On some generalized stopping power sum rules

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Abstract

The Lindhard-Winther (LW) equipartition sum rule shows that within the linear response theory, the stopping power of an energetic point-charge projectile in a degenerate electron gas medium, receives equal contributions from single-particle and collective excitations in the medium. In this paper we show that the LW sum rule does not necessarily hold for an extended projectile ion and for ion-clusters moving in a fully degenerate electron gas. We have derived a generalized equipartition sum rule and some related sum rules for this type of projectiles. We also present numerical plots for He$^+$ ion and He$^+$ ion-clusters.

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1 Introduction

The stopping power (SP), which is a measure of energy loss of energetic charged particles in a target medium, is of continuing theoretical and experimental interest in diverse areas such as interaction of charged particles with solids (see [1-4] for reviews) and beam-heating of fusion plasma [5]. For high-velocity projectile particles or clusters, the energy loss may be mainly due to collective and single-particle excitations in the target medium. It is of fundamental and practical interest to study the extent to which the collective and single-particle excitations each contribute to SP. This is the objective of our work reported here.

The energy loss of a high velocity projectile is formulated, originally due to Lindhard [6], on the justifiable assumption of a weak coupling between the particle and a target medium which is modelled by a degenerate electron gas (DEG), through the linear response function of the DEG. The corresponding dielectric function \( \epsilon(k, \omega) \) contains contributions from both collective excitations (plasmons) and single-particle excitations. For a single point-ion projectile Lindhard and Winther (LW) [7] investigated the respective contributions of these two excitations and found a sum rule which states that both these excitations contribute equally to SP. To our knowledge this type of sum rule has not yet been studied for an extended-charge projectile or a cluster. In this paper we formulate a generalized stopping power sum rule, again in the linear response approach, and present mostly analytical results for a He\(^{+}\) ion and for a diproton cluster as projectiles. We compare and contrast our results with those of LW.

In linear response theory, the stopping power (SP) which is the energy loss per unit length for an external projectile with a spatial charge distribution \( \rho_{\text{ext}}(r, t) = Q_{\text{ext}}(r - Vt) \) moving with velocity \( V \) in a homogeneous isotropic medium characterized by the dielectric function \( \epsilon(k, \omega) \), is given by (see, e.g., [3])

\[
S = \frac{1}{2\pi^2 V} \int dK |G(k)|^2 \frac{k \cdot V}{k^2} \text{Im} \frac{-1}{\epsilon(k, k \cdot V)},
\]

(1)

where \( G(k) \) is the Fourier transform of the stationary charge \( Q_{\text{ext}}(r) \).

Eq. (1) is applicable to any external charge distribution. In Sec. II we discuss a dicluster of two identical He\(^{+}\) ions separated by a variable distance \( R \). The spatial distribution of bound electrons in the ions, \( \rho(r) \), is assumed to be spherically symmetric. We use a 1s-type wave function of the form \( \psi_{1s}(r) = (Z^3/\pi a_0^3)^{1/2} e^{-Zr/a_0} \), to describe the bound electron on each He\(^{+}\) ion, with \( a_0 = 0.529 \) Å as the Bohr radius. Ze is the charge on each of the point-like nuclei (\( Z = 2 \)). It may be remarked that we are considering an unscreened 1s electron. For the projectile systems under study we may write \( G(k) \) as

\[
G(k) = e [Z - \rho(k)] [1 + \exp (-ik \cdot R)],
\]

(2)

where \( \rho(k) \) is the Fourier transform of \( \rho(r) = |\psi_{1s}(r)|^2 \). \( G(k) \) contains \( R \) as a
For a dicluster of He\textsuperscript{+} ions the SP of a dicluster can be written as

\[ S = 2S_{\text{ind}}(\lambda) + 2S_{\text{corr}}(\lambda, R, \vartheta) \]

\[ = \frac{16e^2k_F^2}{\pi\lambda^2} \int_0^\lambda udu \int_0^\infty \mathcal{Z}(z) \text{Im} \left[ \frac{1 + \cos(\mathcal{A}z \cos \vartheta) J_0(\mathcal{B}z \sin \vartheta)}{\varepsilon(z, u)} \right] zdz, \]

where \( \mathcal{A} = (2u/\lambda)k_FR \) and \( \mathcal{B} = 2k_FR\sqrt{1-u^2/\lambda^2} \). \( S_{\text{ind}}(\lambda) \) and \( S_{\text{corr}}(\lambda, R, \vartheta) \) stand for individual and correlated SP, respectively. \( J_0(x) \) is the Bessel function of first kind and zero order and \( \vartheta \) is the angle between the interionic separation vector \( \mathbf{R} \) and the velocity vector \( \mathbf{V} \); \( \lambda = V/v_F \), \( \chi^2 = 1/\pi k_F a_0^3 = (4/9\pi^4)^{1/3} r_s \), \( r_s = (3/4\pi n_0 a_0^3)^{1/3} \). \( n_0 \) is the electron gas density, \( v_F \) and \( k_F \) are the Fermi velocity and wave number of the target electrons respectively. In our calculations \( \chi \) (or \( r_s \)) serves as a measure of electron density. Here, as in Refs. [2-4,6,7], we have introduced the following notations \( z = k/2k_F \), \( u = \omega/kv_F \). In these variables \( \mathcal{Z}(z) = Z - \rho(z) \) and the Fourier transform of the spatial distribution \( \rho(r) \) is expressed as

\[ \rho(z) = \frac{\alpha^4}{(z^2 + \alpha^2)^2}, \]

where \( \alpha = \pi \lambda^2 Z \).

In Eq. (3) the term for correlated stopping power \( S_{\text{corr}} \) vanishes for large \( R \) \( (R \to \infty) \) and SP is the sum of individual stopping powers for the separate ions. For \( R \to 0 \) the two ions coalesce into a single entity. Then \( S_{\text{corr}} = S_{\text{ind}} \) and SP is that for a total charge \( 2e(Z - 1) \).

We will consider the interaction process of a dicluster in a fully degenerate \( (T = 0) \) electron gas. For this purpose we use the exact random-phase approximation (RPA) dielectric response function due to Lindhard [3],

\[ \varepsilon(k, \omega) = 1 + \frac{2m^2\omega^2}{\hbar^2k^2} \sum_{n=1}^N \frac{f(k_n)}{N} \left\{ \frac{1}{k^2 + 2k \cdot \mathbf{k}_n - (2m/\hbar)(\omega + i0^+)} \right\}, \]

\[ + \frac{1}{k^2 - 2k \cdot \mathbf{k}_n + (2m/\hbar)(\omega + i0^+)} \].

Here, \( \mathbf{k}_n \) is the wave vector of the electron in the \( n \)th state. The distribution function \( f(k_n) \) is an even function of \( \mathbf{k}_n \), and normalized so that \( N = \sum_n f(k_n) \) is the total number of electrons. In the case of a fully degenerate free electron gas with Fermi energy \( E_F = \hbar^2k_F^2/2m \) the distribution function is \( f(k_n) = 1 \) for \( k_n < k_F \), and \( f(k_n) = 0 \) for \( k_n > k_F \).

The summation in Eq. (5) can be analytically performed, leading to the characteristic logarithmic expression in \( \varepsilon(z, u) \) first obtained by Lindhard [3].
However, in our further consideration it is convenient to use the form (5) for the dielectric function. This allows a wider investigation of the analytical properties of $\varepsilon(z,u)$ in the complex $z$ plane with applications toward deriving some useful sum rules.

2 Equipartition sum rule

In this section we shall discuss some important properties of the SP integrals, which we call stopping power summation rules (SPSR). In the literature two such sum rules have been widely considered—the familiar Bethe sum rule and the Lindhard-Winther (LW) equipartition rule (see [7]). While the Bethe sum rule concerns the integral of $1/\varepsilon(z,u)$ over $\omega$ (or $u$) for fixed $k$ (or $z$), the LW equipartition rule concerns the integral of $1/\varepsilon(z,u)$ over $z$ for fixed $u$. The latter summation rule states that an integral of the form

$$\int_{0}^{\infty} \Im \frac{-1}{\varepsilon(z,u)} zdz = \Im p(u) + \Im sp(u)$$

receives equal contributions, $\Im p(u)$ and $\Im sp(u)$, respectively, from the plasma resonance (plasmons), $0 < z < u - 1$, and from the region of close collisions (single-particle excitations), $u - 1 < z < u + 1$.

The LW equipartition rule was originally formulated for a single point-like charged projectile. Here we shall examine and generalize this equipartition rule for extended projectiles and their diclusters. As an example we shall consider a dicluster of two He$^+$ ions separated by a variable distance $R$. In order to deal with extended projectiles, as a generalization of Eq. (6), we need to consider an integral proportional to that in Eq. (3),

$$\int_{0}^{\infty} \mathbb{Z}^2(z) \Im \frac{-1}{\varepsilon(z,u)} [1 + \cos (Az \cos \vartheta) J_0 (Bz \sin \vartheta)] zdz,$$

which we decompose as $\Im_p(\alpha,u) + \Im_{sp}(\alpha,u)$, where $\Im_p(\alpha,u)$ and $\Im_{sp}(\alpha,u)$ are the contributions for plasmon and single-particle excitations.

In Eq.(7) the respective contributions for plasmon and single-particle excitations can be written as the sum of individual (first term) and correlated (second term) stopping terms

$$\Im_p(\alpha,u) = \Im_{p}^{ind}(\alpha,u) + \Im_{p}^{corr}(\alpha,u), \hspace{1cm} \Im_{sp}(\alpha,u) = \Im_{sp}^{ind}(\alpha,u) + \Im_{sp}^{corr}(\alpha,u).$$

Here again the terms for correlated stopping contribution, $\Im_{p}^{corr}$ and $\Im_{sp}^{corr}$, for $R \to 0$ tend to $\Im_{p}^{ind}$ and $\Im_{sp}^{ind}$ respectively.

Our objective is to show that the LW equipartition rule, $\Im_p = \Im_{sp}$, is not necessarily satisfied for extended projectiles and their clusters. We may therefore introduce the function
\[ \Delta(\alpha, u) = \Im_{sp}(\alpha, u) - \Im_{p}(\alpha, u), \] (9)

which represents the difference between single-particle and plasmon contributions to the integral given by Eq. (7). In order to calculate the function \( \Delta(\alpha, u) \), it is imperative to consider the integral in the complex \( z \) plane and to find the poles of \( 1/\varepsilon(z, u) \), i.e. the zeros of \( \varepsilon(z, u) \), for fixed \( u \). It is seen from Eq. (5) that there must be \( 4N + 2 \) zeros of \( \varepsilon(z, u) \) for fixed \( u \). For a large real value of \( u \), above the value \( u_0 \) which corresponds to the minimum in the plasma resonance, all \( 4N + 2 \) zeros lie on the real \( z \) axis. Two zeros occur at \( z = \pm z_r(u) \), and are determined by the intersection with the plasma resonance curve. \( 2N \) zeros are grouped together in the intervals \( u - 1 < |z| < u + 1 \), and are responsible for the single-particle contribution, \( \Im_{sp} \), to the integral in Eq. (7). The remaining \( 2N \) zeros are also grouped together near the point \( z = 0 \), but they lie outside of the interval \( u - 1 < |z| < u + 1 \) which is responsible for single-particle excitations.

It can be seen directly from Eq. (5) that at \( z \to 0 \) \( \varepsilon(z, u) \to \infty \). Therefore the contribution of these latter \( 2N \) zeros of \( \varepsilon(z, u) \) to the integral in Eq. (7) vanishes.

It should be noted that in the RPA dielectric function (5), the variable \( u \) has an infinitesimal positive imaginary part which is introduced for causality. It is seen from Eq. (5) that a small positive imaginary part \( i\theta^+ \) being added to \( u \), is equivalent to a displacement of the zeros of \( \varepsilon(z, u) \) in the complex \( z \) plane in such a way that the zeros \( z = \pm z_r(u) \) at plasma resonance lie below the real \( z \) axis while the zeros in the region \( u - 1 < |z| < u + 1 \) lie above this axis. From Eq. (5) it also follows that the slope \( \partial \varepsilon(z, u)/\partial z \) is positive at the plasmon curve, \( z = z_r(u) \) but negative at the other zero curves, \( z = z_j(u) \) in the \( z \) plane.

With these observations we shall now establish a generalized SP equipartition sum rule for a He\(^+\) ion dicluster projectile, and shall present results for two values of the orientation angle \( \vartheta \) made by the projectile velocity vector with the inter-He\(^+\) ion separation vector. The result for a single He\(^+\) ion will subsequently be obtained from the dicluster sum rule.

### 2.1 He\(^+\) ion cluster with \( \vartheta = 0 \)

To derive an expression for a non-zero \( \Delta(\alpha, u) \) and to generalize the LW summation rule we consider the following contour integral

\[ Q_{\pm}(\alpha, u) = \int_{C_1, D_1} Z^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] \left[ 1 + \exp(\pm \text{i}Az) \right] zdz, \] (10)

where the contours \( C_1 \) (for \( Q_+(\alpha, u) \)) and \( D_1 \) (for \( Q_-(\alpha, u) \)) are shown in Fig. 1. These two contours contain the real \( z \) axis \((0, +\infty)\), upper (for \( C_1 \)) or lower (for \( D_1 \)) quarter circles, the imaginary \( z \) axis \((\pm i\infty, 0)\) and infinitesimal semicircles \( C_2 \) or \( D_2 \). The full structure of the integral in Eq. (10), for the cases of He\(^+\) ion and a dicluster, is more involved than for the case of a point-like ion, and it also
contains an exponential function. An analytical evaluation of this integral thus leads us to consider a contour different from the one used in the LW paper (see [7], for details).

For large values of $|z|$, the dielectric function must behave as

$$\varepsilon(z, u) \rightarrow 1 + \frac{\chi^2}{3z^4},$$

according to Eq. (5). Therefore both integrals $Q_{\pm}(\alpha, u)$ vanish within the upper and lower quadrants, respectively and from Eq. (10) we find

$$Q_{\pm}(\alpha, u) = \left( \int_{0}^{\infty} + \int_{\pm i\infty}^{0} + \int_{C_2, D_2} \right) Z^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] \left[ 1 + \exp(\pm iA z) \right] z dz. \quad (12)$$

On the other hand both the integrands in $Q_{\pm}(\alpha, u)$ are analytical functions inside contours $C_1$ and $D_1$ containing single-particle $N$ poles $z_j + i0^+$, $j = 1, 2, ..., N$, (contour $C_1$) or single plasmon pole, $z_r(u) - i0^+$, (contour $D_1$). According to the theorem of residues, for these functions we have

$$Q_{+}(\alpha, u) = -2\pi i \sum_j z_j Z^2(z_j) \left[ 1 + \exp(iAz_j) \right], \quad (13)$$

$$Q_{-}(\alpha, u) = 2\pi i \frac{Z^2(z_r)}{\varepsilon(z_r, u)} \left[ 1 + \exp(iAz_r) \right]. \quad (14)$$

As has been mentioned earlier, $\partial\varepsilon(z_r, u)/\partial z > 0$ for plasmons and $\partial\varepsilon(z_j, u)/\partial z < 0$ for single-particle excitations.

Now let us take the imaginary part of both sides of Eqs. (12)-(14). We find

$$\mathcal{I}_{\pm}(\alpha, u) = \text{Im} \int_{0}^{\infty} Z^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] \left[ 1 + \exp(\pm iA z) \right] z dz \quad (15)$$

where

$$P_{\pm}(\alpha, u) = \text{Im} \int_{C_2, D_2} Z^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] \left[ 1 + \exp(\pm iA z) \right] z dz. \quad (16)$$

In Eq. (15) we have introduced

$$\Im_{sp}(\alpha, u) = -\sum_j \frac{\pi z_j Z^2(z_j)}{\varepsilon(z_j, u)} [1 + \cos(Az_j)] \quad (17)$$

$$= \int_{u-1}^{u+1} Z^2(z) \text{Im} \frac{-1}{\varepsilon(z, u)} [1 + \cos(Az)] z dz,$$
\[ \Im(\pi z_r Z^2(z_r) [1 + \cos(Az)]) \]

\[ = \int_{\alpha-1}^{\alpha+1} Z^2(z) \Im\left(\frac{1}{\varepsilon(z, u)} [1 + \cos(Az)] \right) dz, \]

for single-particle (\( \Im_{sp}(\alpha, u) \)) and plasmon (\( \Im_p(\alpha, u) \)) contributions to the integral (7), respectively. To prove that the sums in Eqs. (17) and (18) are actually equal to the integral forms of \( \Im_{sp}(\alpha, u) \) and \( \Im_p(\alpha, u) \) we use the known expression (see, e.g., [8])

\[ \Im\left(\frac{1}{\varepsilon(z, u)} \right) \bigg|_{\varepsilon(z, u) \to 0^+} = \pi \sum_j \frac{\delta(z - z_j)}{|\partial_{z}\varepsilon(z_j, u)|}, \]

where \( z_j \) are the zeros of \( \varepsilon(z, u) \). Since all \( N \) single-particle poles lie in the interval \( \alpha - 1 < z < \alpha + 1 \), the integration in Eq. (17) over \( z \) results in the summation form for \( \Im_{sp}(\alpha, u) \). However, for plasmon contribution the plasmon pole \( z_r(u) \) lies in the interval \( 0 < z < \alpha - 1 \), only for sufficiently high \( u, \alpha > \alpha_0(\chi) \). The threshold value \( \alpha_0(\chi) \) depends on the electron gas density. For instance, for metallic densities \( \rho_s \sim 2 \) (\( \chi \sim 0.5 \)) for threshold value of \( u \) we have \( \alpha_0 \sim 1.4 \). When \( u < \alpha_0(\chi) \) the plasmon contribution term vanishes, \( \Im_p = 0 \).

Next, we note that the imaginary part of the second terms in Eq. (12) has been omitted, because the function

\[ Z^2(\pm iz) \left[ 1 - \frac{1}{\varepsilon(\pm iz, u)} \right] \]

is real. Consequently

\[ \Im \int_{-\infty}^{\infty} Z^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] [1 + \exp(\pm Az)] dz = \Im \int_{0}^{\infty} Z^2(\pm iz) \left[ 1 - \frac{1}{\varepsilon(\pm iz, u)} \right] [1 + \exp(-Az)] dz = 0. \]

Let us now consider the integrals \( P_{\pm}(\alpha, u) \). From Fig. 1 and Eq. (16) and after evaluating the residues we find

\[ P_{+}(\alpha, u) = -P_{-}(\alpha, u) \]

\[ = \frac{\pi \alpha^3}{2} \left[ \left( Z - \frac{1}{16} \right) \frac{\partial}{\partial \alpha} + \frac{\alpha}{16} \frac{\partial^2}{\partial \alpha^2} - \frac{\alpha^2}{48} \frac{\partial^3}{\partial \alpha^3} \right] \Phi(\alpha, u) \]

where
\[ \Phi(\alpha, u) = [1 + \exp(-A\alpha)] \left[ \frac{1}{\tilde{\varepsilon}(\alpha, u)} - 1 \right], \]  
(23)

\[ \tilde{\varepsilon}(\alpha, u) = \varepsilon(i\alpha, u) = 1 + \frac{\chi^2}{4\alpha^8} \left\{ -2\alpha - \arctan \frac{u-1}{\alpha} + \arctan \frac{u+1}{\alpha} \right. \]
\[ + \left( u^2 - \alpha^2 \right) \left( \arctan \frac{\alpha}{u+1} - \arctan \frac{\alpha}{u-1} \right) + u\alpha \ln \left( \frac{(u+1)^2 + \alpha^2}{(u-1)^2 + \alpha^2} \right) \}. \]

(24)

Therefore from Eqs. (15) and (22) we finally obtain

\[ \Delta_{\varepsilon}^{(h)}(\alpha, u) = P_+(\alpha, u) + \frac{1}{2} [\mathcal{I}_+(\alpha, u) - \mathcal{I}_-(\alpha, u)] \]
\[ = P_+(\alpha, u) + P \int_0^\infty \mathcal{Z}^2(z) \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] \sin (Az) dz. \]

(25)

Note that in Eq. (25) at \( z = z_r(u) \), where \( 0 < z_r(u) < u - 1 \), both the real and imaginary parts of the dielectric function vanish i.e. \( \varepsilon(z_r, u) = 0 \). Therefore one needs to consider the Cauchy principal value (denoted by P) of the integral.

Eq. (25) is the generalized SPSR for a He\(^+\) ion cluster with \( \vartheta = 0 \). From the general expression (25) we shall derive below some particular SPSR for individual He\(^+\) ion and diproton cluster with \( \vartheta = 0 \).

### 2.1.1 Individual He\(^+\) ion

We can derive the SPSR for an individual He\(^+\) ion directly from Eq. (25) if we consider the limit of \( A \to \infty \). In this limit the exponential function in Eq. (23) eventually vanishes and the function \( P_+(\alpha, u) \) is defined by the first term in Eq. (23). The second term in Eq. (25) in the limit of \( A \to \infty \) must behave as \( \cos [a(u)A] \) as can be seen from Eqs. (17) and (18), where \( a(u) \) is some unspecified function of \( u \). Therefore the second term in Eq. (25) oscillates with an increasing \( A \) or interionic distance \( R \); the full integral of this term over \( u \) is damped although not necessarily vanishing as \( A \to \infty \). However, when we include a small damping in the electron gas, which is expected for any real medium, the second term in Eq. (25) vanishes as \( A \to \infty \). Thus for an individual He\(^+\) ion we find:

\[ \Delta_{\varepsilon}^{(h)}(\alpha, u) = P_\infty(\alpha, u), \]

(26)

where \( P_\infty(\alpha, u) \) is the function \( P_+(\alpha, u) \) at \( A \to \infty \).

For individual protons \( (\alpha \to \infty) \) the right-hand side of Eq. (26) behaves as

\[ P_\infty(\alpha, u) \simeq \frac{2\pi\chi^2}{3\alpha^8} (Z - 1) \to 0. \]

(27)
Consequently, in this limit we recover the known Lindhard-Winther equipartition rule (ER), \( \mathcal{I}_{sp} = \mathcal{I}_p \).

### 2.1.2 Diproton cluster with \( \vartheta = 0 \)

For a diproton cluster \((\alpha \to \infty)\) the function \( P_+ (\alpha, u) \) vanishes as in Eq. (27). Therefore for a cluster of point-like particles we find

\[
\Delta_\varepsilon^{(p)}(\alpha, u) = \mathcal{P} \int_0^\infty \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] \sin (zA) \, dz.
\]  

(28)

For individual protons \((R \to \infty \text{ or } A \to \infty)\) the RHS of Eq. (28) vanishes due to a small damping in the electron gas and again we recover the Lindhard-Winther ER.

### 2.2 \( \text{He}^+ \) ion cluster with \( \vartheta = \pi/2 \)

In order to derive an analytical expression for \( \Delta(\alpha, u) \) for a \( \text{He}^+ \) ion dicluster with \( \vartheta = \pi/2 \), we use the same integration contours \( C_1 \) and \( D_1 \) of Fig. 1, and consider the following integrals

\[
Q_\pm (\alpha, u) = \int_{C_1, D_1} \mathcal{Z}^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] \left[ 1 + H_0^{(1,2)}(Bz) \right] \, dz,
\]

(29)

where \( H_0^{(1)}(z) \) and \( H_0^{(2)}(z) \) are the Hankel cylindrical functions of the first and second kind, respectively and of zero order. We may recall that the Hankel functions are analytic inside and on the contours \( C_1 \) (for \( Q_+(\alpha, u) \)) and \( D_1 \) (for \( Q_-(\alpha, u) \)) except at the point \( z = 0 \) where they have a logarithmic singularity. Moreover, the functions \( H_0^{(1)}(z) \) and \( H_0^{(2)}(z) \) vanish on the upper and lower quadrants, respectively.

Using the theorem of residues, the functions \( Q_\pm (\alpha, u) \) are evaluated as

\[
Q_+ (\alpha, u) = -2\pi i \sum_j \frac{z_j \mathcal{Z}^2(z_j)}{\partial_z \varepsilon(z_j, u)} \left[ 1 + H_0^{(1)}(Bz_j) \right],
\]

(30)

\[
Q_- (\alpha, u) = 2\pi i \frac{z_r \mathcal{Z}^2(z_r)}{\partial_z \varepsilon(z_r, u)} \left[ 1 + H_0^{(2)}(Bz_r) \right].
\]

(31)

Then for \( \vartheta = \pi/2 \), we obtain from Eqs. (29)-(31)

\[
\Im_{sp}(\alpha, u) = \sum_j \frac{\pi z_j \mathcal{Z}^2(z_j)}{|\partial_z \varepsilon(z_j, u)|} \left[ 1 + J_0(Bz_j) \right],
\]

(32)

\[
\Im_p(\alpha, u) = \frac{\pi z_r \mathcal{Z}^2(z_r)}{\partial_z \varepsilon(z_r, u)} \left[ 1 + J_0(Bz_r) \right],
\]

(33)
which are different from the corresponding quantities for $\vartheta = 0$ given in Eqs. (17) and (18).

Using a similar procedure of calculation as in the previous section we finally find

$$\Delta_{c}^{(h)}(\alpha, u) = P_{\infty}(\alpha, u) + P \int_{0}^{\infty} Z^2(z) \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] Y_{0}(Bz) zdz \quad (34)$$

$$- \frac{2}{\pi} P \int_{0}^{\infty} \tilde{Z}^2(z) \left[ 1 - \frac{1}{\tilde{\varepsilon}(z, u)} \right] K_{0}(Bz) zdz,$$

where $\tilde{Z}(z) = Z(iz)$, $Y_{0}(z)$ is the Bessel function of the second kind and zero order, $K_{0}(z)$ is the modified Bessel function of the second kind and zero order.

After some algebraic manipulation, the last term in Eq. (34) can be shown to read:

$$\frac{2}{\pi} Z^2 \int_{0}^{\infty} \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] K_{0}(Bz) zdz \quad (35)$$

$$+ \frac{2\alpha^3}{\pi} \left[ (Z - \frac{1}{16}) \frac{\partial}{\partial \alpha} + \frac{\alpha}{16} \frac{\partial^2}{\partial \alpha^2} - \frac{\alpha^2}{48} \frac{\partial^3}{\partial \alpha^3} \right] P \int_{0}^{\infty} \frac{K_{0}(Bz)}{\alpha^2 - z^2} \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] zdz.$$

Eq. (34) is the generalized equipartition sum rule for a He$^+$ dicluster with $\vartheta = \pi/2$. In the limit $\alpha \to \infty$, we obtain the corresponding sum rule for a diproton cluster with $\vartheta = \pi/2$,

$$\Delta_{c}^{(p)}(\alpha, u) = P \int_{0}^{\infty} \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] Y_{0}(Bz) zdz \quad (36)$$

$$- \frac{2}{\pi} \int_{0}^{\infty} \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] K_{0}(Bz) zdz.$$

The first and second terms in Eq. (36) vanish as $B^{-3/2}$ and $B^{-2}$ respectively at large interionic distances. This leads again to the LW equipartition rule for point-like projectiles. Thus, in contrast to the case of an aligned dicluster with $\vartheta = 0$ (see Eq. (28)), for $\vartheta = \pi/2$ there is no need to introduce an infinitesimal damping for plasmons and single-particle excitations to get the correct limit at $B \to \infty$. This is because a fast ion moving in an electron gas excites the wake field which has different structures along and across of the direction of motion [9]. These waves are damped strongly across the direction of motion [9].

2.3 Some simple SPSR

In this subsection we will consider some useful summation rules. To derive the first of them we consider the following contour integral
\[ Q(\alpha, u) = \int_{C_1} Z^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z \ln z dz = -2\pi i \sum_j \frac{z_j Z^2_j(z_j)}{\frac{\partial}{\partial z} \varepsilon(z_j, u)} \ln z_j, \]

where the contour \( C_1 \) is shown in Fig. 1.

Now, in contrast to the previous sections we take the real part of both sides of Eq. (37). Then using similar calculational techniques as in Sec. 2.1 we find

\[ P \int_0^\infty Z^2(z) \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z \ln z dz = \frac{\pi}{2} P_\infty(\alpha, u) - P \int_0^\infty \widetilde{Z}^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z \ln z dz. \]

In a similar way we can obtain some other summation rules

\[ P \int_0^\infty Z^2(z) \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z dz = -P \int_0^\infty \widetilde{Z}^2(z) \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z dz, \]

\[ P \int_0^\infty \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z \ln z dz = -\int_0^\infty \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z \ln z dz \]

and

\[ P \int_0^\infty \Re \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] z dz = -\int_0^\infty \left[ 1 - \frac{1}{\varepsilon(z, u)} \right] zdz. \]

The singularities in the RHS of Eqs. (38) and (39) can be understood in a similar manner as in Eqs. (34) and (35).

In order to illustrate our analytical results, Eqs. (25)-(28) and (34)-(36), in Fig. 2 we present \( \Delta(\alpha, u) \) as a function of the parameter \( u = \omega/kv_F \) \( (u_0 \leq u \leq \lambda) \), where \( u_0 \) is the threshold value for plasmon excitation) for an individual He\(^+\) ion (solid line). The lines with and without circles correspond to He\(^+\) ion \( (R = 3 \text{ Å}) \) and diproton \( (R = 1 \text{ Å}) \) clusters, respectively. \( \vartheta = 0 \) (dashed lines) and \( \vartheta = \pi/2 \) (dotted lines). The numerical results are for fast projectiles \( \lambda = V/v_F = 8 \) and for density parameter \( r_s = 2.07 \) appropriate to the valence electrons in Al. \( \Delta(\alpha, u) \) as a function of \( u \) has interesting features. \( \Delta(\alpha, u) \) remains positive (\( \Im p > \Im sp \)) for He\(^+\) ion and for He\(^+\) ion cluster with \( \vartheta = 0 \) (at \( u > 2 \)) and \( \vartheta = \pi/2 \) and remains negative (\( \Im sp < \Im p \)) for diproton cluster with \( \vartheta = 0 \) and \( \vartheta = \pi/2 \). The curve for He\(^+\) ion cluster with \( \vartheta = 0 \) crosses the zero-axis for \( u \simeq 2 \). From Fig. 2 the oscillatory nature of the function \( \Delta(\alpha, u) \) can be seen for both diproton and He\(^+\) ion clusters with \( \vartheta = 0 \). Note that for a diproton cluster with \( \vartheta = \pi/2 \) at \( u = \lambda \), when the excited wave moves with the phase velocity \( \omega/k = V \), the
parameter $B$ vanishes, $B = 0$. Therefore, from Eqs. (36), (40) and (41) at $B \to 0$ follows $\Delta = 0$, i.e. the LW equipartition strongly holds. While for He$^+$ ion cluster with $\vartheta = \pi/2$ from Eqs. (34), (38) and (39) we find that the function $\Delta$ at $u = \lambda$ is two times greater than for an individual He$^+$ ion projectile. In general for the high velocity domain $\omega/k \gg v_F$ (or $u \gg 1$) all the curves decrease and an approximate LW equipartition rule, $\Im_{sp} \simeq \Im_p$ holds asymptotically. But it is also clear that in this high velocity limit the energy losses due to single-particle ($\Im_{sp}$) and plasmon ($\Im_p$) excitations decrease as well.

We may conclude with the remark that our analytical expressions are well supported by numerical results.

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**Figure Captions**

Fig. 1. Illustration of contours $C_1$ and $D_1$, in complex $z$ plane. Isolated point $P$ below real $z$ axis indicates plasmon pole. Group of crosses above real $z$ axis indicates poles in single-particle excitations.

Fig. 2. The function $\Delta(\alpha, u)$ vs parameter $u$ for $\lambda = 8$. Individual He$^+$ ion (solid line), diproton cluster with $R = 1 \, \text{Å}, \vartheta = 0$ (dashed line without circles) and $\vartheta = \pi/2$ (dotted line without circles), He$^+$ ion cluster with $R = 3 \, \text{Å}, \vartheta = 0$ (dashed line with circles) and $\vartheta = \pi/2$ (dotted line with circles). The density parameter is $r_s = 2.07$ (Al target).
The diagram illustrates a complex plane labeled as $z$-Plane. It contains two closed contours $C_1$ and $C_2$, and two open contours $D_1$ and $D_2$. The points $+i\alpha$ and $-i\alpha$ are marked on the plane, indicating the orientation of these contours.
$\Delta(\alpha, u)$