16th International Conference
on the Physics of Non-Ideal Plasmas

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# NNP16

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September 24-28, 2018
Saint-Malo, France

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# Stopping power in warm dense targets from first principles

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Recent experimental advances enabled the precise measurement of the stopping power of fusion products in warm dense targets. Time-dependent density functional theory coupled with Ehrenfest molecular dynamics is the standard method to predict stopping power in cold targets. We assess its ability to reproduce these experimental measurements in warm dense targets[1], illustrate the computational challenges with this method, and introduce an alternative framework based on time-dependent density functional theory coupled with average-atom models. Our approach facilitates the prediction of the stopping power in future experiments from first principles and advances our empirical and phenomenological understanding of transport properties in this technologically challenging thermodynamic regime.

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# Stopping power of electron gas

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The polarizational stopping power of heavy ions in fully ionized plasmas is described by the Lindhard formula [1]:

$$\left[-\frac{dE}{dx}\right]^{pol}=\frac{2\left(Z_pe\right)^2}{\pi v^2}\int_0^{\infty}\frac{dk}{k}\int_0^{kv}\omega^2\left(-\mathrm{Im}\left[\frac{\varepsilon^{-1}(k,\omega)}{\omega}\right]\right)d\omega,$$

whose high-velocity asymptotic form was found by Bohr, Bethe, and Larkin [2]:

$$\left[-\frac{dE}{dx}\right]^{pol}_{v\to\infty}\cong\left(\frac{Z_pe\omega_p}{v}\right)^2\ln\left[\frac{2m_ev^2}{\hbar\omega_p}\right].$$

The plasma inverse dielectric function (IDF), $\varepsilon^{-1}(k,\omega)$, was determined in [3] within the moment approach [4], complemented by some physical observations in terms of two characteristic frequencies $\omega_1$ and $\omega_2$, which are the ratios of the frequency power moments of the IDF imaginary part, in the following form:

$$\varepsilon^{-1}(k,\omega)=1+\frac{\omega_p^2\left(\sqrt{2}\omega_1\omega+i\omega_2^2\right)}{\sqrt{2}\omega_1\omega\left(\omega^2-\omega_2^2\right)+i\omega_2^2\left(\omega^2-\omega_1^2\right)}.$$

The frequencies $\omega_1$ and $\omega_2$ can be rigorously evaluated using the static structure factor (SSF) of the system. Nevertheless, here we employ the following interpolating expressions [5,6]:

$$\omega_1^2=\omega_1^2(k)=\omega_p^2\left(1+k^2k_D^{-2}+k^4k_q^{-4}\right),\qquad \omega_2^2=\omega_2^2(k)=\omega_p^2\left(1+\frac{\left\langle v_e^2\right\rangle k^2}{\omega_p^2}-\frac{v_{int}^2k^2}{\omega_p^2}\right),$$

The interpolation and fitting parameters introduced are chosen as follows:

$$v_{int}^2=-\frac{4}{15}\frac{\Gamma^{3/2}}{\beta m_e}\left(\frac{-0.9052}{\sqrt{0.6322+\Gamma}}+\frac{0.27243}{1+\Gamma}\right),\ \Gamma=\beta e^2/a,\ k_q^4=12r_s/a^4,\ r_s=a/a_B,$$

$a$ and $a_B$ are the Wigner-Seitz and Bohr radii, respectively, $\beta=1/(k_BT)$, $k_D^{-1}$ is the Debye radius, $k_B$ stands for the Boltzmann constant with $T$ being the plasma temperature.

The numerical results obtained for the energy losses of heavy ions moving in an electron gas are found in good agreement with the PIC simulation data [7].

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