Nuclear collisions effects on H_2^+ energy loss

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Introduction

The energy loss of ion beams in plasmas is an important quantity for the ICF. For atomic ions moving in plasmas, the energy loss is well understood based on various theoretical models, such as the linear Vlasov-Poisson theory [1], the binary collision theory [2], and the nonlinear Vlasov-Poisson theory [3]. For the slowing-down processes of molecular ions in plasmas, however, it has been shown that the energy loss of an molecular ion is strongly influenced by the interference resulting from spatial correlation among the molecule constituent particles. This so-called vicinage effect on the energy loss of molecular ions in plasma targets has been described theoretically by several authors [4] within the framework of the linearized Vlasov-Poisson theory. But to date there is no studies about these vicinage effects considering a full simulation of the transport of the molecular ion.

Here computer simulations of the trajectory followed by the protons resulting from the dissociation of H_2^+ molecules after traversing plasma targets have been performed. Dielectric formalism have been used to describe the forces due to electronic excitations in the medium; the self-retarding proton force and the vicinage force created by its partner proton. Coulomb repulsion between the pair of protons is also considered. Nuclear collisions with target plasma nuclei are incorporated through a Monte Carlo code. The influence of these collisions on the H_2^+ energy loss, the interproton vector angle and interproton separation are discussed for a target plasma.

Electronic stopping of cluster ions in plasmas

In the dielectric formalism, the target is characterized by its dielectric function $\varepsilon(k,\omega)$, which contains relevant information about its response to electronic excitations induced by the charged projectile traversing it. These excitations are characterized by its momentum k and energy ω. To simplify theoretical calculations atomic units (a.u.) will be used, except for results where plasma units will be stated. The dielectric function of a classical electron plasma can be obtained from the random phase approximation [1, 5]

$$\varepsilon(k,\omega)_{QRPA} = 1 + \frac{k_D^2}{k}\left(W(\zeta) + iY(\zeta)\right)$$

with $\quad W(\xi) = 1 - \sqrt{2}\xi\, e^{-\xi^2/2}\int_0^{\xi/\sqrt{2}} e^{-x^2}dx \quad$ and $\quad Y(\xi) = \sqrt{\frac{\pi}{2}}\,\xi\, e^{-\xi^2/2}$

where $\xi=\omega/(kv_{th})$; being $k_D=\omega_p/v_{th}$ the inverse Debye length, $v_{th}=(k_BT)^{1/2}$ the electron thermal velocity and $\omega_p=(4\pi n)^{1/2}$ the plasma frequency. T and n are the temperature in eV and the electronic density in a.u. of the target plasma, respectively.

Following the dielectric formalism, the induced force produced by a pointlike charge Z_{p1} moving at velocity $\mathbf{v}$ inside a uniform electron gas on a neighbor charge is Z_{p2} [6]

$$F_z(z,\rho) = \frac{2Z_{p1}Z_{p2}}{v^2\pi}\int_0^{kx}\frac{dk}{k}\int_0^{kv} d\omega\,\omega\, J_0(\rho\sqrt{k^2-\omega^2/v^2})$$
$$\times\left[\sin(\omega z/v)\,\mathrm{Re}\left(\frac{1}{\varepsilon_{RPA}(k,\omega)}-1\right) + \cos(\omega z/v)\,\mathrm{Im}\left(\frac{1}{\varepsilon_{RPA}(k,\omega)}-1\right)\right]$$

$$F_\rho(z,\rho)=\frac{2Z_{p1}Z_{p2}}{v\,\pi}\int_0^{kx}\frac{dk}{k}\int_0^{kv}d\omega\;\; J_1(\rho\sqrt{k^2-\omega^2/v^2})\sqrt{k^2-\omega^2/v^2}$$
$$\times\left[\cos(\omega\, z/v)\,\mathrm{Re}\left(\frac{1}{\varepsilon_{RPA}(k,\omega)}-1\right)-\sin(\omega\, z/v)\,\mathrm{Im}\left(\frac{1}{\varepsilon_{RPA}(k,\omega)}-1\right)\right]$$

where z and ρ are the coordinates parallel and perpendicular of the neighbor projectile from the projectile that generates the potential in the reference frame of the motion of the last one. $J_0(x)$ and $J_1(x)$ are the zeroth and the first order Bessel function.

Putting $z=\rho=0$ and $Z_{p1}=Z_{p2}$ in former equations results $F_\rho=0$, and F_z yields the self-retarding particle force F_s. The variation of the projectile kinetic energy is $dE=F_s\, v_{p1}dt$ so the electronic stopping, S_e, defined as the energy loss per unit path length, becomes

$$S_e(v)=\frac{2Z_{p1}^2}{v_{p1}{}^2\pi}\int_0^{\infty}\frac{dk}{k}\int_0^{kv}d\omega\;\omega\,\mathrm{Im}\left(\frac{-1}{\varepsilon_{RPA}\;(k,\omega)}\right)$$

Nuclear scattering model

Nuclear interactions are treated within the classical dispersion theory. Let us consider $E_p=m_pv_p^2/2$, m_p and Z as the projectile energy, mass and charge; and m_n and Z_n as the target nucleus mass and charge, in the centre of mass frame. The target nucleus produces a potential energy $V(r)$ at the projectile position during the collision, so the projectile is scattered with an angle θ [7]

$$\theta(s)=\pi-2s\int_{R_{\min}}^{\infty}\frac{dr}{r^2\sqrt{1-V(r)/E_r-s^2/r^2}},$$

where $E_r=4m_pm_nE_p/(m_p+m_n)^2$ is the maximum transferable energy in the collision, r is the distance between the projectile and the force center and R_{min} is the minimum r. It can be seen that θ angles are larger for lower projectile velocities.

The interatomic potential energy $V(r)$ is written as

$$V(r)=\frac{ZZ_n}{r}\Phi(\frac{r}{a})$$

For a fully ionized plasma Φ is the Debye potential $\Phi(r/a)=exp(-r/a)$ and a is the dynamical adiabatic screening length, which depends on temperature

$$a=\frac{\sqrt{v_{th}^2+v^2}}{\omega_p}$$

For a partially ionized plasma, Φ and a are obtained from the average atom model [8].

The elastic collision induces an energy E_T transferred to the nucleus, and therefore lost by the projectile. It is related to the scattering angle θ by

$$E_T=\frac{4m_pm_nE_p}{(m_p+m_n)^2}\sin^2(\frac{\theta}{2})$$

so the greater the scattering angle, the greater the energy loss. In our energy regime, nuclear collisions introduce only a small correction to the inelastic proton energy loss. This nuclear scattering model is included in our computer code, TAMIM, through a Monte Carlo method described by Möller et al. [9].

Results

This section shows the effects of considering or not considering the nuclear scattering in the slowing down process of a H_2^+ ion. The H_2^+ ion will lose its electron just entering the target and dissociates into two protons, $Z_{p1}=Z_{p2}=1$ and $m_p=1$ in proton units (p.u.), separated by an initial distance $r_0=1.08\times10^{-8}$ cm [10]. This gives two protons that move in close proximity, interacting between them and with the target electrons and nuclei. The target is considered to be deuterium, $Z_n=1$ and $m_n=2$ in p.u., in a plasma state characterized by its density, $n=10^{23}$ cm^{-3}, and its temperature, $T=10$ eV. H_2^+ velocities inciding on the plasma target are low enough to see the effects of nuclear scattering in its slowing down, $v_p \approx v_{th}$.

The main difference on the energy loss between two correlated or isolated protons is the due to the Coulomb and vicinage forces. So we are going to analyze how nuclear collisions influence two fundamental quantities for calculating these forces: the interproton distance, r, and the angle between the interproton vector and the motion direction, α.

It is worth to introduce the logarithm of the dimensionless dwell time (t) $\tau=log_{10}(t/t_c)$, where $t_c=1.47$ fs is the characteristic Coulomb explosion time of the two protons fragmented from the H_2^+ ion.

Figure 1 shows that vicinage forces always delay Coulomb explosions when nuclear collisions are not included. This screening is consequence of the asymmetry of these forces that try to join the two protons in ρ and z direction. This is more significant in the late dwell times when the two protons are quite separated and the Coulomb force is smaller than the vicinage forces. When nuclear collisions are included, the delay produced by the vicinage forces is canceled, indeed r increases faster than for bare Coulomb explosion. This growth is bigger for low impact projectile velocities as nuclear scattering effects are more significant.

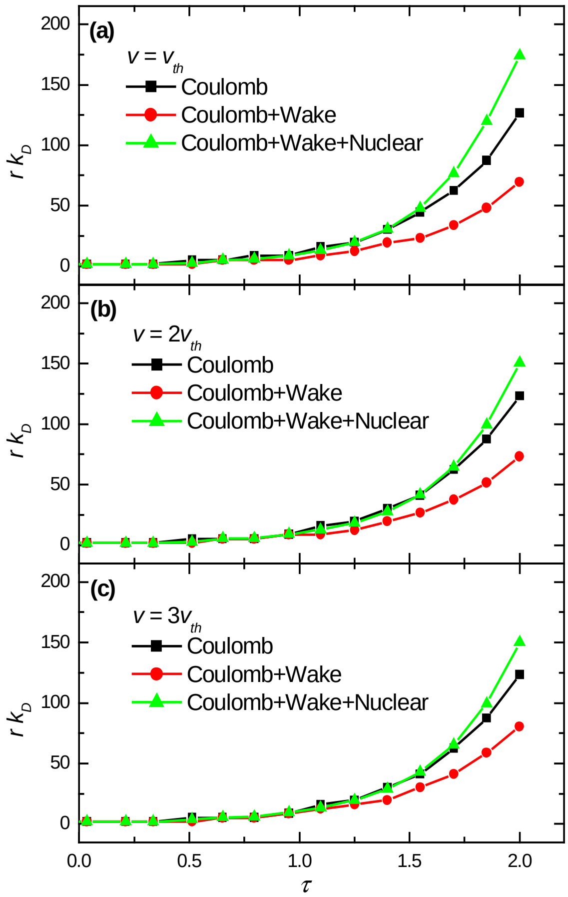

Figure 1. Evolution of the adimensional interproton distance rk_D as a function of the logarithm of dwell time ▯ during the Coulomb explosion of a H_2^+ ion with the initial angle $\alpha_0=60°$ traversing the plasma with different velocities (a) $v_p=v_{th}$, (b) $v_p=2v_{th}$ and (c) $v_p=3v_{th}$. Only considering the bare Coulomb force, the Coulomb and wake forces, and the Coulomb force, wake force and nuclear collisions.

Many published works (see [11] for a complete list) have mentioned that vicinage forces tend to align the interproton vector in the motion direction due to its asymmetry. Figure 2 shows that when these forces are considered the azimutal angle diminishes to indicate an alignment along motion direction. It means that the averaged F_ρ force is higher than the averaged F_z one during proton travel. When nuclear collisions are included in the calculations the interproton vector misaligns and cancel the effects of the vicinage forces. This misalignment is more significant for low velocities as the nuclear scattering becomes more relevant.

Finally we are going to analyse the nuclear scattering effects on the energy loss of the H_2^+ ion. The H_2^+ energy loss ratio could be defined as $R_2=\Delta E^*_{H2+}/\Delta E_{H2+}$, where ΔE^*_{H2+} and ΔE_{H2+} means the H_2^+ energy loss with and without vicinage forces, respectively. In Fig. 3 it can be seen that for longer dwell times the stopping ratio tends to 1 while for early

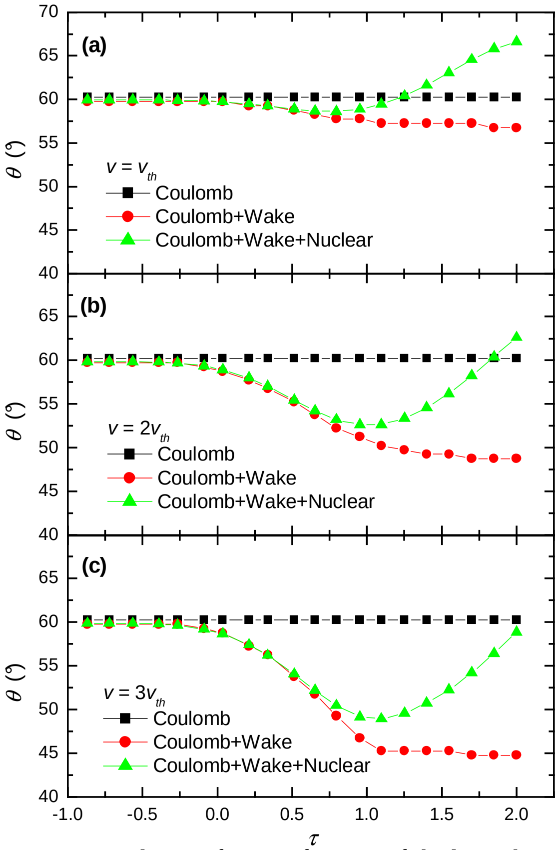

Figure 2. Evolution of α as a function of the logarithm of dwell time τ when the initial azimutal angle is α_0=60°; for the same conditions as in Fig. 1.

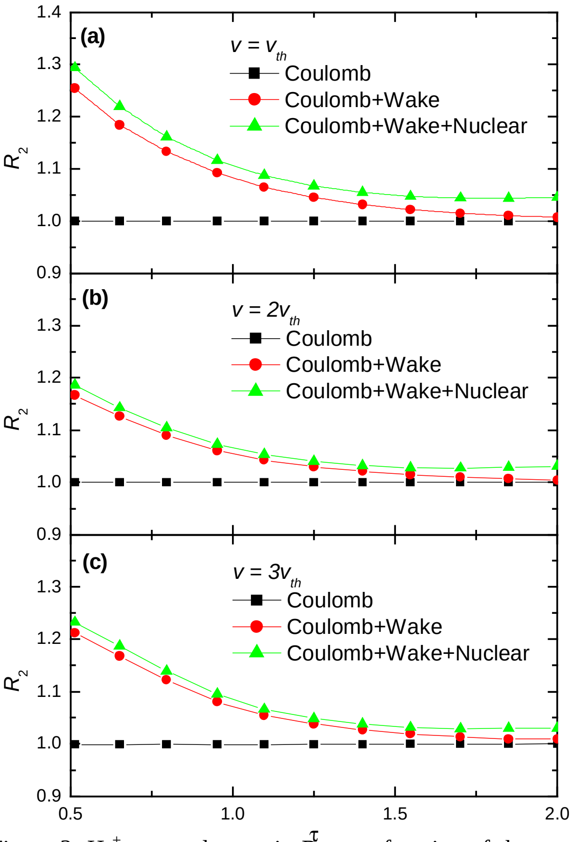

Figure 3. H_2^+ energy loss ratio R_2 as a function of the logarithm of dwell time τ for the same conditions as in Fig. 1.

times the ratio is higher than 1. This is because the two protons in the early stages are very close and they feel greater vicinage forces while in the last stages the protons are completely separated and they travel as isolated ions. When nuclear collisions are included in the computer code, they contribute moderately to increase the energy loss of the fragmented H_2^+ ion for all velocities, so the stopping ratios for last dwell times do not tend to 1. This last event is more prominent for lower velocities as expected from our nuclear scattering model.

The main conclusion of this work is that many vicinage effects can not be obtained realistically as nuclear collisions shade them; unless vicinage forces could be also isolated experimentally from nuclear scattering. Experiments concerning cluster beams cannot be investigated without taking into account the collisions with the target nuclei, for this purpose we have created the computer code TAMIM.

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