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Dynamic screening of an ion in a degenerate electron gas within the second-order Born approximation

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ABSTRACT

The dynamic Friedel sum rule (FSR) is derived within the second-order Born (B2) approximation for an ion that moves in a fully degenerate electron gas and for an arbitrary spherically-symmetric electron–ion interaction potential. This results in an implicit equation for the dynamic B2 screening parameter which depends on the ion atomic number Z_1 unlike the first-order Born (B1) dynamic screening parameter reported earlier by some authors. Furthermore, for typical metallic densities our analytical results for the Yukawa and hydrogenic potentials are compared, for both positive and negative ions, to the exact screening parameters calculated self-consistently by imposing the exact dynamic FSR requirement to the scattering phase shifts. The B1 and B2 screening parameters agree excellently with the exact values at large velocities, while at moderate and low velocities the B1 approximation deviates from the exact solution whereas the B2 approximation still remains close to it. In addition, a Padé approximant to the Born series yields a further improvement of the perturbative approach, showing an excellent agreement on the whole velocity range in the case of antiprotons.

1. Introduction

The dynamic screening of swift heavy charged particles in condensed matter is a phenomenon that is important to understand the electronic stopping power and related projectile-target interaction properties. The screening experienced by an intruder charge arises from the electron density induced in the traversed medium and affects the stopping properties of the particles. It is therefore of interest to determine how this screening effect varies with the projectile velocity.

An approach commonly used to describe dynamic screening effects is based on the dynamic Friedel sum rule (FSR) proposed in [1,2] which uses the concept of the shifted Fermi sphere [3]. This rule is very useful to adjust in a self-consistent way the electron–ion interaction potential and the related screening length. In this paper we study the dynamic FSR for a point-like ion that moves in a fully degenerate electron gas (DEG) within the framework of the second-order Born (B2) approximation. The Born approximation has been previously used in conjunction with the static [4] or dynamic FSR [1,2], but only within the first-order Born (B1) approximation. This is somewhat unsatisfactory because the resulting B1 screening length is independent of the ion atomic number and is therefore identical for a particle and its antiparticle. Recently, the static screening length has been deduced within the B2 approximation [5,6]. The static B2 screening lengths pertaining to protons and antiprotons agree satisfactorily with the exact numerical solutions at electron densities typical of metals. In this context, our main purpose is to go beyond the B1 approximation, and consider the B2 approximation for the dynamic FSR. This generalizes the previous results obtained within the static B1 [4] or B2 [5,6] and the dynamic B1 approximations [1,2] and hence furnishes useful numerical estimates of the influence of both the ion charge and its velocity on the screening length in a DEG.

2. Self-consistent formulation of the dynamic FSR

Let us revisit the dynamic FSR first formulated by Nagy and Bergara [1] and later studied in more detail by Lifschitz and Arista [2] for a DEG. To this end, consider an ion with charge $Z_1 e$ (Z_1 is the ion atomic number) and constant velocity $\mathbf{v}$ that moves through a DEG of density n_e [Fermi wave number $k_F = (3\pi^2 n_e)^{1/3}$]. An elec-

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tron whose wave vector is $\mathbf{k}_e$ collides elastically with the ion. The relative velocity of the colliding particles is denoted as $\mathbf{v}_r = \mathbf{v}_e - \mathbf{v}$, where $\mathbf{v}_e = \hbar\mathbf{k}_e/m_e$ is the electron's initial velocity. The relative wave vector is $\mathbf{k}_r = \mathbf{k}_e - \mathbf{k}$ with $\mathbf{k} = m_e\mathbf{v}/\hbar$ (note that $\mathbf{k}$ is not the wave vector of the ion). In the center of mass (c.m.) frame of reference the wave function of the incoming free electron is $\phi_{\mathbf{k}_r}(\mathbf{r}) = e^{i\mathbf{k}_r\cdot\mathbf{r}}$ whereas its wave function after the collision is given by the partial-wave expansion (see, e.g., [7])

$$\psi_{\mathbf{k}_r}(\mathbf{r}) = \sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)\,e^{i\delta_\ell(k_r)}\,\mathfrak{R}_{k_r,\ell}(r)P_\ell(\cos\theta), \quad (1)$$

where $\mathfrak{R}_{k_r,\ell}(r)$ and $\delta_\ell(k_r)$ are, respectively, the radial wave function and the scattering phase shifts corresponding to the angular momentum ℓ and depending only on k_r (the modulus of $\mathbf{k}_r$), θ is the scattering angle in the c.m. reference frame (i.e., the angle between $\mathbf{k}_r$ and $\mathbf{r}$), and P_ℓ are the Legendre polynomials.

Following [1] we introduce now the electron density induced in the DEG by the moving ion

$$n_{\mathrm{ind}}(\mathbf{r}) = \frac{2}{(2\pi)^3}\int_{k_e\leqslant k_F}\left(|\psi_{\mathbf{k}_r}(\mathbf{r})|^2 - |\phi_{\mathbf{k}_r}(\mathbf{r})|^2\right)d\mathbf{k}_e, \quad (2)$$

where the integration is performed in the domain $k_e \leqslant k_F$ as a consequence of the Pauli exclusion principle. Let us stress that $n_{\mathrm{ind}}(\mathbf{r})$ is not isotropic because of the motion of the ion. This fact is expressed in averaging of the induced density with respect to the unit-step distribution function of a DEG in the laboratory frame of reference (wave vector $\mathbf{k}_e$) while $|\psi_{\mathbf{k}_r}(\mathbf{r})|^2$ and $|\phi_{\mathbf{k}_r}(\mathbf{r})|^2$ are calculated in the c.m. reference frame. In the case of an ion at rest $\mathbf{k}_r = \mathbf{k}_e$ and Eq. (2) becomes the equation addressed by Friedel in [8], which yields the well-known static FSR [8] and an isotropic induced electron density.

Next we calculate the total charge induced in a spherical volume Ω_R around the ion, which is $Q_{\mathrm{ind}} = -eN_{\mathrm{ind}}(v)$ with

$$N_{\mathrm{ind}}(v) = \int_{\Omega_R} n_{\mathrm{ind}}(\mathbf{r})\,d\mathbf{r} = \frac{2}{(2\pi)^2}\int_{k_e\leqslant k_F} A(k_r)\,\frac{d\mathbf{k}_e}{k_r^2}, \quad (3)$$

where R (with $R\to\infty$) is the radius of the volume Ω_R and

$$A(k_r) = \frac{k_r^2}{2\pi}\int_{\Omega_R}\left(|\psi_{\mathbf{k}_r}(\mathbf{r})|^2 - |\phi_{\mathbf{k}_r}(\mathbf{r})|^2\right)d\mathbf{r}; \quad (4)$$

notice that the function $A(k_r)$ differs from the definition adopted in [9,1] by a factor $k_r^2/2\pi$. From Eqs. (1) and (4) it is seen that $A(k_r)$ is isotropic and depends only on k_r. This enables the angular integration in Eq. (3) which results in

$$N_{\mathrm{ind}}(v) = \frac{2}{\pi}\left\{\Theta(k_F-k)\int_0^{k_F-k}A(q)\,dq + \frac{1}{4k}\int_{|k-k_F|}^{k+k_F}\left[k_F^2-(k-q)^2\right]A(q)\,\frac{dq}{q}\right\}, \quad (5)$$

$\Theta(\kappa)$ is the Heaviside unit-step function. The quantity $A(q)$ can be evaluated in closed form using Servadio's general relation [9]. When $R\to\infty$ this function can be expressed through the scattering amplitude $f(q,\theta)$ as follows

$$A(q) = \frac{\partial}{\partial q}[qf^*(q,0)] + i\int_0^{\pi} qf(q,\theta)\,\frac{\partial}{\partial q}[qf^*(q,\theta)]\sin\theta\,d\theta \quad (6)$$

$$= \sum_{\ell=0}^{\infty}(2\ell+1)\,\delta'_\ell(q). \quad (7)$$

Here $f(q,0)$ is the scattering amplitude for $\theta=0$, the asterisc denotes complex conjugation and the prime indicates derivation with respect to the argument. The second part of Servadio's relation, Eq. (7), is easily found by substitution of the partial-wave expansion of the scattering amplitude (see, e.g., [7]) into Eq. (6).

At this point we impose the condition that the intruder ion has to be completely screened at large distances, $Z_1e + Q_{\mathrm{ind}} = 0$, which serves as the basic constraint for the scattering theory. It was first suggested by Friedel [8] and can be viewed as the conservation of the total charge of a many-electron system. In this sense the FSR is similar to the optical theorem of scattering theory [7] which requires the conservation of particle number (for inelastic scattering the number of the particles participating in the elastic scattering). Using Eq. (5) the condition of complete screening can be rewritten in the explicit form

$$Z_1 = N_{\mathrm{ind}}(v) \quad (8)$$

with $v = \hbar k/m_e$. If the projectile carries with it N_b bound electrons, in Eq. (8) one should simply replace Z_1 with $Z_1 - N_b$ [8]. In order to represent the dynamic FSR, Eq. (8), in a more familiar form (as a sum over partial waves) we insert Eq. (7) into Eq. (5) and integrate by parts assuming that $\delta_\ell(0)=0$, which yields

$$Z_1 = \frac{2}{\pi}\sum_{\ell=0}^{\infty}(2\ell+1)\,\Delta_\ell(v) \quad (9)$$

with the "dynamic phase shifts"

$$\Delta_\ell(v) = \frac{1}{4k}\int_{|k-k_F|}^{k+k_F}\left(1+\frac{k_F^2-k^2}{q^2}\right)\delta_\ell(q)\,dq. \quad (10)$$

Eqs. (9) and (10) are identical to the "extended" FSR of Lifschitz and Arista [2] for a DEG, which was deduced having recourse to geometrical arguments about the Galilean transformation of the Fermi sphere. The extension of the dynamic FSR to an electron gas at high temperature has been outlined by Nagy and Bergara [1].

It is straightforward to see that in the limit $v\to 0$ Eq. (10) reduces to $\Delta_\ell(0) = \delta_\ell(k_F)$ which together with Eq. (9) constitutes the static FSR [8]. In the high-velocity limit, within the leading order from Eq. (10) one gets $\Delta_\ell(v) = (v_F^2/3v^2)k_F\delta'_\ell(k)$, where $v_F = \hbar k_F/m_e$ is the Fermi velocity [2]. Interestingly, the dynamic phase shifts are expressed in the high-velocity regime through the momentum derivative of the ordinary phase shifts.

3. First- and second-order Born approximations

With the theoretical formalism presented in Section 2, we take up the main topic of this paper, namely to study the dynamic FSR for a point-like ion moving in a DEG within up to the B2 approximation. Hence we look for the scattering amplitude in Eq. (6) in a perturbative manner writing $f = f_{B1} + f_{B2}$, where f_{B1} and f_{B2} are the first- and second-order scattering amplitudes, respectively. Similarly, we expand Servadio's function perturbatively to the second order, $A = A_{B1} + A_{B2}$. Introducing in Eq. (7) the corresponding expansion of the phase shifts, $\delta_\ell = \delta_{\ell,B1} + \delta_{\ell,B2}$, we get with the help of Eq. (19) in [6]

$$A_{B1}(q) = \frac{\partial}{\partial q}\{qf_{B1}(q,0)\}, \quad (11)$$

$$A_{B2}(q) = \frac{\partial}{\partial q}\{q\,\mathrm{Re}[f_{B2}(q,0)]\}, \quad (12)$$

where $f_{B1}(q,0)$ and $f_{B2}(q,0)$ are the B1 and B2 forward-scattering amplitudes. Then, using Eqs. (23) and (26) in [6] we arrive at

$$A_{B1}(q) = -\frac{m_e}{2\pi\hbar^2}\,\widetilde{V}(0), \quad (13)$$

$$A_{B2}(q) = \frac{4m_e^2}{(2\pi)^3\hbar^4}\int_0^{\infty}\widetilde{V}^2(\kappa)\,\frac{\kappa^2\,d\kappa}{\kappa^2-4q^2}, \quad (14)$$

where $\widetilde{V}(q)$ is the Fourier transform of the electron–ion interaction potential $V(r)$ given by

$$\widetilde{V}(q) = \int_0^{\infty} V(r)j_0(qr)4\pi r^2\,dr \quad (15)$$