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Mermin dielectric function versus local field corrections on proton stopping in degenerate plasmas

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Abstract

If plasmas are considered fully ionized, the electronic stopping of a charged particle that traverses them will only be due to free electrons. This stopping can be obtained in a first view through the random phase approximation (RPA). But free electrons interact between them affecting the stopping. These interactions can be taken into account in the dielectric formalism by means of two different ways: the Mermin function or the local field corrections (LFCs). LFCs produce an enhancement in stopping before the maximum and recover the RPA values just after it. Mermin method also produces firstly a high increase at very low energies, then a small enhancement at low energies and finally decreases below RPA values before and after the maximum. Differences between the two methods are very important at very low energies and by 30% around the stopping maximum.

Keywords: Electron collisions; Energy loss; Fast ignition; Local field correction

1. INTRODUCTION

The energy loss of charged particles in a free electron gas is of considerable interest to actual slowing-down problems. This is a topic of relevance to understand the beam-target interaction in the contexts of particle driven fusion (Deutsch, 1984; Hoffmann *et al.*, 1990; Roth *et al.*, 2001; Deutsch & Popoff, 2006; Nardi *et al.*, 2006; Nardi *et al.*, 2007). Energy losses of ions moving in an electron gas can be studied through the stopping power of the medium (Eisenbarth *et al.*, 2007). Dielectric formalism has become one of the most used methods to describe this stopping power. The use of this formalism was introduced by Fermi (1940). Subsequent developments made it possible to extend the dielectric formalism to provide a more comprehensive description of the stopping of ions in matter (Lindhard, 1954; Lindhard & Winther, 1964). For dilute plasmas, the dielectric formulation of the energy-loss rate was first studied by Pines and Bohm (1952), Akhiezer and Sitenko (1952), and other scientists. Large number of calculations of electronic stopping forces of ions and electrons in plasmas has been carried out since then using the random phase approximation (RPA) (see Zwicknagel *et al.*, (1999) for a complete list). The RPA is usually valid for high-velocity projectiles and in the weak coupling limit of an electron gas. But for partially coupled plasmas, which are subject of much interest for current studies of inertial confinement fusion (ICF), RPA it is not sufficient and the electronic interactions have to be taken into account. The coupling parameter, Γ, is a measure of target electron interactions. It is defined, in a degenerate electron gas, as the ratio between potential and kinetic energies of the electrons, $\Gamma \equiv e^2/r_s m v_F^2$, where r_s is the Wigner-Seitz radius and v_F is the Fermi velocity. In this article, the coupling will be treated through two different ways: the Mermin function or the local field corrections (LFCs).

Mermin (1970), and later Das (1975), derived an expression for the dielectric function taking into account the target electron interactions and also preserving the local particle density. Recently, extended dielectric function has been considered which conserves momentum and energy (Selchow *et al.*, 2000; Morawetz & Fuhrmann, 2000; Atwal & Ashcroft, 2002), but it is somewhat involved and it has only small differences with Mermin dielectric function. Mermin dielectric function has been successfully applied to solids (Barriga-Carrasco & Garcia-Molina, 2003, 2004) and to plasmas (Barriga-Carrasco, 2006*a*, 2006*b*, 2007; Barriga-Carrasco & Maynard, 2006; Barriga-Carrasco & Deutsch, 2006).

On the other hand, some authors (Hubbard, 1957; Singwi *et al.*, 1968; Vashishta & Singwi, 1972; Vaishya & Gupta,

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1973; Pathak & Vashishta, 1973; Ichimaru & Utsumi, 1980) have introduced the local field corrections to improve previous results based on the RPA theory. Mostly static approximations have been proposed (SLFC), as it was considered that greater part of the local field corrections will succeed for the static limit. Hubbard obtained an explicit expression for the static local field correction, which takes into account the exchange effects but neglects correlations (Hubbard, 1957). Next step was made by Singwi *et al.* (1968) which related the local field corrections with the static structure function. This last result had some deficiencies, as it violates the compressibility sum rule. Latter deficiency was removed by Vashishta and Singwi (1972), and improved by Pathak and Vashishta (1973) demanding that the response function fulfills the third-order frequency sum rule. Ichimaru and Utsumi (1980) present a simple fitting formula for the static local field correction of coupled electron gas. But in Vaishya and Gupta (1973) it was shown that one cannot construct a SLFC which fulfills both limits, the compressibility and the third-order sum rule. Therefore the concentration was mostly focused on the construction of dynamical local field corrections (DLFC). Then Yan *et al.* (1985) proposed a parametrization of the DLFC that takes into account the asymptotic behaviors in their frequency dependence. We will use in this work the Ichimaru and Utsumi, and the Yan et al. parametrizations for SLFC and DLFC functions, respectively.

Mermin dielectric function is derived in Section 2 while local field corrections are in Section 3. This two methods are compared in Section 4 for the electronic stopping of a proton traversing a degenerate plasma.

2. MERMIN DIELECTRIC FUNCTION

In this section, we are going to develop the Mermin dielectric function $\varepsilon_{\rm M}(k, \omega)$ in terms of the wave number k and of the frequency ω provided by a consistent quantum mechanical analysis. First the dielectric response of the electronic medium is calculated in the random phase approximation (RPA). We use atomic units (a.u.), $e = \hbar = m_e = 1$, to simplify formulas. The RPA analysis yields to the expression (Lindhard, 1954)

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

where $E_{\vec{k}} = k^2/2$. For degenerate plasmas, the distribution function is $f(\vec{k}) = 0$ for $k > k_F$ and $f(\vec{k}) = 1$ for $k < k_F$, where k_F is the Fermi wave number. In this part of the analysis, we assume the absence of collisions so the damping constant approaches zero, $\nu \to 0^+$.

Dielectric function can be separated into its real and imaginary parts

$$\varepsilon(k, \omega) = \varepsilon_r(k, \omega) + i\varepsilon_i(k, \omega). \qquad (2)$$

$\varepsilon_r(k, \omega)$ can be directly obtained from Eq. (1), (Arista & Brandt, 1984)

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

where $g(x)$ corresponds to

$$g(x) = x + \frac{1}{2}(1 - x^2)\ln\left|\frac{1+x}{1-x}\right|, \qquad (4)$$

and $u = \omega/kv_F$ and $z = k/2k_F$ are the common dimensionless variables (Lindhard, 1954). $v_F = k_F = \sqrt{2E_F}$ is Fermi velocity in a.u.

The function $\varepsilon_i(k, \omega)$ also follows from Eq. (1), (Arista & Brandt, 1984)

$$\varepsilon_i(k, \omega) = \begin{cases} \dfrac{1}{8z^3 k_F}\dfrac{\omega}{E_F}, & (u \pm z)^2 < 1 \\ \dfrac{1}{8z^3 k_F}[1 - (u-z)^2], & (u-z)^2 < 1 < (u+z)^2 \\ 0, & 1 < (u-z)^2 \end{cases} \qquad (5)$$

We will see in Section 4 that for ion stopping considerations, it is worth defining the energy loss function (ELF)

$$\mathrm{ELF} \equiv \mathrm{Im}\left[\frac{-1}{\varepsilon(k, \omega)}\right]. \qquad (6)$$

As mentioned in the introduction, the RPA it is not sufficient for partially coupled plasmas and the target electron interactions have to be taken into account. Mermin dielectric function (1970) is derived taking care of these interactions and also preserving the local particle density

$$\varepsilon_{\rm M}(k, \omega) = 1 + \frac{(\omega + i\nu)[\varepsilon(k, \omega + i\nu) - 1]}{\omega + i\nu[\varepsilon(k, \omega + i\nu) - 1]/[\varepsilon(k, 0) - 1]}, \qquad (7)$$

where $\varepsilon(k, \omega)$ is the RPA dielectric function from Eq. (2). Electron collisions are considered through their collision frequency, ν. It is easy to see that when $\nu \to 0$, the Mermin function reproduces the RPA one.

The collision frequency ν in solids can be determined experimentally, but in plasmas, nowadays, it must be calculated theoretically (Barriga-Carrasco, 2008). It is known that in a fully ionized plasma, the collision frequency is determined by electron-electron (e-e) and electron-ion (e-i) Coulomb collisions (if we do not consider impurities). We can assert that the total effective frequency can be obtained as the sum of these collisions $\nu = \nu_{ee} + \nu_{ei}$ (this is an extension of the Matthiessen rule to partially degenerate plasmas, Cassisi *et al.*, 2007). Then ν can be easily divided into e-e collisions and e-i collisions to study their effects separately.

The e-e collision frequency of nonrelativistic degenerate electrons was first analyzed by Lampe (1968*a*, 1968*b*) using the formalism of the dynamic screening of the e-e interaction. After that, Flowers and Itoh (1976) obtained the expression for the relativistic degenerate electrons. Recently, Shternin and Yakovlev (2006) obtained an analytical formula for nonrelativistic and relativistic electrons at high degeneracy

$$\nu_{ee} = \frac{m_e c^2}{\hbar}\frac{6\alpha^{3/2}}{\pi^{5/2}} xy\sqrt{\beta_r} I(\beta_r, y), \tag{8}$$

where $y = \sqrt{3}\omega_p/k_B T$, $\beta_r = x/(1+x^2)^{1/2}$, $x = p_F/m_e c$ is the relativistic parameter of degenerate electrons, ω_p is the plasma frequency, and α is the fine-structure constant. On the other hand, $I(\beta_r, y)$ function is

$$\begin{aligned} I(\beta_r, y) = {} & \frac{1}{\beta_r}\left(\frac{10}{63} - \frac{8/315}{1+0.0435y}\right) \\ & \times \ln\left(1 + \frac{128.56}{37.1y + 10.83y^2 + y^3}\right) \\ & + \beta_r^3\left(\frac{2.404}{B} + \frac{C - 2.404/B}{1 + 0.1\beta_r y}\right) \\ & \times \ln\left(1 + \frac{B}{A\beta_r y + (\beta_r y)^2}\right) \\ & + \frac{\beta_r}{1+D}\left(C + \frac{18.52\beta_r^2 D}{B}\right) \\ & \times \ln\left(1 + \frac{B}{Ay + 10.83(\beta_r y)^2 + (\beta_r y)^{8/3}}\right), \end{aligned} \tag{9}$$

where $A = 12.2 + 25.2\beta_r^2$, $B = A\exp[(0.123636 + 0.016234\beta_r^2)/C]$, $C = 8/105 + 0.05714\beta_r^4$, and $D = 0.1558y^{1-0.75\beta_r}$.

The effective e-i collision frequency for degenerate plasmas was also derived by Flowers and Itoh (1976) and lately by Shternin and Yakovlev (2006)

$$\nu_{ei} = \frac{4\pi Z_i^2 e^4 m_e (1+x^2)^{1/2}}{p_F^3} n_i \Lambda_{ei}.$$

where n_i is the ion density, Z_i is the ion atomic number, and Λ_{ei} is the Coulomb logarithm. Then the total electron frequency results from

$$\nu = \nu_{ee} + \nu_{ei}, \tag{10}$$

Figure 1 shows RPA and Mermin energy loss function dependence with ω/ω_p when $k/k_F = 1$, for a $n_e = 10^{23}\,\mathrm{cm}^{-3}$ degenerate plasma. The collision frequency used in Mermin case is $\nu = 3.6\,\mathrm{fs}^{-1}$; it is obtained from the last procedure. Solid line represents RPA ELF while dashed line represents Mermin ELF. When collisions are considered through Mermin dielectric function, the ELF increases around $\omega = 0$. Also its maximum and the edge at $\omega/\omega_p = 2$ smooth in a great deal. In next sections, Mermin method will be compared with the local field corrections.

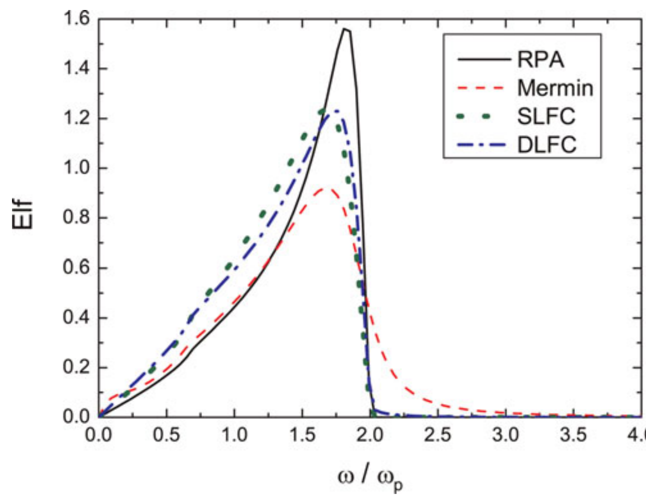

Fig. 1. (Color online) RPA, Mermin, SLFC and DLFC energy loss function dependence with ω/ω_p when $k/k_F = 1$, for a $n_e = 10^{23}\,\mathrm{cm}^{-3}$ degenerate plasma.

3. LOCAL FIELD CORRECTIONS

If LFCs are considered the dielectric function reads

$$\varepsilon_{\mathrm{LFC}}(k,\omega) = 1 - \frac{[1-\varepsilon(k,\omega)]}{1 + [1-\varepsilon(k,\omega)]G(k,\omega)}, \tag{11}$$

where $\varepsilon(k,\omega)$ is the RPA dielectric function and $G(k,\omega)$ is the local field corrections of the electron gas. Mostly static approximations (SLFC), $G(k) = G(k, 0)$, have been proposed in the past, as it is considered that greater part of the local field corrections will succeed for the static limit, $\omega = 0$. It has started with the pioneering work of Hubbard (1957) who first introduced the notation of local field corrections and took into account the exchange contributions

$$G_H(k) = \frac{1}{2}\frac{k^2}{k^2 + k_F^2}. \tag{12}$$

This expression has established a remarkable improvement of the RPA but it was insufficient due to its self-inconsistency which leads the pair correlation function still to unphysical negative values. This has been repaired by Singwi *et al.* (STLS) (1968) by using the correlation contribution

$$G_{STLS}(k) = -\frac{1}{n_e}\int \frac{dq}{(2\pi)^3}\frac{qk}{q^2}(S(q-k) - 1), \tag{13}$$

where the static structure factor is

$$S(k) = \int \frac{d\omega}{n_e \pi V(k)} \mathrm{Im}\varepsilon_{\mathrm{LFC}}^{-1}(k,\omega), \tag{14}$$

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. Eq. (13) has been improved further by Pathak and Vashista (1973) demanding that the response function should fulfill the third-order frequency sum rule, which resulted in

$$G_{PV}(k) = -\frac{1}{n_e}\int \frac{dq}{(2\pi)^3}\frac{(qk)^2}{q^4}\frac{V(k)}{V(q)}(S(q-k)-S(k)), \tag{15}$$

leading to the improved small-distance limit. At the same time, there have been different improvements to the derivation of LFC from the virial formula (Vashishta & Singwi, 1972; Vaishya & Gupta, 1973) which have resulted in expressions known from density variations

$$G_{VS}(k) = \left(1 + an_e\frac{\partial}{\partial n_e}\right)G_{STLS}(k), \tag{16}$$

for the degenerate electron liquids at metallic densities $a = 2/3$.

The self-consistent (Singwi *et al.*, 1968; Pathak & Vashishta, 1973) and the variational (Vashishta & Singwi, 1972; Vaishya & Gupta, 1973) formulations need of non-linear integral equations and computer simulations to obtain the SLFC. For coupled degenerate electron liquids it will be useful to derive a parametrized expression which accurately fits the results of the self-consistent formulation as well as the variational calculations. On the suggestion of their microscopic calculations, Ichimaru and Utsumi (IU) (1980) adopted the formula

$$G_{IU}(k) = \frac{Ak^4}{k_F^4} + \frac{Bk^2}{k_F^2} + C + \left[\frac{Ak^4}{k_F^4} + \left(B + \frac{8}{3}\right)\frac{k^2}{k_F^2} - C\right] \times \frac{4k_F^2 - k^2}{4kk_F}\ln\left|\frac{2k_F + k}{2k_F - k}\right|. \tag{17}$$

The parameters are $A = 0.029$, $B = 9/16\gamma_0 - 3/64[1-g_0] - 16/15A$ and $C = -3/4\gamma_0 + 9/16\,[1-g_0] - 16/5A$, where

$$g_0 = \frac{1}{8}\left[\frac{z}{I(z)}\right], \tag{18}$$

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 $r_s = (3/4\pi n_e)\, me^2/\hbar^2$. Also γ_0 is defined as

$$\gamma_0 = \frac{1}{4} - \frac{\pi\alpha r_s^5 b_0}{24}\frac{d}{dr_s}\left(\frac{r_s^{-3} + b_1 r_s^{-2.5}}{1 + b_1 r_s^{0.5} + b_2 r_s + b_3 r_s^{1.5}}\right), \tag{19}$$

where $b_0 = 0.0621814$, $b_1 = 9.81379$, $b_2 = 2.82224$, and $b_3 = 0.736411$.

But in Vaishya and Gupta (1973) 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), $G(k,\omega)$. The formulation of the DLFC for a coupled degenerate plasma is a difficult task, then Yan *et al.* (1985) proposed a parametrization that takes into account the asymptotic behaviors of the DLFC in their frequency dependence

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

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

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

$$G_Y(k,\omega) = \frac{\omega G_{PV}(k) + i\omega_p G_{IU}(k)}{\omega + i\omega_p}. \tag{20}$$

Figure 2 shows the LFC as a function of k/k_F, for a $n_e = 10^{23}$ cm^{-3} degenerate coupled plasma ($\Gamma = 0.686$). Solid lines represents IU parametrization, $G_{IU}(k)$, and PV function, $G_{PV}(k)$. Other curves in Figure 2 represent Yan *et al.* (1985) parametrization, $G_Y(k,\omega)$, for different frequency values; dashed line, $\omega = 0$, dotted line, $\omega = \omega_p$, and dashed-dotted line, $\omega = 10\omega_p$. As it is seen $G_Y(k,\omega)$ tends to $G_{IU}(k)$ for low frequencies while it tends to $G_{PV}(k)$ for high frequencies.

The corresponding SLFC y DLFC energy loss functions are drawn in Figure 1 with dotted and dashed-dotted lines, respectively. The SLFC is based on the UI parametrization and the DLFC is based on the Yan et al. one. When collisions are considered in both cases, the ELF increases for low frequencies up to the frequency at maximum, even with higher values than in the Mermin case. Then it decreases suddenly at $\omega/\omega_p = 2$ as in the RPA case. Differences between SLFC and DLFC corrections are minimal. This is because our calculated DLFC function has a low frequency dependence, as it can be seen in Figure 2; for enough high

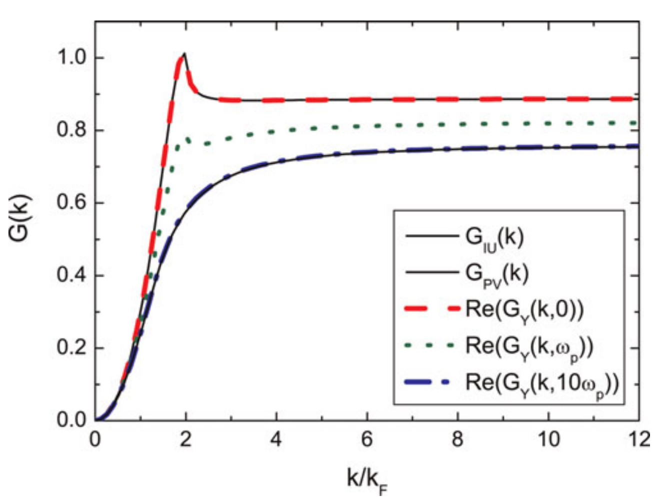

Fig. 2. (Color online) $G_Y(k,\omega)$ as a function of k/k_F, for a $n_e = 10^{23}$ cm^{-3} degenerate coupled plasma ($\Gamma = 0.686$). It tends to $G_{IU}(k)$ for low frequencies while it tends to $G_{PV}(k)$ for high frequencies.

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k values it changes only by 15% along all frequency range, $0 \le \omega < \infty$.

4. ELECTRONIC STOPPING

In the dielectric formalism, the formula to calculate the ion electronic stopping in any target is very well known. The electronic stopping for a swift pointlike ion with charge Z travelling with constant velocity v through a target plasma defined by its energy loss function is

$$S_e(v) = \frac{2Z^2}{\pi v^2} \int_0^{\infty} \frac{dk}{k} \int_0^{kv} d\omega\omega \, \mathrm{Im}\left[\frac{-1}{\varepsilon_x(k,\omega)}\right], \qquad (21)$$

where $\mathrm{Im}[-1/\varepsilon_x(k,\omega)]$ is the energy loss function of any dielectric function stated before. Then it is easy to compare the electronic stopping that results from the use of the Mermin or the local field correction dielectric function.

Figure 3 represents the proton electronic stopping as a function of the proton energy in a $n_e = 10^{23}$ cm^{-3} degenerate plasma normalized to $S_0 = (Zk_F)^2$. The coupling parameter value is obtained from plasma electron density $\Gamma = 0.686 \lesssim 1$ which indicates that we are in the limit of coupled plasmas. The electronic stoppings are contrasted with Bethe formula at high energies. Solid line corresponds to the calculation with the RPA dielectric function, i.e., not considering collisions. Dashed line is the calculation with the Mermin dielectric function, Eq. (7), where the collision frequency is $\nu = 3.6$ fs^{-1}. Dotted line is the calculation with the LFC dielectric function, Eq. (11), with the static IU parametrization, Eq. (17). Finally, dashed-dotted line is the electronic stopping obtained with the LFC dielectric function, Eq. (11), but with the Yan *et al.* (1985) DLFC function, Eq. (20). Also relative deviations, $(S_x - S_{\mathrm{RPA}})/S_{\mathrm{RPA}}$, are shown to see clearly the differences between methods. Both kinds of LFC, static and dynamic, produce an enhancement in the stopping at low energies. But for the static case, this enhancement arrives at the maximum while for the dynamic case, this enhancement disappears before the maximum. After the maximum, both LFC cases recover the RPA values tending to the Bethe limit at high energies. Mermin method produces a high increase at very low energies, higher than the one produced by the LFC ones, but this increase is less significant than the LFC one at lower energies than the energy at maximum. Around and just after the maximum, Mermin values drop below RPA values. Finally, they also tend to Bethe limit at high energies. We see important differences between Mermin and LFC methods; they are very important at very low energies and by 30% around the maximum. Similar results for LFC approach have been recognized for nondegenerate cases (Yan et al., 1985).

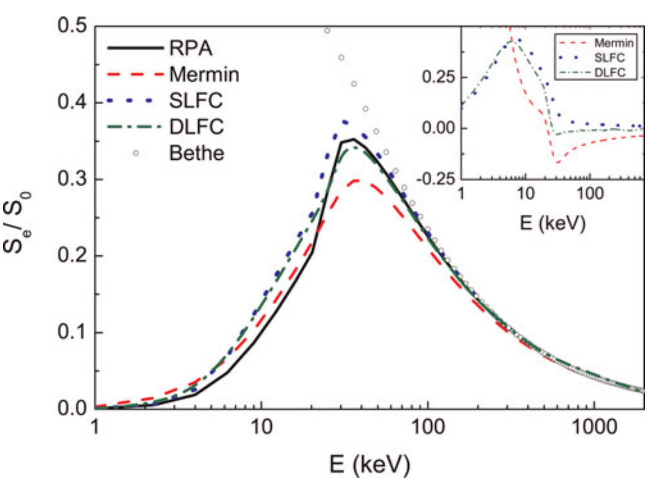

Fig. 3. (Color online) Proton electronic stopping as a function of its energy, in a $n_e = 10^{23}$ cm^{-3} degenerate plasma, normalized to $S_0 = (Zk_F)^2$. Solid line corresponds to RPA calculation, dashed line to Mermin calculation, dotted line to SLFC calculation and dashed-dotted line to the DLFC one. Relative deviations, respect to the RPA calculation, are also shown.

5. CONCLUSIONS

In this work, the effects of target electron collisions on the electronic stopping of protons in degenerate plasmas have been examined by means of two methods: the Mermin dielectric function or the local field corrections. The electronic stopping is due to the free electrons as the plasma target is considered fully ionized. Its electronic density is around solid values $n_e \simeq 10^{23}$ cm^{-3}, which are very interesting for ICF studies. To calculate the electronic stopping, we have used the random phase approximation for degenerate plasmas, i.e., the Lindhard dielectric function. Then we have considered electron collisions through two methods: the Mermin dielectric function and the local field corrections. The LFC methods produce an enhancement in stopping before the maximum. But for the static case, this enhancement arrives at the maximum while for the dynamic case, this enhancement disappears before the maximum. On the other hand, Mermin method produces a high increase at very low energies, higher than the one produced by the LFC, but this increase is less significant than the LFC at lower energies than the energy at maximum. Around and just after the maximum, Mermin values are damped below RPA values. Finally, all of them tend to Bethe limit at high energies. Differences between Mermin and LFC methods are very important at very low energies and by 30% around the maximum.

But it is not easy to decide which method is better. LFC methods usually fulfil the sum rules as LFC functions are defined in order to fulfil them. But it was demonstrated that one cannot construct a SLFC which fulfills the compressibility and the third-order sum rules. That is why we propose to use a DLFC which is parameterized between one SLFC, which takes into account the compressibility sum rule, and another SLFC, which takes into account the third-order sum rule. On the other hand, Selchow and Morawetz (1999) 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 long-wavelength limit. Then it is not easy to manifest which method is better from this point of view. Difference between the Mermin approach and the LFC approach has been tested for nondegenerate, classical plasmas by comparing with computer simulations (Pschiwul & Zwicknagel, 2003). They found that LFC method works only for low coupling but fails for strong one, while Mermin method works also for strong coupling if an appropriate collision frequency is applied. One can thought that it will be the same for degenerate plasmas, but the comparison of our results with computer simulations is out of our possibilities.

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