Dynamical local field corrections on energy loss in plasmas of all degeneracies

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Random phase approximation (RPA) has become one of the most used methods to describe the energy loss of charged particles in plasmas. The RPA is usually valid for high-velocity projectiles and in the weak coupling limit of the electron gas. However, for partially coupled plasmas RPA is not sufficient and the electronic coupling must be taken into account. This coupling can be considered through local field corrections. In this work, we have constructed a dynamical local field correction (DLFC) function from Mermin dielectric function. This DLFC function has the advantage to describe plasmas at any degeneracy. Mermin DLFC function is compared with other DLFC functions from the literature in the energy loss calculation. We see important differences between them; they are significant at low velocities and very relevant around the maximum, almost 30%.

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The energy loss of charged particles in plasmas is a topic of relevance to understand the energy deposition in the contexts of a particle driven in the inertial confinement fusion (ICF) [1,2]. Dielectric formalism has become one of the most used methods to describe this energy loss. The use of this formalism was introduced by Fermi [3] and large number of calculations have been carried out since then using the random phase approximation (RPA) (see [4] for a complete list). The RPA is usually valid for high-velocity projectiles and in the weak coupling limit of the electron gas. But for partially coupled plasmas, which are subject of much interest for current studies of ICF, RPA is not sufficient and the electronic coupling must be taken into account. The aim of this work is to study the influence of the plasma coupling on the energy loss of a proton moving through a plasma at any degeneracy. The nonlinear coupling effects are beyond the scope of this Brief Report.

Dielectric formalism is based on the dielectric function of the target medium. First, we are going to calculate this dielectric function in the random phase approximation provided by a consistent quantum mechanical analysis. Using atomic units (a.u.), $e=\hbar=m_e=1$, to simplify formulas, we obtain [5]

$$\epsilon(k,\omega) = 1 + \frac{1}{\pi^2 k^2}\int d^3k' \frac{f(\vec{k}+\vec{k}') - f(\vec{k}')}{\omega + i\nu - (E_{\vec{k}+\vec{k}'} - E_{\vec{k}'})}, \quad (1)$$

where $E_{\vec{k}}=k^2/2$. The temperature dependence is included through the Fermi-Dirac function

$$f(\vec{k}) = \frac{1}{1+\exp[\beta(E_k-\mu)]}, \quad (2)$$

being $\beta=1/k_BT$ and μ the chemical potential of the plasma with electron density n_e and temperature T. In this part of the analysis we assume the absence of collisions so that the damping constant approaches zero, $\nu\to 0^+$.

Dielectric function can be separated into its real and imaginary parts,

$$\epsilon(k,\omega) = \epsilon_r(k,\omega) + i\epsilon_i(k,\omega). \quad (3)$$

$\epsilon_r(k,\omega)$ can be directly obtained from Eq. (1) [6],

$$\epsilon_r(k,\omega) = 1 + \frac{1}{4z^3\pi k_F}[g(u+z) - g(u-z)], \quad (4)$$

where $g(x)$ corresponds to

$$g(x) = \int_0^\infty \frac{ydy}{\exp(E_F\beta y^2 - \beta\mu) + 1} \ln\left|\frac{x+y}{x-y}\right|, \quad (5)$$

and $u=\omega/kv_F$ and $z=k/2k_F$ are the common dimensionless variables [5]. $v_F=k_F=\sqrt{2E_F}=(3\pi^2 n_e)^{1/3}$ is the Fermi velocity in a.u.

The function $\epsilon_i(k,\omega)$ also follows from Eq. (1) [6–8]:

$$\epsilon_i(k,\omega) = \frac{1}{8z^3k_F}\theta \ln\left(\frac{1+\exp[\beta\mu - E_F\beta(u-z)^2]}{1+\exp[\beta\mu - E_F\beta(u+z)^2]}\right). \quad (6)$$

However, as mentioned before, the RPA is not sufficient to describe partially coupled plasmas, where electron coupling interactions must be taken into account. These interactions could be considered through the local field corrections (LFCs), and then the target dielectric function is modified as

$$\epsilon_{\mathrm{LFC}}(k,\omega) = 1 - \frac{[1-\epsilon(k,\omega)]}{1+[1-\epsilon(k,\omega)]G(k,\omega)}, \quad (7)$$

where $\epsilon(k,\omega)$ is the RPA dielectric function obtained before and $G(k,\omega)$ is the local field correction function. Mostly static local field corrections (SLFC), $G(k)=G(k,0)$, have been proposed in the past, as it was considered that the greater part of the LFCs would succeed for the static limit, $\omega=0$.

Pathak and Vashista [9] developed an SLFC function, which took into account the exchange and the correlation contributions, demanding that the dielectric function should fulfill the third-order frequency sum rule, which resulted in

$$G_{\mathrm{PV}}(k) = -\frac{1}{n_e}\int \frac{dq}{(2\pi)^3}\frac{(qk)^2}{q^4}\frac{V(k)}{V(q)}[S(q-k) - S(k)], \quad (8)$$

where the static structure factor is

$$S(k) = \int \frac{d\omega}{n_e \pi V(k)} \frac{\mathrm{Im}\ \epsilon_{\mathrm{LFC}}^{-1}(k,\omega)}{1-\exp(-\beta\omega)}, \tag{9}$$

$\beta = 1/k_B T$ is the inverse temperature and $V(k) = 4\pi/k^2$ is the Coulomb potential. This provides a self-consistent problem in solving the dielectric function and the static structure factor.

However, this procedure does not satisfy the compressibility sum rule, and is in need of nonlinear integral equations and computer simulations to obtain the SLFC. For coupled electron liquids, it is possible to derive a parametrized expression, which accurately fits the results of the self-consistent formulation. On the suggestion of their microscopic calculations, Ichimaru and Utsumi (IU) [10] adopted the formula

$$G_{\mathrm{IU}}(k) = \frac{Ak^4}{k_F^4} + \frac{Bk^2}{k_F^2} + C + \left[\frac{Ak^4}{k_F^4} + \left(B + \frac{8}{3}\right)\frac{k^2}{k_F^2} - C\right]\frac{4k_F^2 - k^2}{4kk_F} \ln\left|\frac{2k_F + k}{2k_F - k}\right|. \tag{10}$$

The parameters are $A = 0.029$, $B = \frac{9}{16}\gamma_0 - \frac{3}{64}(1-g_0) - \frac{16}{15}A$ and $C = \frac{-3}{4}\gamma_0 + \frac{9}{16}(1-g_0) - \frac{16}{5}A$, where

$$g_0 = \frac{1}{8}\left(\frac{z}{I(z)}\right), \tag{11}$$

and $I(z)$ is the modified Bessel function of the first order of $z = 4(\alpha r_s/\pi)^{1/2}$, with $\alpha = (4/9\pi)^{1/3}$ and $r_s = (3/4\pi n_e)^{1/3} me^2/\hbar^2$. Also γ_0 is defined as

$$\gamma_0 = \frac{1}{4} - \frac{\pi\alpha r_s^5 b_0}{24}\frac{d}{dr_s}\left(\frac{r_s^{-3} + b_1 r_s^{-2.5}}{1 + b_1 r_s^{0.5} + b_2 r_s + b_3 r_s^{1.5}}\right), \tag{12}$$

where $b_0 = 0.062\,1814$, $b_1 = 9.813\,79$, $b_2 = 2.822\,24$, and $b_3 = 0.736\,411$.

Nevertheless, in [11] it was shown that one cannot construct a SLFC which fulfills the compressibility and the third-order sum rules. Therefore, the concentration was mostly focused on the construction of dynamical local field corrections (DLFC), $G(k,\omega)$. Then Yan *et al.* [12] proposed a parametrization that takes into account the asymptotic behaviors of the DLFC in their frequency dependence

$$\lim_{\omega\to 0} G(k,\omega) = G_{\mathrm{IU}}(k), \tag{13}$$

$$\lim_{\omega\to\infty} G(k,\omega) = G_{\mathrm{PV}}(k). \tag{14}$$

The proposed formula for $G(k,\omega)$, satisfying these two constraints, is

$$G_Y(k,\omega) = \frac{\omega G_{\mathrm{PV}}(k) + i\omega_p G_{\mathrm{IU}}(k)}{\omega + i\omega_p}. \tag{15}$$

Dabrowski [13] proposed another parametrization for the DLFC function, $G_D(k,\omega)$, which imaginary part could be calculated as

$$\mathrm{Im}\ G_D(k,\omega) = \frac{a(k)\omega}{(1 + b(k)\omega^2)^{5/4}}, \tag{16}$$

where

$$a(k) = Ck^2\left(\frac{G_{\mathrm{IU}}(k) - G_{\mathrm{PV}}(k)}{CDk^2}\right)^{5/3}, \tag{17}$$

$$b(k) = \left(\frac{G_{\mathrm{IU}}(k) - G_{\mathrm{PV}}(k)}{CDk^2}\right)^{4/3}, \tag{18}$$

and $D \simeq 0.763$. The real part, $\mathrm{Re}\ G_{\mathrm{D}}(k,\omega)$, is obtained by the use of the Kramers-Kronig relation. Then,

$$G_D(k,\omega) = \mathrm{Re}\ G_D(k,\omega) + i\ \mathrm{Im}\ G_D(k,\omega). \tag{19}$$

Other DLFC functions have been established since then, as [14], but they are not easy to handle. Here in this work, we propose an easy DLFC function obtained from the Mermin dielectric function. Mermin [15] derived an expression for the dielectric function, taking into account the target electron coupling and preserving the local particle density. We have successfully applied this dielectric function to solids [16] and to plasmas [17]. Mermin dielectric function $\epsilon_M(k,\omega)$, in terms of the wave number k and of the frequency ω, can be written as

$$\epsilon_M(k,\omega) = 1 + \frac{(\omega + i\nu)[\epsilon(k,\omega+i\nu) - 1]}{\omega + i\nu[\epsilon(k,\omega+i\nu) - 1]/[\epsilon(k,0) - 1]}, \tag{20}$$

where $\epsilon(k,\omega)$ is the RPA dielectric function from Eq. (3). Electron interactions are considered through their collision frequency, ν. It is easy to see that when $\nu \to 0$, Mermin dielectric function reproduces the RPA one. The collision frequency ν in solids can be determined experimentally, but in plasmas, nowadays, it must be calculated theoretically [18]. To obtain the Mermin DLFC function, we consider Mermin dielectric function as the DLFC dielectric function in Eq. (7), then

$$G_M(k,\omega) = \frac{1}{1 - \epsilon_M(k,\omega)} - \frac{1}{1 - \epsilon(k,\omega)}. \tag{21}$$

This DLFC function can be used for plasmas at any temperature, as it depends on a RPA dielectric function that takes into account the plasma degeneracy.

We will see later that for proton energy loss calculations, it is worth defining the energy loss function (ELF)

$$f_{\mathrm{ELF}} \equiv \mathrm{Im}\left(\frac{-1}{\epsilon_x(k,\omega)}\right), \tag{22}$$

where $\epsilon_x(k,\omega)$ is any of the dielectric functions stated before.

Figure 1 shows the different ELF dependence with ω/ω_p when $k/k_F = 1$, for a $T = 1$ eV and $n_e = 10^{23}$ cm^{-3} partially coupled plasma. The coupling for a partially degenerate plasma is measured through the parameter $\Gamma \equiv E_F/[\pi k_F a_0 (E_F + k_B T)]$ [19], where E_F and k_F are Fermi energy and Fermi wave number, and a_0 is the Bohr radius. In this case, $\Gamma = 0.372 \lesssim 1$, which indicates that we are in the limit of coupled plasmas. Solid line represents RPA calcula-

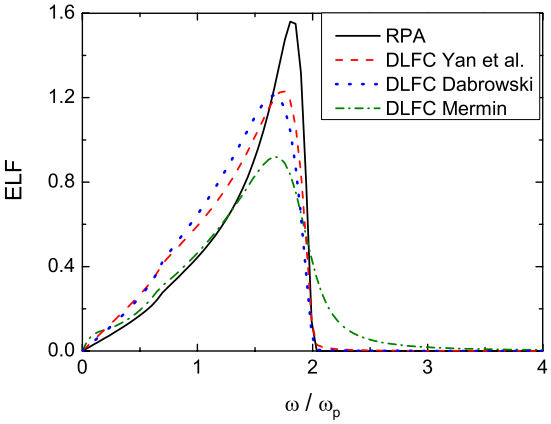

FIG. 1. (Color online) Different ELFs as a function of ω/ω_p when $k/k_F=1$, for a $T=1$ eV and $n_e=10^{23}$ cm^{-3} partially coupled plasma ($\Gamma=0.372$). Solid line represents RPA calculation, dashed line is the result by Yan *et al.*, and dotted line is the one by Dabrowski. Finally, dashed-dotted line is the ELF obtained with Mermin DLFC.

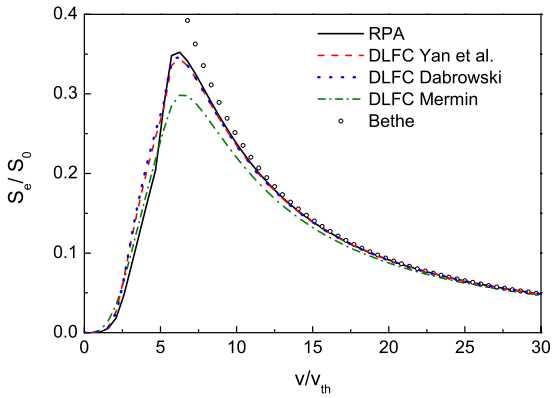

FIG. 2. (Color online) Proton electronic stopping, as a function of its velocity, normalized to $S_0=(Zk_F)^2$. The plasma target is the same as in Fig. 1. Solid line corresponds to RPA calculation, dashed line is the result with Yan *et al.* DLFC and dotted line is the one with Dabrowski DLFC. Finally, dashed-dotted line is the electronic stopping obtained with Mermin DLFC.

tion with dielectric function from Eq. (3). Dashed line is the result with DLFC function by Yan *et al.*, Eq. (15), and dotted line is the one with DLFC function by Dabrowski, Eq. (19). Finally, dashed-dotted line is the energy loss function obtained with Mermin DLFC, Eq. (21). The collision frequency needed in the Mermin case, which depends on plasma temperature and electron density, is obtained from [18], $\nu=3.6$ fs^{-1}. Results for Yan *et al.* and Dabrowski are very similar as both are parametrizations based on the same asymptotic behaviors of the DLFC function frequency dependence and this dependence is slight. These DLFC function values change only by 15% along all frequency ranges, $0\leqslant\omega<\infty$, for not very small k. On the order hand, when Mermin DLFC function is considered, the energy loss function peak is greatly damped, more than the former two cases. Though it increases for small frequencies, it returns to RPA values until its maximum, that takes place shortly before the RPA one, and finally it diminishes smoothing the ridge at $\omega/\omega_p=2$. The Mermin case is the only one, which ELF is not canceled for $\omega/\omega_p>2$.

Once we have calculated the plasma energy loss function, which takes into account its coupling through the dynamical field corrections, we can measure the energy loss by a proton that traverses our plasma. This energy loss will be mostly due to proton interaction with the plasma electrons. To calculate this electronic energy loss we use again the dielectric formalism. In the dielectric formalism, we can determine the energy loss by the electronic stopping, defined as the electronic energy loss per path unit, $S_e=dE/dx$. The formula to calculate the electronic stopping for a pointlike ion with charge Z traveling with constant velocity v through a plasma is very well known [3,5],

$$S_e(v)=\frac{2Z^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon_x(k,\omega)}\right), \qquad (23)$$

which depends on the plasma only through its energy loss function $\mathrm{Im}[-1/\epsilon_x(k,\omega)]$. Then, we can compare the electronic stopping that results from the different DLFC functions.

Figure 2 represents different proton electronic stoppings, normalized to $S_0=(Zk_F)^2$, as a function of its velocity, normalized to electron thermal velocity, $v_{th}=\sqrt{k_BT}$. The plasma target is the same as in Fig. 1. All stopping calculations are contrasted with Bethe formula at high velocities. Solid line corresponds to the calculation with the RPA dielectric function, i.e., not considering coupling. Dashed line is the result with DLFC function by Yan *et al.*, Eq. (15), and dotted line is the one with DLFC function by Dabrowski, Eq. (19). Finally, dashed-dotted line is the electronic stopping obtained with Mermin DLFC, Eq. (21). The collision frequency used is the same as in Fig. 1, $\nu=3.6$ fs^{-1} [18]. Results for Yan *et al.* and Dabrowski are very similar as their energy loss function are also very similar, see Fig. 1. Both corrections generate an enhancement for lower velocities as the velocity at maximum, recovering RPA values just after it. Similar effects for the Yan *et al.* approach have been recognized for nondegenerate cases [12]. A completely different result is achieved when coupling is considered by Mermin DLFC function, Eq. (21). Mermin method produces a high increase at very low velocities, higher than the one produced by the other ones; but the most significant effect is the damping around the maximum stopping. Finally, the Mermin calculation tends to the same values as RPA ones for higher velocities. Obviously all stoppings fit the Bethe formula at high velocities. We see important differences between Yan *et al.*, or Dabrowski, and Mermin results. They are significant at low velocities and very relevant around the maximum, nearly 30%.

In conclusion, we must say that even though differences between the parametrized DLFC functions and the Mermin DLFC function are very relevant, it is not easy to decide which method is better. The dielectric functions from Yan *et al.* or Dabrowski usually fulfill the sum rules as their DLFC functions are defined in order to fulfill them. On the other hand, Selchow and Morawetz [20] showed that Mermin dielectric function carries out the strongest sum rules; the

longitudinal frequency, the conductivity, the compressibility and the screening sum rules, and recovers Drude formula for the long-wavelength limit. Then, one cannot manifest which method is better from this point of view. The difference between parametrized DLFC functions and Mermin DLFC approach has been tested for nondegenerate, classical plasmas by comparing with computer simulations [21]. They found that parametrized DLFC functions work only for low coupling but fail for strong coupling, while Mermin DLFC function works also for strong coupling if an appropriate collision frequency is applied. One can think that it will be the same for plasmas at any degeneracy, but the comparison of our results with computer simulations is beyond the scope of this paper.

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