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Local Field Correction Effect on Dicluster Stopping Power in a Strongly Coupled Two-Dimensional Electron Gas System

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Abstract

We calculate the stopping power for heavy-ion diclusters moving in a strongly coupled two-dimensional electron gas system by using the local field corrected dielectric function at finite temperature. We obtain a parameterized local field correction factor based on a relation between the thermal compressibility and exchange-correlation energy in two-dimension. The interpolated parameter is derived from the Monte-Carlo data for the exchange-correlation energy of a two-dimensional electron gas system. We compare our results with those of previous calculations which used a local field factor that satisfied the compressibility sum rule in three-dimension. In general, the stopping power increases by taking into account the short-range interactions. In addition, it is found that the dicluster stopping power (in particular the uncorrelated part) obtained from our calculations is smaller than the previous work.

Keywords: Stopping power; Dicluster; Local field correction; Finite temperature; Monte-Carlo

Introduction

In recent years, the phenomena related to the interaction of particles (atoms, molecules, electrons, neutrons,…) with plasma and condensed matter systems have been attracted the attention of many scientists [1-20]. Projectile ions moving through a dense target or near a solid surface may lose their energy mainly due to the interaction with the nucleus or electrons. Stopping power which is defined as the mean energy loss per unit path can be used to characterize these physical processes. The electronic stopping power for the single-ion and cluster-ion projectiles passing through the three and two dimensional electron gas (3DEG and 2DEG) systems has been investigated by several authors [21-26]. In a strongly coupled 2DEG, the stopping power of heavy-ion diclusters which composed of two point-like charges was theoretically studied by Ballester et al. [27]. They computed the polarizational stopping power from the imaginary part of the dielectric function for both fast and slow projectiles at zero and finite temperatures. In addition, they went beyond the random-phase-approximation (RPA) and considered the effect of the exchange-correlation (XC) interaction which is expected to be important in the strongly coupled systems. In their work, the short range electron-electron interactions were included by introducing an interpolated expression for the static local field

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correction (LFC) factor which satisfies the compressibility sum rule. They used an interpolation parameter which was determined from an equation relating the thermal compressibility to the XC energy per electron in a 3DEG [28]. However, their formula for the XC energy was derived from the Totsuji Monte-Carlo results for a 2DEG system [29].We believe that the correct analytical expression for the LFC factor in a 2DEG is obtained from a relation between the 2D (not 3D) compressibility and the XC energy per electron.

Here, we follow the method outlined in Ref. [27] but make use of the correct parameterized 2D LFC to calculate the electronic stopping power of a slow dicluster-ion in a 2DEG system at high temperatures.

The outline of this paper is as follows. In section 2, we review the theory of the dicluster stopping power based on the dielectric function formalism. Also, the interpolation method that we use to obtain the 2D LFC factor is introduced in this section. Finally the results of our calculations are given in section 3 and discussed there.

Materials and Methods

1. Stopping Power Formalism

We consider heavy-ion diclusters consisting of two point-like charges Z_1e and Z_2e moving with a velocity V randomly oriented in the plane of a 2DEG. with an inter-ion separation vector **R**. We suppose that the diclusters are randomly oriented in the plane of a 2DEG and moving with a velocity V. Because of heavy projectile approximation, we can assume the projectile trajectory to be a straight line. The corresponding surface charge distribution, σ, is given by [26]:

$$\sigma(\mathbf{k}) = Z_1 e + (Z_2 e) e^{i\mathbf{k}.\mathbf{R}} \quad (1)$$

where $\mathbf{k}$ is a 2D wave vector. Using the linear-response dielectric theory, the dicluster stopping power is then obtained as [26]:

$$-\frac{dw}{dx} = \frac{2e^2}{\pi v}\int_0^{+\infty} dk \int_0^{kv} \frac{\omega d\omega}{\sqrt{(kv)^2-\omega^2}} \mathrm{Im}\left(-\frac{1}{\varepsilon(k,\omega)}\right) \left[Z_1^2 + Z_1^2 + 2Z_1 Z_2 \cos(\mathbf{k}.\mathbf{R})\right] \quad (2)$$

Here $\varepsilon(k,\omega)$ is the dynamic dielectric function of a 2DEG system.

The above expression for stopping power can be divided into two parts; uncorrelated and correlated parts:

$$-\frac{dw}{dx} = (-\frac{dw}{dx})_{uncorr} + (-\frac{dw}{dx})_{corr} \quad (3)$$

The uncorrelated contribution which is independent of the inter-ion distance defined as:

$$(-\frac{dw}{dx})_{uncorr} = \frac{2e^2}{\pi v}(Z_1^2 + Z_2^2) \int_0^{\infty} dk \int_0^{kv} d\omega \frac{\omega}{\sqrt{(kv)^2-\omega^2}} \mathrm{Im}\left(-\frac{1}{\varepsilon(k,\omega)}\right) \quad (4)$$

By taking the average over in-plane **R** orientations

$$\frac{1}{2\pi}\int_0^{2\pi} \cos(kR\cos\theta) d\theta = J_0(kR) \quad (5)$$

we can write the following expression for the correlated part:

$$(-\frac{dw}{dx})_{corr} = \frac{2e^2}{\pi v}(2Z_1 Z_2) \int_0^{\infty} dk \int_0^{kv} d\omega \frac{\omega J_0(kR)}{\sqrt{(kv)^2-\omega^2}} \mathrm{Im}\left(-\frac{1}{\varepsilon(k,\omega)}\right) \quad (6)$$

where J_0 is the usual first-kind Bessel function. The dielectric function of a 2DEG system which includes the short range XC corrections is given by [30]:

$$\varepsilon(\mathbf{k},\omega) = 1 + \frac{\phi(\mathbf{k})\,\chi_0(\mathbf{k},\omega)}{1-\phi(\mathbf{k})\,G(\mathbf{k})\,\chi_0(\mathbf{k},\omega)} \quad (7)$$

Here $\phi(\mathbf{k}) = 2\pi e^2/k$, $\chi_0(\mathbf{k},\omega)$ and $G(\mathbf{k})$ are the 2D Coulomb potential, non-interacting polarizability (Lindhard) function and static LFC factor, respectively. By defining $\chi_0 = \chi_0' + i\chi_0''$, we get the following relation for the imaginary part of inverse dielectric function:

$$\mathrm{Im}\left(\frac{-1}{\varepsilon(\mathbf{k},\omega)}\right) = \frac{\phi(\mathbf{k})\chi_0''(\mathbf{k},\omega)}{\left[1+\phi(\mathbf{k})\chi_0'(\mathbf{k},\omega)\right]^2 + \left[\phi(\mathbf{k})H(\mathbf{k})\chi_0''(\mathbf{k},\omega)\right]^2} \quad (8)$$

The RPA limit is recovered by setting $H(\mathbf{k}) = 1$. The Lindhard function in two-dimension [31] is obtained from:

$$\chi_0(\mathbf{k},\omega) = \lim_{\eta\to 0}\iint \frac{d^2q}{(2\pi)^2}\frac{n(\mathbf{q}+\mathbf{k})-n(\mathbf{q})}{\varepsilon(\mathbf{q}+\mathbf{k})-\varepsilon(\mathbf{q})-\hbar\omega-i\eta} \quad (9)$$

where $n(\mathbf{q})$ being the Fermi-Dirac distribution function, $\varepsilon(\mathbf{q}) = \hbar^2 q^2/2m$, m is the electron mass and η is an infinitesimal small positive number. After some algebra, one gets the following simple relation for the finite temperature Lindhard function:

$$\chi_0(\mathbf{k},\omega) = \frac{k_F^2}{2\pi k_B T}\left[1 - 2Ue^{-U^2}\psi(U) + i\sqrt{\pi}Ue^{-U^2}\right] \quad (10)$$

where $\psi(U) = \int_0^U e^{t^2} dt$, $U = \omega / kv_{th}$, $v_{th} = \sqrt{2k_B T/m}$, k_F being the Fermi wave vector and k_B is the Boltzmann constant.

At finite temperature, it is common to define two characteristic quantities in the degenerate electron gas; the coupling parameter, Γ:

$$\Gamma = \frac{e^2}{a k_B T} \quad (11)$$

and the degeneracy parameter, D:

$$D = \frac{E_F}{k_B T} \quad (12)$$

where a and E_F are the Wigner-Seitz radius and Fermi energy, respectively. The strongly coupled regime is determined by value of Γ higher than unity.

As it is mentioned in the previous section, we are interested in the case of high temperatures and slow diclusters i.e. the projectile velocity, v, is smaller than the Fermi velocity, v_F. Under these conditions, the uncorrelated and correlated parts of stopping power are given by [27]:

$$\left(-\frac{dw}{dx}\right)_{uncorr} = \frac{\hbar v k_D \sqrt{\pi}(Z_1^2 + Z_2^2)}{a_B}\int_0^\infty \frac{x^2 e^{-x^2} dx}{\left[x + \Gamma\sqrt{D/2}H(x/\sqrt{D})\right]^2} \quad (13)$$

and

$$\left(-\frac{dw}{dx}\right)_{corr} = \frac{2\hbar v k_D \sqrt{\pi} Z_1 Z_2}{a_B}\int_0^\infty \frac{x^2 e^{-x^2} J_0(\bar{R}x) dx}{\left[x + \Gamma\sqrt{D/2}H(x/\sqrt{D})\right]^2} \quad (14)$$

where $k_D = e^2 k_F^2 / k_B T$, $\bar{R} = 2R / \sqrt{\hbar^2 / 2mk_B T}$ and a_B is the Bohr radius. The spatial correlation between two ions is taken into account in the expression for correlated stopping. The vicinage function, γ, which is defined as the ratio of correlated to uncorrelated parts of stopping power

$$\gamma = \frac{(-dw/dx)_{corr}}{(-dw/dx)_{uncorr}} \quad (15)$$

measures the interference effects on the energy loss of a cluster.

2. Interpolated Expression for LFC

In order to calculate the short range interactions effects on the stopping power, we introduce the interpolation method which we use to obtain the correct 2D LFC factor, $G^{2D}(\mathbf{k})$. Following the work of [27], we consider the below parameterized expression for the LFC factor

$$G^{2D}(\mathbf{k}) = \frac{A^{2D}(k/k_F)}{1 + A^{2D}(k/k_F)} \quad (16)$$

This relation reproduces the asymptotic behavior of the LFC at both short and long wavelengths. The interpolation parameter, A^{2D}, can be determined via the compressibility sum rule [28]

$$A^{2D} = \frac{1}{\sqrt{2}\Gamma}\left(1 - \frac{\kappa_0^T}{\kappa^T}\right) \quad (17)$$

where $\kappa_0^T = 1/nk_B T$ and κ^T is the finite temperature compressibility of the interacting electron gas system. Here, we make use of the correct relation between κ^T and the XC energy per electron, E_{xc}, for a 2DEG system [28]:

$$\frac{1}{\kappa^T} = nk_B T\left[1 + \frac{E_{xc}}{2k_B T} + \frac{\Gamma}{4}\frac{d}{d\Gamma}\left(\frac{E_{xc}}{k_B T}\right)\right] \quad (18)$$

And from it, the correct expression for A^{2D} can be obtained as follows:

$$A^{2D} = -\frac{\left(E_{xc}(\Gamma)/k_B T\right) + \frac{\Gamma}{2}\frac{d}{d\Gamma}\left(E_{xc}(\Gamma)/k_B T\right)}{2\sqrt{2}\Gamma} \quad (19)$$

Using the Totsuji Monte-Carlo data for 2D XC energy per electron [29]

$$E_{xc}(\Gamma) = k_B T(-1.12\Gamma + 0.71\Gamma^{1/4} - 0.38) \quad (20)$$

which is valid for $\sqrt{2} < \Gamma < 50$, we are able to calculate the correct parameterized 2D LFC factor.

Results and Discussions

We are ready to perform the numerical calculations on the dicluster stopping power for a strongly coupled 2DEG system at low velocities and finite temperatures. We assume that the dicluster consists of two identical ions $Z_1 = Z_2$ which are separated by a distance R .

First, we plot the correct static 2D LFC, G^{2D}, for two different values of coupling parameter, $\Gamma = 2$ and 10 , in Fig. 1. For comparison, we also show the interpolated LFC factor proposed in Ref. [27] which we refer to as G^{B} in our figures.

As this figure shows, although the values of G^{2D} are up to 10% smaller than those of G^{B}, the change of coupling parameter has a small effect on both LFC factors.

In Fig. 2, we display the ratio of the local field corrected to the RPA stopping power of a dicluster-ion projectile as a function of Γ for two different values of the degeneracy parameter, D . Again we compare our results (based on the G^{2D}) with those obtained from the Ref. [27]. According to this figure, the inclusion of the short range interactions in the calculations enhances the stopping power and this effect become more important at large coupling parameter and high degeneracy parameter. Also, it can be observed that the stopping power calculated via G^{B} is greater than those computed using G^{2D} as expected from the results of Fig. 1.

We compare the vicinage functions, γ, calculated within three different approaches, G^{2D}, G^{B} and $G = 0$ (RPA) in a 2DEG system for $\Gamma = 2$ and $D = 0.01$ in Fig. 3. As shown in this figure, the

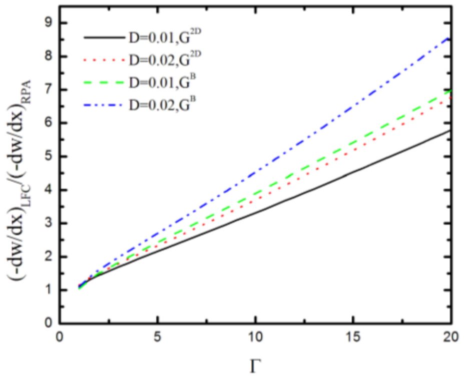

Figure 2. The ratio of local field corrected (both G^{2D} and G^{B}) to RPA stopping powers of a dicluster in a 2DEG system with R=1nm and for two different values of degeneracy parameter, D=0.01 and 0.02.

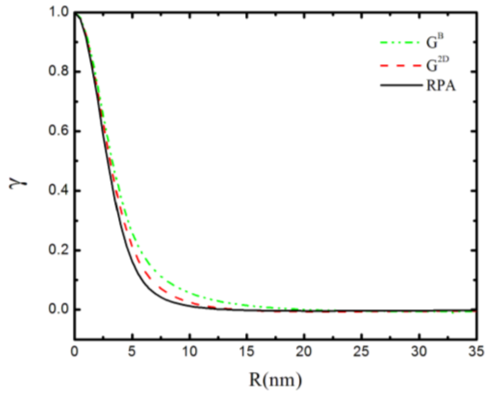

Figure 3. The vicinage function of a dicluster-ion moving in a 2DEG as a function of inter-ion distance R calculated within three different static LFC factors, G^{2D}, G^{B} and G=0 (RPA) with R=1nm and for D=0.01.

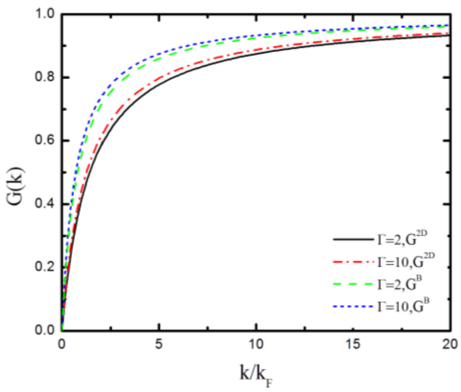

Figure 1. Two different interpolated static LFC of the 2DEG as functions of k/k_F for two distinct values of coupling parameter, Γ=2 and 10.

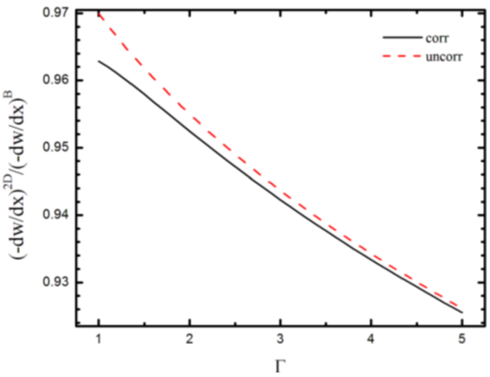

Figure 4. The ratio of the correlated (uncorrelated) part of stopping obtained from G^{2D}, $(-dw/dx)^{2D}$, to the corresponding one calculated from G^{B}, $(-dw/dx)^{B}$, as functions of coupling parameter, Γ, with R=1nm and for D=0.01.

vicinage function increases by considering the XC interaction between electrons. Furthermore, the difference between the G^{2D} and G^{B} results is small.

In order to discover which part of the dicluster stopping power, the correlated contribution or uncorrelated one, is more sensitive to the change of LFC factor, we display the ratio of the correlated (uncorrelated) stopping obtained from the G^{2D} calculations, $(-dw/dx)^{2D}$, to the corresponding one given by G^{B}, $(-dw/dx)^{B}$, in Fig. 4. As this figure indicates, the uncorrelated part of stopping power is more affected by the LFC expression than the uncorrelated one, specially for small coupling parameters.

In conclusion, we investigate the effect of a parameterized static LFC factor which satisfies the compressibility sum rule in two-dimension on the dicluster stopping power in a 2DEG system at high temperatures. The interpolation parameter is derived from the Monte-Carlo data. We make a comparison with the results of Ref. [27] which is based on a formula for the 3DEG compressibility. We find that the stopping power increases by including the LFC factor in the dielectric function, although this enhancement is smaller when the correct 2D LFC is used.

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