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Inelastic scattering of low-energy electrons in metals: the role of kinematics in screening

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Abstract

The inelastic scattering of low-energy electrons with the mobile part of the electron density of free-electron-like materials is investigated. Based on the dielectric theory for the homogeneous electron gas, the concept of Bohm and Pines is adopted in order to separate the single-particle and collective basic channels of the total inelastic rate. An effective screened potential is introduced to describe the separated single-particle part. The role of the relative motion of electrons, a kind of dynamical correlation effect, is modelled in this potential via a physical argument. The results obtained show that the nontrivial correlated motion of electrons may have a measurable influence on the result of dynamical probing of a degenerate electron gas.

1. Introduction

The dynamical probing of correlated motions of the constituents of a many-body fermion system is currently a very active subfield in physics. It is the subject of experiments based on a variety of sophisticated methods and gives a challenge for theoretical attempts [1].

It is reasonable to suppose that at very low temperatures and in pure metals the damping mechanism for an excited electron is due to inelastic transitions mediated by the coupling to electronic excitations in the target. The first theoretical work [2] for metals investigated this mechanism by using the electron gas model for the target, and the (linearized) self-consistent field approximation to characterize the excitations [3]. Experiments performed to find the lifetime [4] τ or inelastic mean free path l_{in} in free-electron-like metals show, however, remarkable and consistent deviations in comparison with this usual estimation in the low-energy range, where the role of the relative motion of electrons is expected to be important.

It is not the subject of the present theoretical work to discuss the inherent difficulties of direct measurements on these quantities. For example, a measured attenuation length may involve different effects in addition to the pure electronic one [5, 6]. We consider the mentioned deviations as *experimental* motivation for a refined calculation within a basically dielectric theory, which will also rest on the electron gas model [2].

Generally, for an interacting electron gas, the excitation spectrum is characterized by dynamical structure functions $S(q,\omega)$ [7, 8], the spacetime Fourier transforms of correlation functions. The basic electronic excitations, obtained from the density–density correlation function, consist of screened single-particle excitations (particle–hole pairs) as well as plasmons. The (linearized) self-consistent time-dependent Hartree approximation (random-phase approximation, RPA) attempts a unified characterization of these basic excitations [2, 3, 8]. The approximation treats the exact density–density response function $\chi(q,\omega)$ via its inverse; i.e., it models the dielectric function $\epsilon(q,\omega)$ of the assembly. The RPA theory contains only quite globally those details of the many-body system that are related to the relative motion and interaction of electrons. This observation provides the *theoretical* motivation for a refinement. This refinement will consider the possible influence of the relative motion of scattering electrons on measurable quantities of dynamical probing. The electron system is characterized by its density n_0; the Fermi velocity v_F and the Wigner radius r_s are $v_F = (3\pi^2 n_0)^{1/3}$ and $r_s = (1.92/v_F)$, respectively. Hartree atomic units are used throughout this work.

2. Theory and results

The inelastic mean free path (l_{in}) is defined as the distance which the intruder (or excited) particle with kinetic energy E travels within its lifetime: $l_{in} = \tau\sqrt{2E} = \tau v$ [8, 9]. The lifetime (τ) is related to the total rate of inelastic transitions that result in damping.

The perturbative description, based on the fluctuation–dissipation theorem ($S(q,\omega) \propto \operatorname{Im}\chi(q,\omega)\Theta(\omega)$), gives the standard expression [10]:

$$\frac{1}{\tau} = \frac{1}{2\pi^2}\frac{1}{v}\int_0^{\Delta E} \mathrm{d}\omega \int_{q_-}^{q^+} \mathrm{d}q\, q\, |V(q)|^2 \operatorname{Im}\chi(q,\omega), \tag{1}$$

where $\Delta E = E - E_F \geqslant 0$ at $T = 0$, due to the Pauli principle, and $q_\pm = v \pm (v^2 - 2\omega)^{1/2}$ due to the energy conservation $\omega = \boldsymbol{q}\boldsymbol{v} - q^2/2$. The basic interaction is $V(q) = 4\pi/q^2$. For our electron target system the Dyson-like form for the density–density response function, which is a physical quantity, is [8]

$$\frac{1}{\chi(q,\omega)} = \frac{1}{\chi_0(q,\omega)} + V(q), \tag{2}$$

in which $\chi_0(q,\omega)$ is the noninteracting response function, the electron–hole propagator.

By taking the prescribed imaginary part for $\chi(q,\omega)$ in equation (2) one obtains for the integrand in equation (1) the following:

$$|V(q)|^2 \operatorname{Im}\chi(q,\omega) = |V(q)|^2 \frac{\operatorname{Im}\chi_0(q,\omega)}{|1 + V(q)\chi_0(q,\omega)|^2}. \tag{3}$$

The interaction-mediated real transitions are weighted by the Lindhard dielectric function. A free electron responds, in this picture, to a well behaved common external field [1–3].

As we are interested in the possible role of the relative motion of colliding electrons at low and intermediate energies of the projectile (or excited) electron, we shall consider the electron–hole and plasmon excitations *separately*. In other words, we adopt the concept of Bohm and Pines [11]. They described the interacting electron gas as 'individual' electrons

interacting with the collective, plasmon field at long range and with one another (decoupled from the collective field) through short-range *screened* Coulomb collisions.

Therefore, by shifting the denominator of equation (3) under the first, coulombic factor, we reinterpret the obtained expression as a dynamically screened ($V_{sc}(q,\omega)$) effective interaction to single-particle excitations. The independent particles interact, in this adopted picture, via an effective potential as in the kinetic theory [8]. Of course, we shall use the complete Im $\chi_0(q,\omega)$ expression in equations (3) and (1), which is the proper kinematical factor for allowed ($T=0, \omega \geqslant 0$) real excitations.

Furthermore, and here is our physical motivation, in the small-ω range a straightforward interpretation of the effective screening to the important particle–particle collision via a static Lindhard dielectric function $V_{sc}^{RPA}(q)$ is questionable. This static screening would correspond, in a self-consistent field treatment, to the fixed-impurity case. The effect of relative motion needs a refined consideration, because the Pauli principle not only controls the kinematically allowed transitions but restricts the momentum state of the probe fermion, too. We have a 'mobile' scattering pair embedded into the system.

In order to treat this problem [12], the screened potential is now modelled as [13, 14]

$$V_{sc}(q) = \frac{4\pi}{q^2}\left[1 - \frac{\omega_p^2}{(q^2/2)^2 + b(q^2/2) + \omega_p^2}\right], \tag{4}$$

where $\omega_p^2 = 4\pi n_0 = 3/r_s^3$.

The conventional $b = (2/3)v_F^2$ value would refer to the screening of a static unit-charge impurity. By *this* value of b one could obtain pair functions which should be most appropriate for electrons with zero wavenumbers. For 'mobile' charges the $b = 2 \times (2/3)v_F^2$ modified value was deduced [12, 14]. We adopt this enhanced value of b to characterize the separated single-particle (sp) part of the damping (τ_{sp}). We note that a recent work of Holm and von Barth [15] also emphasized the need of consistent modifications in a dielectric theory for both the short- and long-range limits.

The long-range Coulomb interaction leads to a collective, *classical* mode: the plasmon in an electron gas. It is the oscillation of the electrons as a whole and reflects an overall polarization effect. In order to include this channel, here we employ the usual expression [16] for the corresponding τ_{pl}:

$$\frac{1}{\tau_{pl}} = \frac{\omega_p}{v} \ln \frac{q_c}{v - (v^2 - 2\omega_p)^{1/2}}. \tag{5}$$

Quinn's original estimation for the cut-off momentum is $q_c = (v_F^2 + 2\omega_p)^{1/2} - v_F$. Our real-space potential $V_{sc}(r)$ gives, using the standard screening-length argumentation [11], the $q_c = \omega_p/[(b/2) + \sqrt{\omega}_p]^{1/2}$ form. The two forms yield, practically, the same q_c values at metallic densities. The above expression (equation (5)) is obtained from the RPA. As is well known the plasmon pole is properly described in this simple (based on Hartree-only Green functions) approximation.

The illustrative numerical results obtained for $l_{in} = v\tau$ ($\tau^{-1} = \tau_{sp}^{-1} + \tau_{pl}^{-1}$) are exhibited in figures 1 and 2 for $r_s = 2$ and 4, respectively. The inset of figure 1 shows the inverse lifetime in units of femtoseconds (fs). The small black dots are taken from the experimental work on an Al target [4]. For further details on the role of intrinsic transport effects in these data, we refer to that work. Our results show that the proper treatment of relative motions (an inherent dynamical effect of system electrons) leads to *reduction* in the lifetime and the mean free path. At low energies (a few eV above E_F), where the influence of the relative motion is expected to be more important, the deviations are in the range of 50–60%. These *tendencies* are in accord with those found in [5] by using different methods to estimate l_{in} in the alkalis. The reduction

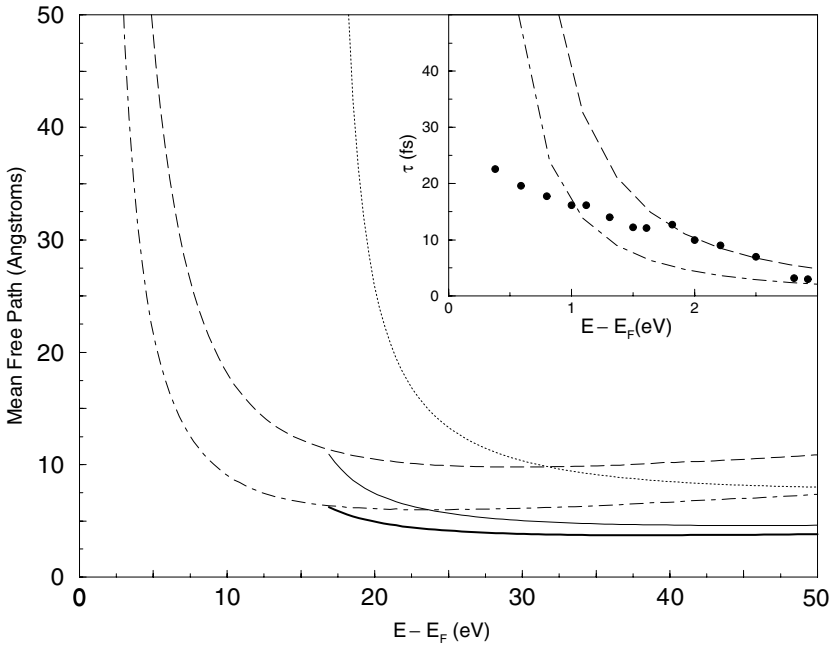

Figure 1. Numerically determined l_{in} and τ functions to characterize the inelastic electron interaction with an electron gas of $r_s = 2$. The black dots refer to 'uncleaned' experimental data obtained for an Al target [4]. Dashed and dash–dotted curves are based on τ_{sp} with $b = (2/3)v_F^2$ and $b = (4/3)v_F^2$ in equation (4), respectively. The dotted curve is based on the common τ_{pl}, Thin and thick solid curves are based on the corresponding total τ values.

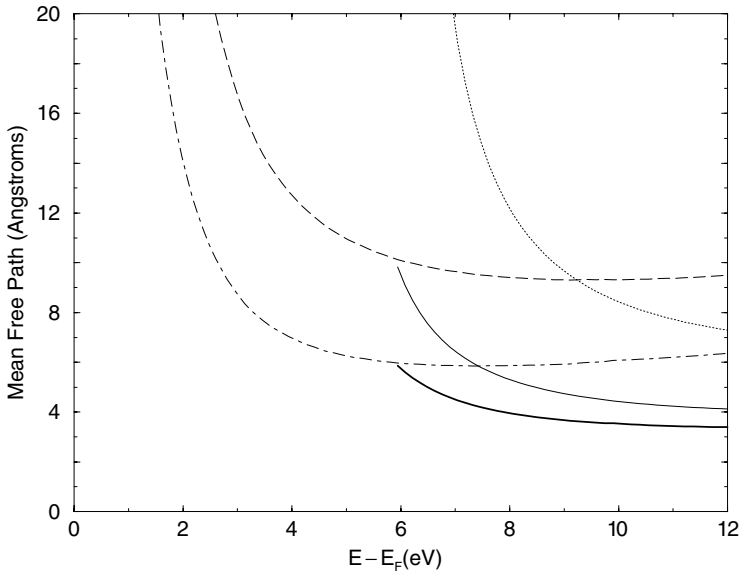

Figure 2. Theoretical l_{in} functions, at the $r_s = 4$ value of the Wigner–Seitz parameter. The meanings of the curves are the same as in figure 1.

found is due to the reduced screening in the present model. Remarkably, similar reductions in the effective screening for electron–electron interaction were deduced from a numerical simulation on electron relaxation dynamics [17], and via a consistent theoretical calculation for the (static) screened exchange energy [18]. The correctly screened interaction is one of the basic problems in many-body calculations [19].

In conclusion, based on a basically dielectric theory for the homogeneous electron gas and the concept of separated single-particle and collective density excitations, the role of electron kinematics in screening is quantified. It is found that the effect studied may have a measurable influence on the results of dynamical probing of inherent excitations.

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