs. (3) and (4). These results are given in the relevant columns of Table I.

We compared our values for the transport cross section with results obtained by a standard calculation performed within the ground-state density-functional theory (DFT). In this latter treatment[18] the complete shielding is satisfied via an explicit construction of the induced charge, using auxiliary Kohn-Sham stationary-state representation for the one-electron wave functions whose occupation is prescribed by the *whole* Fermi distribution function. The comparison shows an essentially perfect agreement at the lower r_s values and differences about 10–15% at the low-density range, where the present values for $\sigma_{tr}(p_F)$ are slightly higher. Considering the statement of Mann and Brandt[19] on the remarkable accuracy of DFT-based results[18] for slow protons in comparison with collected experimental data (deviations within $\pm 15\%$), we can conclude that our results are also very reasonable ones. The agreement may give a firm base in the planned stopping-range measurements using epithermal positive muon beams.[9]

Now, we turn to the application of our K_∞ values, shown in Table I. Well-established experimental results for the overlap parameter are available for aluminum and copper. For the lighter metal (Al, $r_s=2.07$) the recommended (see Ref. 2 for further details) value is about 0.32. Our prediction is in good agreement with this. For copper the experiments give results in the 0.16–0.22 range.[2] If we use (as it is ususal in stopping measurements by ions) the value of about $r_s \simeq 1.5$, we can also establish a very satisfactory agreement with our theoretical result. This choice of r_s value mimics the role of *d*-band electrons of a real Cu target, in an average manner. Note, that the nonmonotonic behavior of $K_\infty(r_s)$ is due to the theoretical[4,6] prescription: $\delta_l^*=\tan^{-1}(\tan\delta_l)$ which results in $|\delta_l^*|\leq\pi/2$.

We continue the representation and discussion of our theoretical results by considering the third important area of application of positive muons in metal physics: the problem of Knight shift. One key quantity to calculate $\Delta H/H$ is the scattering wave-function enchancement $E(p_F)$, as discussed at Eq. (5). For our Hulthén-like potential the enchancement is given in a closed analytical form (a physical motivation for the use of this model) as follows:[15,20]

$$E(p_F)=\frac{2\pi Z}{p_F}\frac{e^{\alpha}-e^{-\alpha}}{e^{\alpha}+e^{-\alpha}-2\cos(\alpha\beta)}. \tag{8}$$

In this equation we have introduced, as short-hand notations, $\alpha=(2\pi p_F/\lambda)$, and $\beta^2=[(2Z\lambda/p_F^2)-1]$, respectively. The so-called reduced enchancements, defined as $E^*(p_F)=(p_F/2\pi)E(p_F)$, are given in Table I for our case $Z=1$. Our screened potential, optimized for scatterings at the Fermi level via a nontrivial sum rule, produces almost exactly Coulomb-like enchancements. For scatterings in an attractive (bare) Coulomb field: $E_c^*(p_F)=[1-e^{-2\pi/p_F}]^{-1}$, as it is well known.

The second key quantity in calculating $\Delta H/H$ is the magnetic susceptibility χ_P. The measurable shifts are proportional to a product, $E(p_F)\chi_P$, where both quantities are to be determined. In the present model calculation we use the theoretical results for χ_P from Ref. 21, where the enchancement factors for the Pauli susceptibility were determined for an interacting electron system, as a function of r_s. We apply the results of Ref. 21 by writing χ_P as $\chi_P = E_P(p_F)\chi_P^0$, where χ_P^0 refers to the ideal-gas value.[11] The theoretical susceptibility enchancements $E_P(p_F)$ are given in the last column of Table I. Using the above-introduced notations, we rewrite Eq. (5) into a transparent form:

$$\frac{\Delta H}{H} = 71 \times E_P(p_F) E^*(p_F), \tag{9}$$

in ppm (parts per million) units. Experimental predictions (see Ref. 22; for further discussions, see Refs. 14 and 20) for $\Delta H/H$ are in the range of 79–88 ppm for Cu ($\Delta H/H = 81$; $r_s \simeq 1.5$), Mg ($\Delta H/H = 87$; $r_s \simeq 2.7$), Na ($\Delta H/H = 79$; $r_s \simeq 3.9$), and K ($\Delta H/H = 88$; $r_s \simeq 4.9$). The product, $E^*(p_F)E_P(p_F)$, is a moderately growing function in our description. This is due to the interesting behavior of the present $E^*(p_F)$ function. Earlier theoretical calculations[14,20] resulted in higher, by 50–60% in the low-density range, $E^*(p_F)$ factors, and thus in essentially overestimated Knight-shift values.

We conclude with an outlook on the applicability of the present results in cases of ferromagnetic metals. Assuming a homogeneous spin-polarized electron gas model for these materials, Jena, Singwi, and Nieminen,[14] by extending a simple earlier calculation,[23] investigated the problem of the hyperfine field at a muon site. They concluded that in this model, at least for small initial polarization and within the practical framework of DFT, the important relative spin-density enchancement is directly related to the $E(p_F)$ factor of Eq. (5). A more general model for the mentioned problem in ferromagnetic metals is based on the combination of a spin-dependent potential arising from the exchange scattering of conduction electrons at localized magnetic moments of the host and a common screened potential of the positive muon.[24,25] The investigation of the capability of our screened potential along this line (with incorporation of lattice dynamics) by calculating spin-density enchancement factors for electron scattering in a combined field is left for future work.

In conclusion, we have applied a sum rule to determine the screening of slow positive muons in an electron gas. We used this consistent model in three experimentally important areas (overlap parameter in quantum diffusion, longitudinal retarding force, and Knight shift) of muon interactions with metals. The obtained theoretical results are in nice agreement with different experimental predictions. The main physical conclusion is the following: our screened potential, optimized via a nontrivial sum rule, results in an almost perfect Coulombic enchancement of scattered waves at the muon site, for electron scattering at the Fermi level of metallic electron gases.

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