Self-energy of a moving charged particle in the presence of a metal surface

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The general expression for the self-energy of a moving charged particle interacting with a metal surface has been derived for its above-threshold speed. The dispersion of the surface as well as bulk plasmon has been taken into account. Expressions for the energy loss and the effective mass of the incident charged particle have been also derived. Numerical results for the self-energy, energy loss, and the effective mass of the incident charged particle have been presented. It is found that effects of plasmon dispersion are quite significant.

I. INTRODUCTION

There has been considerable interest in the study of the interaction of a moving charged particle with a polarizable medium, which can be a solid surface, metal-insulator interface, etc. The knowledge of the interaction potential is useful in the interpretation of a large number of experiments, such as reflection electron-energy-loss experiments and low-energy electron-diffraction experiments. Attempts have been made to study the interaction potential in the classical[1-3] semiclassical[4] as well as in the quantum-mechanical framework. The interaction of the incident charged particle (ICP) with the excitations of the medium has been considered a quantum-mechanical description and related to the self-energy of the ICP.[5-8]

The self-energy is a function of the distance between the ICP and the metal surface and is a complex quantity. The real part of the self-energy saturates to a finite negative value at the surface and this becomes equal to the classical image-potential value very far away from the metal surface. There are two factors which are responsible for this saturation. One of them is the dispersion of the plasmons which leads to the screening of the ICP when it is inside or outside the metal surface. The second factor is a quantum-mechanical one, arising out of the real emission or reabsorption of the plasmons, depending upon the speed of the ICP. If the ICP has a speed above a certain threshold value, it is capable of creating real surface- and bulk-plasmon excitations (see Fig. 1) in the medium. On the other hand if its speed is below the threshold value, it creates virtual plasmon excitations in the medium. The imaginary part of the self-energy can be divided into conservative and nonconservative parts. The conservative imaginary part of the self-energy is antisymmetric in energy when ICP comes outside from the surface compared to the case when it enters in the metal surface. The nonconservative imaginary part is associated with the energy loss by the ICP. Mahanty, Pathak, and Paranjape[10,11] and Pathak and Paranjape[12] have calculated the self-energy of the ICP, taking dispersion effects into account for a below-threshold speed of the ICP. For the case of above-threshold speed, they have neglected the dispersion effects. In the present work, we derive general expressions for the self-energy of a moving charged particle for speeds of the ICP above the threshold value, taking dispersion effects into account.

The plan of the paper is as follows. In Sec. II we derive a general expression for the self-energy. In Sec. III we derive an expression for the energy loss and effective mass of the ICP. Section IV contains results and discussions.

II. GENERAL EXPRESSION FOR THE SELF-ENERGY

A. Interaction Hamiltonian

The Hamiltonian of the ICP of charge Q and mass M and the metal surface is

$$H=\frac{p^2}{2M}+\sum_{\lambda}\hbar\omega_{\lambda}(a_{\lambda}^{\dagger}a_{\lambda}+\tfrac{1}{2})+H^1 , \tag{1}$$

where $a_{\lambda}^{\dagger}$ and a_{λ} are the creation and annihilation operators of the quanta of plasmons in the metallic electron gas, λ being the index $\boldsymbol{\kappa}$ and $\boldsymbol{\kappa},q$ specifying the surface and bulk plasmon, respectively. The interaction Hamiltonian $H^1(=H_s^1+H_B^1)$ between the ICP and the metal surface is given in the hydrodynamical model as

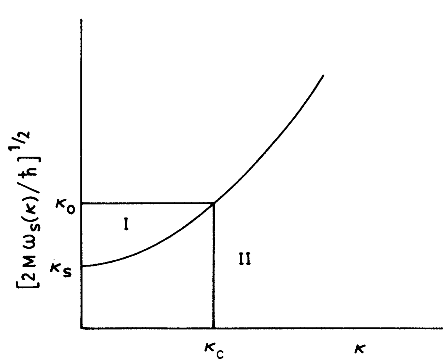

FIG. 1. Dispersion curve for surface and bulk plasmons (schematic).

$$H_s^1 = -Q \sum_{\kappa} \exp(i\boldsymbol{\kappa}\cdot R)(a_{-\kappa}+a_{\kappa}^{\dagger})\{\Theta(-z)B_1 \exp(-\kappa z)+\Theta(z)[B_2 \exp(\kappa z)+B_3 \exp(\gamma z)]\} , \tag{2}$$

$$H_B^1 = -Q \sum_{\kappa,q} \exp(i\boldsymbol{\kappa}\cdot R)(a_{-\kappa,q}+a_{\kappa}^{\dagger},q)\{\Theta(-z)c_1 \exp(-\kappa z)+\Theta(z)[c_2 \exp(\kappa z)+c_3 \cos(qz)+c_4 \sin(qz)]\} , \tag{3}$$

where B_1, B_2, B_3, c_1, c_2, c_3, and c_4 are the coupling parameters and can be obtained from the work of Barton.[13] These are explicitly given by Pathak and Paranjape.[12] In Eqs. (2) and (3) $\boldsymbol{\kappa}$ and $\mathbf{q}$ are the wave vectors of plasmon parallel and perpendicular to the metal surface and $\Theta(z)=1$ for $z>0$ and $\Theta(z)=0$ otherwise.

B. Self-energy of the particle

Manson and Ritchie[5] have expressed the self-energy in terms of the interaction Hamiltonian which is given as

$$E(k_0,z)=\sum_{n,k} \frac{\exp[ir\cdot(\mathbf{k}_0-\mathbf{k})]\langle 0,\mathbf{k}0|H^1|n,\mathbf{k}\rangle\langle n|H^1|0\rangle}{\varepsilon_0(k_0)-\varepsilon_n(k)+i\delta} , \tag{4}$$

where $\varepsilon_n(k)$ is the energy of the system with the plasmon in the state $|n\rangle$ and the ICP in the plane-wave state $|k\rangle\cdot|0\rangle$ and $|k_0\rangle$ are the initial state of the plasmons and the ICP with momentum $\hbar k_0$, respectively. The speed of the ICP is described by $k_0=(\kappa_0,q_0)$, where κ_0 is its component parallel to the metal surface and q_0 is the component perpendicular to the metal surface. After inserting the interaction Hamiltonian and evaluating the matrix elements in Eq. (4) we get the expression for the surface and bulk part of the self-energy given as

$$E_s(z)=-\frac{2M}{\hbar^2}\frac{1}{2\pi}\sum_k \int \frac{dk_3}{D_1} \exp(ik_3 z)[\Theta(-z)B_1 \exp(+\kappa z)+\Theta(z)B_2 \exp(-\kappa z)+B_3 \exp(=\gamma z)]$$
$$\times\left[\frac{B_1}{\kappa-ik_3}+\frac{B_2}{\kappa+ik_3}+\frac{B_3}{\gamma+ik_3}\right] , \tag{5}$$

where $D_1=k_3^2+2q_0k_3+\kappa^2+k_s^2+2\kappa_0\cdot\kappa-i\delta$, $k_s^2=2M\omega_s/\hbar$, and

$$E_B(z)=-\frac{2M}{\hbar^2}\frac{1}{2\pi}\sum_{k,q}\int \frac{dk_3}{D_2} \exp(ik_3 z)\{\Theta(-z)c_1 \exp(\kappa z)+\Theta(z)[c_2 \exp(-\kappa z)+c_3 \cos(qz)+c_4 \sin(qz)]\}$$
$$\times\left[\frac{c_1}{\kappa-ik_3}+\frac{c_2}{\kappa+ik_3}+\frac{c_4-ic_3}{2(k_3-q+i\varepsilon)}-\frac{c_4+ic_3}{2(k_3+q-i\varepsilon)}\right] , \tag{6}$$

where $D_2=k_3^2+2q_0k_3+\kappa^2+k_B^2+2\kappa_0\cdot\kappa-i\delta$, $k_B^2=2M\omega_B/\hbar$. Here δ and ε are infinitesimally small positive quantities. The limit of $\varepsilon\rightarrow 0^+$ is taken after the integration over k_3 in Eq. (6). The above expressions for the self-energy of the ICP are quite general and are valid for any arbitrary speed of the ICP.

In order to integrate over k_3 in Eqs. (5) and (6) we have to proceed separately depending upon whether the speed of the ICP is above threshold at some value. If the speed of the ICP is below threshold the integration in Eqs. (5) and (6) can be done by closing the contour in the upper or lower half of the k_3 plan depending upon whether $z>0$ or $z<0$. Expressions thus obtained are exactly the same as that obtained by Mahanty, Pathak, and Paranjape.[10]

The integration in Eqs. (5) and (6) can be done for the above-threshold speed of the particle with the help of Fig. 1. In this figure we plot $[2M\omega_s(\kappa)/\hbar]^{1/2}$ vs κ or $[2M\omega_B(k)/\hbar]^{1/2}$ vs k. For a given speed of the incident charged particle the k_0 line divides the dispersion curve for surface and bulk plasmons into two regions I and II. Region I corresponds to excitations of the real surface or bulk plasmons whereas region II corresponds to the virtual surface or bulk-plasmon excitations. The point of intersection of the k_0 line with the dispersion curve is obtained by solving equation $(\hbar^2k_0^2)/2M=\hbar\omega_s(\kappa)$, which gives

$$\kappa_c^2=M^2\left[\frac{\hbar^2k_0^4}{2M^2}-\omega_p^2\right]^2\Big/\beta^2\hbar^2k_0^4 .$$

A similarly critical wave number dividing regions I and II for the bulk-plasmon case is found to be

$$k_c^2=\left[\left[\frac{\hbar^2k_0^2}{2M}\right]^2-\omega_p^2\right]\Big/\beta^2 .$$

Now the integration in Eqs. (5) and (6) for the above-threshold case can be done easily by choosing the appropriate contour. The results for the surface part of the self-energy are

$$E_s(z)=-Q^2\left[\frac{M}{\hbar^2}\right]\sum_k [B_2\exp(-\kappa z)+B_3\exp(-\gamma z)]\Theta(\kappa_c^2-\kappa^2)$$
$$\times\left\{\Theta\frac{(u_s^2)}{u_s}\left[e^{-i(q_0-u_s)z}\left[\frac{B_1}{q_0-u_s-i\kappa}-\frac{B_2}{q_0-u_s+i\kappa}-\frac{B_3}{q_0-u_s+i\gamma}\right]\right.\right.$$
$$\left.-\frac{2B_2u_s\exp(-\kappa z)}{(\kappa-iq_0)^2+u_s^2}-\frac{\exp(-\gamma z)2B_3u_s}{(\gamma-iq_0)^2+u_s^2}\right]$$
$$+\frac{\Theta(v_s^2)}{v_s}\left[e^{-(v_s+iq_0)z}\left[\frac{B_1}{\kappa+v_s-iq_0}+\frac{B_2}{\kappa-v_s-iq_0}+\frac{B_3}{\gamma-v_s+iq_0}\right]\right.$$
$$\left.\left.-\frac{\exp(-\kappa z)2B_2v_s}{(\kappa-iq_0)^2-v_s^2}-\frac{2B_3v_s\exp(-\gamma z)}{(\gamma-iq_0)^2-v_s^2}\right]\right\} \tag{7a}$$

for $z>0$. The corresponding self-energy for $z<0$ is

$$E_s(z)=-Q^2\left[\frac{M}{\hbar^2}\right]\sum_k B_1\exp(-\kappa|z|)\Theta(\kappa_c^2-\kappa^2)\left\{\frac{\Theta(u_s^2)}{u_s}\left[e^{i(q_0+u_s)|z|}\left[\frac{B_1}{q_0+u_s-i\kappa}-\frac{B_2}{q_0+u_s+i\kappa}-\frac{B_3}{q_0+u_s+i\gamma}\right]\right.\right.$$
$$\left.+\frac{2B_1u_s\exp(-\kappa|z|)}{(q_0-i\kappa)^2-u_s^2}\right]$$
$$+\frac{\Theta(v_s^2)}{v_s}\left[e^{i(q_0+iv_s)|z|}\left[\frac{B_1}{\kappa+iq_0-v_s}+\frac{B_2}{\kappa+v_s-iq_0}+\frac{B_3}{\gamma+v_s+iq_0}\right]\right.$$
$$\left.\left.-\frac{2B_1v_s\exp(-\kappa|z|)}{(\kappa+iq_0)^2-v_s^2}\right]\right\}. \tag{7b}$$

The bulk contribution can be obtained from Eq. (6) and is given by

$$E_B(z)=-\frac{2M}{\hbar^2}\frac{1}{2\pi}\sum_{k,q}[c_2\exp(-\kappa z)+c_3\cos(qz)-c_4\sin(qz)]\Theta(k_c^2-k^2)$$
$$\times\left\{\Theta(u_B^2)\frac{e^{-i(q_0-u_B)z}}{2u_B}\left[\frac{c_1}{q_0-u_B-i\kappa}-\frac{c_2}{q_0-u_B+i\kappa}-\frac{c_3+ic_4}{2(q_0+q-u_B-i\delta)}-\frac{c_3-ic_4}{2(q_0-q-u_B-i\delta)}\right.\right.$$
$$\left.+\frac{c_2\exp(-\kappa z)}{(q_0+i\kappa)^2-u_B^2}+\frac{(c_3+ic_4)e^{-iqz}}{2[(q_0-q)^2+u_B^2-i\delta]}+\frac{(c_3+ic_4)e^{iqz}}{2[(q_0+q)^2-u_B^2-i\delta]}\right]$$
$$+\Theta(v_B^2)\left[\frac{e^{-v_Bz}}{2v_B}e^{iq_0z}\left[\frac{c_1}{\kappa+v_B+iq_0}+\frac{c_2}{\kappa-v_B-iq_0}-\frac{c_4-ic_3}{2(q_0+q-iv_B)}+\frac{c_4+ic_3}{2(q_0-q-iv_B)}\right]\right.$$
$$\left.\left.+\frac{c_2\exp(-\kappa z)}{(q_0+i\kappa)^2+v_B^2}+\frac{(c_3+ic_4)e^{iqz}}{2[(q_0+q)^2+v_B^2]}+\frac{(c_3-ic_4)e^{-iq|z|}}{2[(q_0-q)^2+v_B^2]}\right]\right\},$$

$$u_B^2=q_0^2-\kappa^2-k_B^2\ ;\ v_B^2=-u_B^2., \tag{8a}$$

for $z>0$. Similarly the corresponding expression for $z<0$ is given by

$$E_B(z)=-\frac{2M}{\hbar^2}\frac{1}{2\pi}\sum_{k,q} c_1\exp(-\kappa|z|)\Theta(k_c^2-k^2)$$

$$\times\Bigg\{\Theta(u_B^2)\left[\frac{e^{i(q_0+u_B)|z|}}{2u_B}\left\{\frac{c_1}{q_0+u_B-i\kappa}-\frac{c_2}{q_0+u_B+i\kappa}-\frac{c_3+ic_4}{2(q_0+q+u_B+i\delta)}-\frac{c_3-ic_4}{2(q_0-q+u_B+i\delta)}\right\}+\frac{c_1e^{-\kappa|z|}}{(q_0-i\kappa)^2-u_B^2}\right]$$

$$+\Theta(v_B^2)\left[\frac{e^{-v_B|z|}}{2v_B}e^{iq_0|z|}\left\{\frac{c_1}{\kappa-v_B+iq_0}+\frac{c_2}{\kappa+v_B-iq_0}-\frac{c_4-ic_3}{2(q_0+q+iv_B)}+\frac{c_4+ic_3}{2(q_0-q+iv_B)}+\frac{c_1e^{-\kappa|z|}}{(q_0-i\kappa)^2+v_B^2}\right\}\right]\Bigg\}\,. \tag{8b}$$

Expressions for the self-energy given by Eqs. (7) and (8) take into account quantal motion of the incident charged particle as well as dispersion effects of surface and bulk plasmons. In the dispersionless limits expressions for the surface, and bulk contribution to self-energy can be easily obtained from Eqs. (7) and (8). These agree with that obtained by Mahanty, Pathak, and Paranjape. [The energy denominator in the fifth and sixth term of the bulk part of the self-energy, i.e., Eq. (14a), should have $+i\delta$ instead of $-i\delta$.] However, the more useful form of these expressions is given as

$$E_s(z)=-\frac{\kappa_p^2}{2}\left[\int_0^\infty\frac{e^{-2\kappa z}}{\kappa_p^2+2iq_0\kappa}d\kappa+e^{-iq_0z}\int_0^{(q_0^2-\kappa_s^2)^{1/2}}\frac{e^{(iu_s-\kappa)z}\kappa}{u_s(2q_0^2-\kappa_s^2-2q_0u_s)}d\kappa+e^{-iq_0z}\int_{(q_0^2-\kappa_s^2)^{1/2}}^\infty\frac{\kappa}{v_s}\frac{e^{-(k+v_s)z}}{(2q_0^2-\kappa_s^2-2iq_0v_s)}d\kappa\right], \tag{9a}$$

for $z>0$ and

$$E_s(z)=-\frac{\kappa_p^2}{2}\left[\int_0^\infty\frac{e^{-2\kappa|z|}}{\kappa_p^2-2iq_0\kappa}d\kappa+e^{iq_0|z|}\int_0^{(q_0^2-k_s^2)^{1/2}}\frac{\kappa}{u_s}\frac{e^{(iu_s-\kappa)|z|}}{(2q_0^2-\kappa_s^2+2q_0u_s)}d\kappa+e^{iq_0|z|}\int_{(q_0^2-\kappa_s^2)^{1/2}}^\infty\frac{\kappa}{v_s}\frac{e^{-(\kappa+v_s)|z|}}{(2q_0^2-\kappa_s^2+2iq_0v_s)}d\kappa\right], \tag{9b}$$

for $z<0$. The corresponding bulk contribution for $z<0$ is

$$E_B(z)=-\frac{Q^2\kappa_B^2}{4}\int_0^\infty\frac{\kappa_B^2}{(\kappa_B^4+4\kappa^2q_0^2)}d\kappa-\frac{Q^2\kappa_B^2}{2}\int_0^\infty\frac{\kappa}{u_B}\frac{(2q_0^2-\kappa_B^2)}{(\kappa_B^4+4\kappa^2q_0^2)}d\kappa+\frac{Q^2\kappa_B^2}{(4\pi)^2}$$

$$\times\int_0^\infty d^2\kappa\left[\Theta(u_B^2)\left[\frac{e^{-2\kappa z}}{\kappa(\kappa_B^2+2i\kappa q_0)}+\frac{i}{u_B}\frac{e^{-\kappa z}e^{-i(q_0-u_B)z}}{2q_0^2-\kappa_B^2-2q_0u_B}\right]+\frac{\Theta(v_B^2)}{v_B}\frac{e^{-v_Bz}e^{-iq_0z}}{2q_0^2-\kappa_B^2-2iq_0v_B}\right], \tag{10}$$

where $u_s^2=q_0^2-\kappa^2-\kappa_s^2$; $v_s^2=-u_s^2$, for $z<0$, $E_B(z)=0$. The above expressions contained in Eqs. (9) and (10) can be easily separated into its real and imaginary parts and can be cast in the same form as recently given by Sols and Ritchie.[14] At the surface (i.e., $z=0$) the imaginary part of the self-energy is given as

$$E_s''(z=0^\pm)=-\frac{\kappa_s^2Q^2}{4\pi}\int_0^{(q_0^2-\kappa_s^2)^{1/2}}\frac{\kappa}{u_s}\frac{(2q_0^2-\kappa_s^2)}{\kappa_s^4+4\kappa^2q_0^2}d\kappa \tag{11}$$

which can be evaluated analytically to be as

$$E_s''(z=0^\pm)=\frac{\kappa_s^2Q^2}{8q_0}\left[\ln\left[1-\frac{2q_0(q_0^2-\kappa_s^2)^{1/2}}{2q_0^2-\kappa_s^2}\right]-\ln\left[1+\frac{2q_0(q_0^2-\kappa_s^2)^{1/2}}{2q_0^2-\kappa_s^2}\right]\right]. \tag{12}$$

Equation (12) is the total contribution of imaginary part of the self-energy at the surface. It can be shown by manipulation that Eq. (12) contains both conservative and nonconservative imaginary parts of the self-energy in agreement with the results of Mahanty, Pathak, and Paranjape.[10]

III. EXPRESSION FOR THE ENERGY LOSS OF THE ICP

The self-energy for all speeds of the ICP can be obtained either from Eq. (8b) or from Eq. (12b) of Mahanty, Pathak and Paranjape. It is given as

$$E_B(z\to\infty,k_0)=-\frac{Q^2\kappa_p^2}{2\pi k_0}\int_0^\infty dk\frac{1}{(1+Ak^2/\kappa_p^2)^{1/2}}\ln\left[\frac{k^2+\kappa_p^2(1+Ak^2/\kappa_p^2)^{1/2}+2kk_0}{k^2+\kappa_p^2(1+Ak^2/\kappa_p^2)^{1/2}-2kk_0}\right] . \quad (13)$$

It can be seen from Eq. (13) that $E_B(z\to+\infty,k_0)$ is always real for $k_0>\kappa_p$ and is given by

$$E_B'(z\to\infty,k_0)=-\frac{Q^2\kappa_p^2}{2\pi k_0}\int_0^\infty \ln\left|\frac{k^2+\kappa_p^2(1+Ak^2/\kappa_p^2)^{1/2}+2kk_0}{k^2+\kappa_p^2(1+Ak^2/\kappa_p^2)^{1/2}-2kk_0}\right|dk . \quad (14)$$

On the other hand it is imaginary for $k_0>\kappa_p$ which is

$$E_B''(z\to+\infty,k_0)=-\frac{Q^2\kappa_p^2}{2k_0}\int_{k_{\min}}^{k_{\max}}dk\frac{1}{(1+Ak^2/\kappa_p^2)^{1/2}} , \quad (15)$$

where $k_{\min}$ and $k_{\max}$ are obtained from the argument of the logarithmic term in Eq. (13). The result obtained is

$$E_B''(z\to\infty,k_0)=-\frac{Q^2\kappa_p^2}{2k_0}\left[\ln\left[\frac{k_0+(k_0^2-\kappa_p^2)^{1/2}}{k_0-(k_0^2-\kappa_p^2)^{1/2}}\right]+\ln\left[\frac{k_p+\{\kappa_p^2+A[2q_0^2-\kappa_p^2-2k_0(k_0^2-\kappa_p^2)^{1/2}]^{1/2}\}}{\kappa_p+\{\kappa_p^2+A[2q_0^2-\kappa_p^2+2k_0(k_0^2-\kappa_p^2)^{1/2}]^{1/2}\}}\right]\right] . \quad (16)$$

The first term in Eq. (16) is the result when dispersion effects are neglected and the second term is the contribution due to the plasmon dispersion effects. The energy loss of the ICP is related with the imaginary part of the self-energy according to the relation

$$\frac{dE}{dz}=\frac{w_p}{2\pi u_0}E_B''(z\to+\infty,k_0) . \quad (17)$$

In the dispersionless limits our result for the energy loss of the ICP reduces to that obtained by Mahanty, Pathak, and Paranjape and by Sols and Ritchie.[14]

Effective mass of the ICP

It is also of interest to calculate the effective mass of the ICP in the presence of a metal surface. Obviously the effective mass of the ICP in the presence of a metal surface depends upon its distance from the metal surface. It will approach the free-particle mass when the ICP is very far away from the metal surface. The depth inside the metal effective mass can be obtained from Eq. (14) by expanding it to the $O(k_0^2)$ and using the definition

$$\frac{1}{M^*}=-\frac{1}{\hbar^2}\frac{d^2E}{dk_0^2} . \quad (18)$$

It is given by

$$M^*=\frac{M}{1+\alpha} , \quad (19)$$

where

$$\alpha=-\frac{4\kappa_p^2}{3\pi}k_0^2M\int_0^\infty dk\frac{k^2}{(1+Ak^2/\kappa_p^2)^{1/2}}\times\frac{1}{[k^2+\kappa_p^2(1+Ak^2/\kappa_p^2)^{1/2}]^3} . \quad (20)$$

The integral given in Eq. (20) can be calculated analytically but it is too lengthy to be of practical value. However in the dispersionless case it is simple and is equal to

$$\alpha=-\frac{Q^2M}{6\kappa_p\hbar^2}=-\left[\frac{M}{m}\right]^{1/2}\frac{Q^2}{e^2}\frac{r_s^{3/4}}{6\sqrt{2}3^{1/4}} , \quad (21)$$

where r_s is the dimensionless electron density parameter. Our result in Eq. (21) agrees with that obtained by Sols and Ritchie.[14] The value of the α can be easily calculated in Eq. (20) when dispersion effects are included by numerical integration.

IV. RESULTS AND DISCUSSIONS

We now proceed to the numerical calculation of the complex self-energy of the ICP for its above-threshold speed. Its real and imaginary parts are easily separated for Eqs. (7a) and (7b). There are poles on the real axis in some term of the bulk contribution to the self-energy given by Eqs. (8a) and (8b). For these terms the real and the imaginary parts are obtained by using the identity

$$\frac{1}{x+i\delta}=\mathrm{P}(x)-i\pi\delta(x)\ , \tag{22}$$

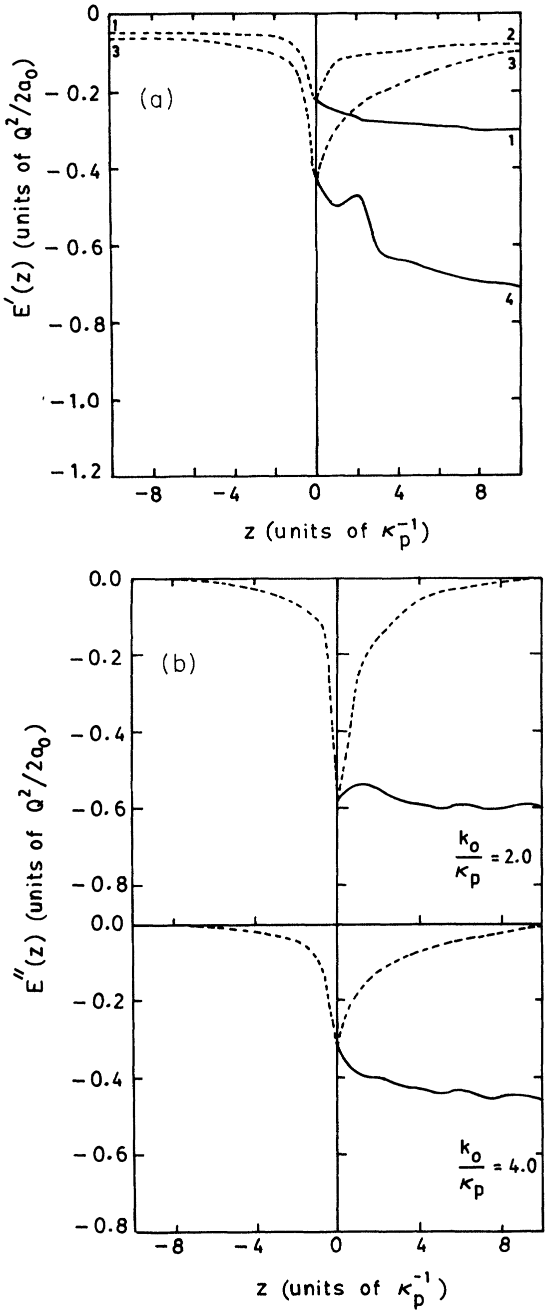

FIG. 2. (a) Real part of the self-energy for the dispersionless case. Dashed (3,3) and solid (3,4) lines represent the surface and the total contribution for speed $k_0=2\kappa_p$ of the incident charged particle. Curves (1,2) and (1,1) represent the same contribution but for speed $k_0=4\kappa_p$. (b) Imaginary part of the self-energy for the dispersionless case. Dashed and solid curves represent the surface and the total contribution for speed $k_0=2\kappa_p$ and $4\kappa_p$, respectively.

where P stands for the principal value. The real and the imaginary parts arising from Eq. (22) do not have a fixed parity with respect to k_0 whereas other terms do have a fixed parity. We replace the summation in Eqs. (7) and (8) by integration as

$$\sum_{k}\to\int_0^\infty\int_0^{2\pi}k\,dk\,d\Theta,\quad \sum_{k,q}\to\int_0^\infty\int_0^\infty\int_0^{2\pi}k\,dk\,dq\,d\Theta$$

and we use the Simpson method for numerical integration.

The self-energy has been calculated for two speeds of the ICP, namely, $k_0/\kappa_p=2$ and 4. In Figs. (2a) and (2b)

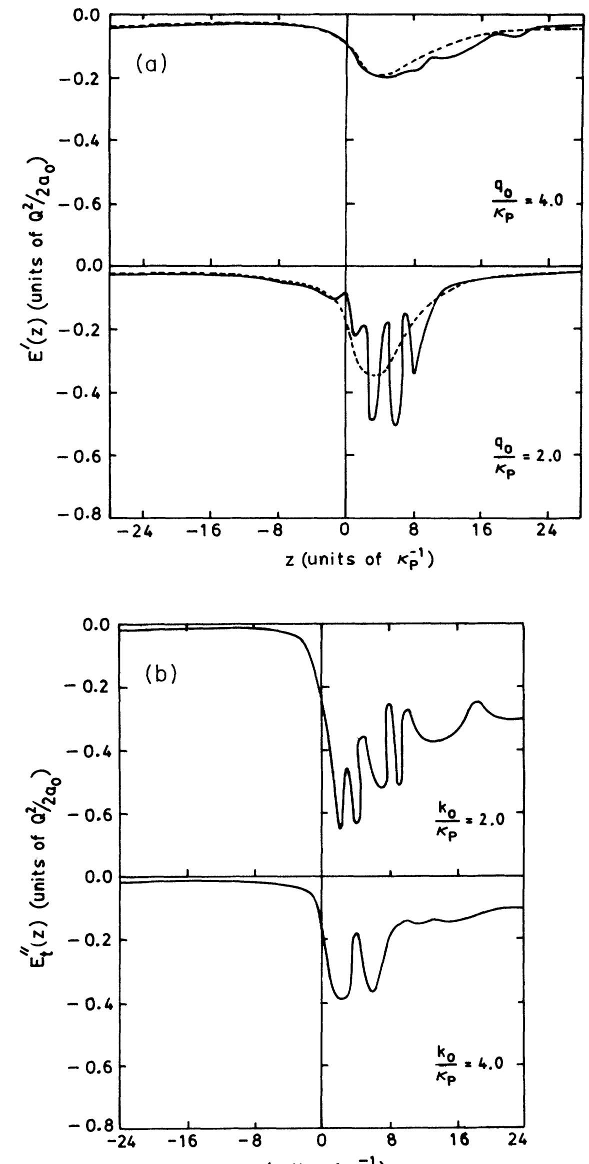

FIG. 3. (a) Real part of the self-energy for the dispersion included case. Dashed and solid curves represent the surface and total contribution for speed $k_0=2\kappa_p$ and $4\kappa_p$, respectively. (b) Imaginary part of the self-energy for the dispersion included case. Dashed and solid curves represent the surface and total contribution for speed $k_0=2\kappa_p$ and $4\kappa_p$, respectively.

we have plotted the real and the imaginary parts of the self-energy of the ICP for the dispersionless case. Surface and total contribution are shown by dashed and solid curves, respectively. At the surface and outside the surface bulk contribution to the self-energy is zero for the dispersionless case. From Figs. 2(a) and 2(b) we observe small oscillation in the real and the imaginary parts of the self-energy when the particle is inside the surface. In Figs. 3(a) and 3(b) we have plotted the real and the imaginary parts of the self-energy when the dispersion of the surface as well as bulk plasmons are included. Here also the dashed and the solid curves represent the surface and the total contribution to the self-energy. It is seen from Figs. 2 and 3 that the numerical value of the self-energy decreases when we take dispersion effects that are included. At the surface for the dispersionless case the numerical value of the real and imaginary parts of the self-energy of the ICP are equal to -0.43 and -0.58, respectively, for speed $k_0=2\kappa_p$. For the dispersion included case these values reduce to -0.09 and -0.28, respectively. Therefore effects of plasmon dispersions are very significant.

We have separated the total imaginary part into conservative and nonconservative imaginary parts. The conservative imaginary part does not represent any dissipation effects while the nonconservative imaginary part is associated with the energy loss by the ICP. In Fig. 4 we have plotted the total conservative and nonconservative imaginary part of the self-energy by dashed and solid curves, respectively, when the dispersion effects of the plasmons are taken into account. It is seen from Fig. 4 that the nonconservative imaginary part oscillates when the ICP is inside the metal surface and oscillations decrease when we increase the speed of the ICP. The oscillatory nature of the imaginary part of the self-energy is because of the quantum nature of the interaction and partly due to finite speed of the ICP.

We calculate the energy loss of the ICP when it is very deep inside the metal surface from Eq. (16) for its speed $k_0=2\kappa_p$. In Eq. (16) we have obtained an analytic result

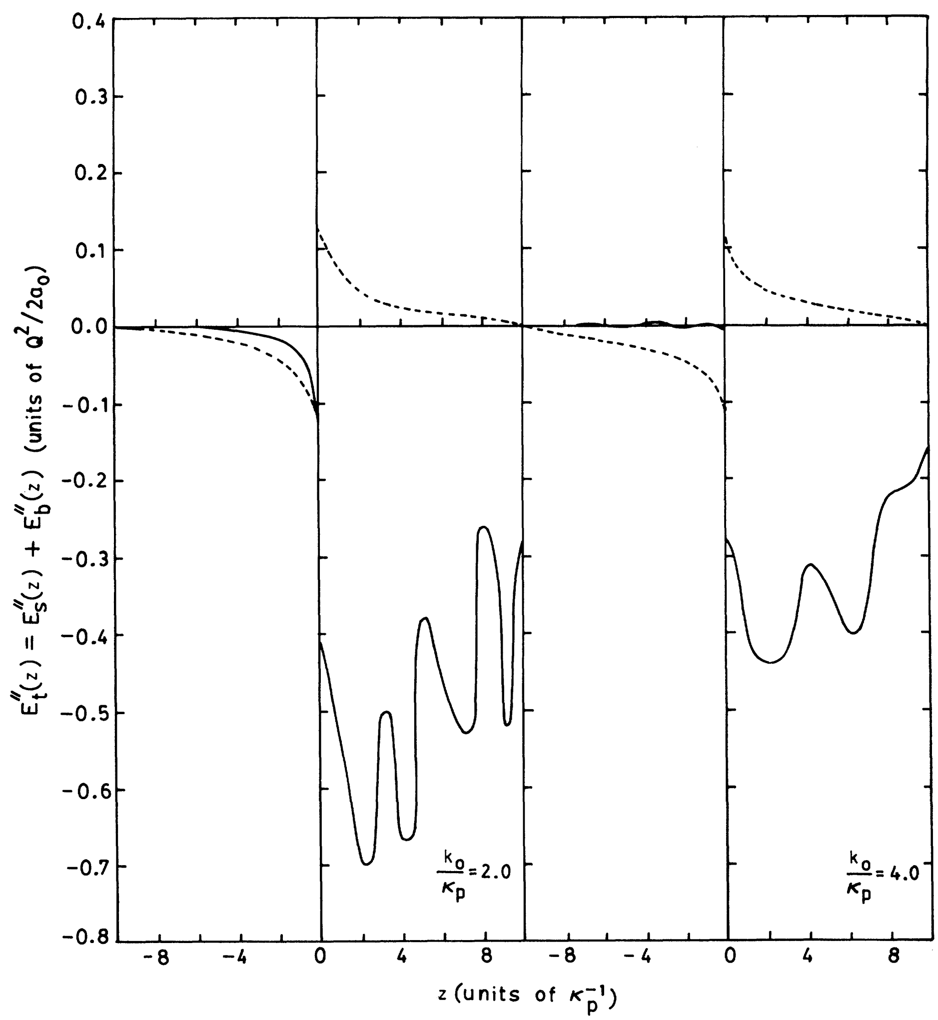

FIG. 4. (a) Dashed and solid curves represent the total conservative and nonconservative imaginary parts of the self-energy for the dispersion included case for speed $k_0=2\kappa_p$. (b) is the same as (a) except for speed $k_0=4\kappa_p$.

for the imaginary part of the self-energy when ICP goes very deep inside the metal surface (i.e., $z \rightarrow +\infty$). From this we obtain the values of the imaginary part of the self-energy equal to -0.58 and -0.35 for dispersion effects excluded and included, respectively. This implies that the value of the energy loss by the ICP decreases by 39% when dispersion effects are included for its speed equal to $2\kappa p$. Our computed results for the real and the imaginary parts of the self-energy also attain a constant value in the $z \rightarrow \infty$ limits as shown in the Figs. 3(a) and 3(b) and are in good agreement with the results obtained from Eq. (16).

We also calculate the effective mass of the ICP when it is deep in the bulk from Eq. (20). For the case of the ICP being an electron it is found that $M^* = 1.14M$ and $M^* = 1.24M$ for the dispersion effects included and excluded, respectively. This amounts to about a 9% decrease in the value of the effective mass of the electron when dispersion effects are included.

In this paper we have derived the general expressions for the self-energy of the ICP interacting with a metal surface within the hydrodynamical model. The numerical results are presented for two speeds of the charged particle for the above-threshold case and for excluding as well as for including dispersion effects. It is found that the contribution to the self-energy arising due to spatial dispersion effects of plasmons is quite substantial and must be taken into account. This work along with the earlier work of Mahanty, Pathak, and Paranjape provides a complete theory for the complex self-energy of moving charged particles interacting with a metal surface.

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[1]P. M. Echenique and J. B. Pendry, J. Phys. C **8**, 2936 (1976).

[2]N. Takimoto, Phys. Rev. **146**, 366 (1966).

[3]J. Harris and R. O. Jones, J. Phys. C **7**, 3751 (1974).

[4]F. Flores and F. Garcia-Molinear, J. Phys. C **12**, 907 (1979).

[5]J. R. Manson and R. H. Ritchie, Phys. Rev. B **24**, 4867 (1981).

[6]W. L. Schaich, *Many-Body Phenomena at Surfaces,* edited by D. Langreth and H. Suhl (Academic, New York, 1984), p. 265.

[7]J. Henrich, Phys. Rev. B **8**, 1316 (1973).

[8]A. G. Equiluz, Phys. Rev. B **23**, 1542 (1981).

[9]R. E. Dietz, E. G. McRae, and R. L. Campbell, Phys. Rev. Lett. **45**, 1280 (1980).

[10]J. Mahanty, K. N. Pathak, and V. V. Paranjape, Phys. Rev. B **33**, 2333 (1986).

[11]J. Mahanty, K. N. Pathak, and V. V. Paranjape, Solid State Commun. **54**, 649 (1985).

[12]K. N. Pathak and V. V. Paranjape II, Nuovo Cimento **8**, 52 (1986).

[13]G. Barton, Rep. Prog. Phys. **42**, 963 (1979).

[14]F. Sols and R. H. Ritchie, Surf. Sci. **194**, 275 (1988).