Self-energy of a moving charge in the presence of a metal surface

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Quantum-mechanical expressions for the potential energy of a moving charged particle interacting with a metal surface are derived using the self-energy formalism. The expressions include the contributions of the surface and the bulk plasmons in the hydrodynamic model. It is found that the saturation of the image potential at $z=0$ arises due to both the plasma dispersions and quantum recoil arising from the plasmon exchange and that the contributions of these two are not additive. Numerical results for the real and imaginary parts of the self-energy are presented for four speeds of the incident particle moving normal to the surface.

I. INTRODUCTION

The interaction of a charged particle with a polarizable medium has been the subject of extensive studies in the past, first in the framework of classical electrodynamics where the medium is regarded as a dielectric continuum, and later in the quantum-mechanical framework where the response of the medium through the interaction of the charged particle with the excitations of the system is considered. The interaction energy of the charged particle is of direct relevance to the interpretation of experimental data on surface excitations obtained through electron-energy-loss spectroscopy and through reflection electron-energy-loss spectroscopic experiments. This interaction energy can be interpreted as the self-energy of the charged particle originating from the induced charge polarizations associated with the excitations of the medium.[1–4]

In the presence of a surface, the real part of the self-energy at a large distance from the surface approaches to its classical image-potential value, while the imaginary part is related with the damping of the scattered particles from the incident beam. When the particle approaches the surface the interaction energy saturates to a finite negative value. This has been recently demonstrated experimentally[5] and has stimulated analysis[1] of the interaction potential in close proximity of the surface. There are two factors leading to this saturation. The first is the dispersion of plasmons, both bulk and surface. This leads to screening of the charge when it is at the surface or inside the metal, and hence to a finite self-energy. This effect has been analyzed in various semiclassical approaches to the problem.[3,4] The second factor is essentially quantum mechanical, arising out of the virtual or real emission and reabsorption of plasmons by the particle, depending on whether its energy is below or above the threshold energy for production of plasmons. This effect has been analyzed for a model of surface plasmons which do not have dispersion.[1]

The purpose of this paper is to present an analysis of the interaction potential of a moving charge particle in the presence of a metal surface using the self-energy formalism[1] and the hydrodynamical model for the metallic electrons. We obtain the explicit variation of the interaction potential of the charged particle with distance from the surface by considering the combined effects of the plasmon dispersion and the quantum recoil, the two effects being nonadditive.

In spite of the known limitations of the hydrodynamical model, it provides the main effects associated with the collective excitations of the metallic electrons rather easily. It is known that the model does not include the effect of the excitation of the electron-hole pairs. The effect should be included in a more complete theory. Since the image-type interaction arises primarily from the interaction of the external charge with the collective plasmon modes of the metal, most of the work in this field use models that give the correct collective behavior of the metallic electrons. A phenomenological way of including the effect of the electron-hole pairs would be through introducing the damping of plasmons. This alters the value of the imaginary part of the self-energy somewhat, but does not affect the real part significantly.

There have been several attempts to calculate the interaction energy between a charged particle and a metal surface. These approaches differ from ours in their approaches to the problem and in their assumptions. Mills[6] calculated the retardation effect on the image potential, but in his calculations he neglected the dispersion effects. His paper therefore is not directly related to ours. Although Equiluz[4] formulated the self-energy of the particle by including both the dispersion and the quantum recoil, he evaluated his results in the limiting case of the infinite mass of the particle. His results therefore are valid in the semiclassical limit. Ekardt[7] by his own admission used Equiluz's work and derived results which are valid for the dispersionless plasmons. His work therefore is less general than ours.

We use the definition of the self-energy of the particle as introduced by Manson and Ritchie, which is different from the form used for the self-energy in the electron-gas theory. The latter nonlocal form arises from the nonlocality of the exchange-correlation potential by the electron. In the formalism of Manson and Ritchie[1] and in ours, the self-energy is defined directly in terms of the energy shift of the charged-particle—metal system. The formal connection between the nonlocal self-energy and our self-energy is known.[8] We will not deal with this question because it would be peripheral to our objective of evaluating the form of the interaction potential.

The plan of the paper is as follows. In Sec. II we derive the general expressions for the self-energy, valid for an arbitrary angle of incidence and for the particle energy below and above the threshold plasmons energies. Separate expressions for the self-energy are given for the surface- and bulk-plasmon contributions. Some limiting cases for the self-energy are also derived. In Sec. III we present the calculations and discuss the results.

II. THEORY

A. Metal-particle interaction

The Hamiltonian of the charged particle of charge Q and mass M and the metal is

$$H=H_{\rm met}+\frac{p^2}{2M}+V\ , \tag{1}$$

$$H_{\rm met}=\sum_{\lambda}\hbar\omega_\lambda(a_\lambda^\dagger a_\lambda+\tfrac{1}{2})\ , \tag{2}$$

$$V=Q\sum_{\lambda}[\varphi_\lambda^*(\mathbf{r})a_\lambda^\dagger+\varphi_\lambda(\mathbf{r})a_\lambda]\ . \tag{3}$$

$a_\lambda^\dagger$ and a_λ are the creation and annihilation operators of the quanta of plasmons in the metallic electron gas, λ being the index specifying the kind of plasmon (surface or bulk), its wave number, etc. $\varphi_\lambda(\mathbf{r})$ is the electrostatic potential that a plasmon with index λ produces.

Explicit forms of $\varphi_\lambda(\mathbf{r})$ for the hydrodynamic model of the metallic electron gas have been by Barton.[9] For the surface plasmons they are

$$\varphi_\kappa(\mathbf{r})=-\frac{m}{e}N_\kappa[\omega_p^2\kappa\exp(\gamma z)-\omega_s^2\gamma\exp(\kappa z)]\exp(i\boldsymbol{\kappa}\cdot\boldsymbol{\rho})\ ,\quad z<0 \tag{4a}$$

$$=-\frac{m}{e}N_\kappa(\omega_p^2\kappa-\omega_s^2\gamma)\exp(i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}-\kappa z),\quad z>0\ . \tag{4b}$$

Here $\omega_p^2=4\pi e^2 n/m$,

$$\omega_s^2\equiv\omega_s^2(\kappa)=\tfrac{1}{2}[\omega_p^2+\beta^2\kappa^2+\beta\kappa(2\omega_p^2+\beta^2\kappa^2)^{1/2}]\ ,$$

$\boldsymbol{\kappa}$ is the wave vector parallel to the surface, $\mathbf{r}\equiv(\boldsymbol{\rho},z)$ and the semi-infinite metal exists for $z<0$, and

$$\gamma^2=\kappa^2+(\omega_p^2-\omega_s^2)/\beta^2\ ,$$

β being the parameter describing plasmon dispersion. As is customary in such problems, β^2 can be chosen to be $3v_F^2/5$, v_F being the Fermi velocity of the electron gas, to be consistent with its high-frequency behavior. The normalization factor N_κ is

$$|N_\kappa|^2=\frac{\omega_p^2(2\omega_s^2-\omega_p^2)^2\hbar}{16\pi^2 mn\omega_s(\omega_p^2+2\omega_s^2)(\omega_s^2-\omega_p^2)^2\kappa^3}\ . \tag{4c}$$

For the bulk plasmons the corresponding expressions are

$$\varphi_{\kappa q}(\mathbf{r})=-\frac{m}{e}\omega_p^2 M_{\kappa q}\left[\cos(qz)+\frac{\kappa\omega_p^2\sin(qz)}{q(2\omega_B^2-\omega_p^2)}-\frac{\omega_B^2\exp(\kappa z)}{2\omega_B^2-\omega_p^2}\right]\exp(i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}),\quad z<0 \tag{5a}$$

$$=-\frac{m}{e}\omega_p^2 M_{\kappa q}\frac{\omega_B^2-\omega_p^2}{2\omega_B^2-\omega_p^2}\exp(i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}-\kappa z),\quad z>0\ . \tag{5b}$$

Here,

$$|M_{\kappa q}|^2=\frac{\beta^4 q^2(2\omega_B^2-\omega_p^2)^2\hbar}{4\pi^3 mn\omega_B(\omega_B^2-\omega_p^2)^2[(2\omega_B^2-\omega_p^2)^2-4\beta^2\kappa^2\omega_B^2]} \tag{5c}$$

and

$$\omega_B^2\equiv\omega_B^2(\kappa,q)=\omega_p^2+\beta^2(\kappa^2+q^2)\ ,$$

q being the wave number along z direction.

B. The self-energy of the particle

The definition of the self-energy $E(\mathbf{r})$ of the particle, as has been demonstrated by Manson and Ritchie,[1] is through the equation

$$\Delta E_0=\int d^3r\langle\mathbf{k}_0|\mathbf{r}\rangle E(\mathbf{r})\langle\mathbf{r}|\mathbf{k}_0\rangle\ , \tag{6}$$

where $|\mathbf{k}_0\rangle$ is the state of the particle moving with momentum $\hbar\mathbf{k}_0$ and ΔE_0 is the change in the energy of the metal-particle system due to the interaction V. Up to second order in perturbation theory,

$$\Delta E_0=\left\langle\mathbf{k}_0\left|\sum_{n,\mathbf{k}}{}'\frac{\langle 0|V|n,\mathbf{k}\rangle\langle n,\mathbf{k}|V|0\rangle}{E_{0,\mathbf{k}_0}-E_{n,\mathbf{k}}+i\delta}\right|\mathbf{k}_0\right\rangle$$

$$=\int d^3r\langle\mathbf{k}_0|\mathbf{r}\rangle\left[\int d^3r'\left\langle\mathbf{r}\left|\sum_{n,\mathbf{k}}{}'\frac{\langle 0|V|n,\mathbf{k}\rangle\langle n,\mathbf{k}|V|0\rangle}{E_{0,\mathbf{k}_0}-E_{n,\mathbf{k}}+i\delta}\right|\mathbf{r}'\right\rangle\frac{\langle\mathbf{r}'|\mathbf{k}_0\rangle}{\langle\mathbf{r}|\mathbf{k}_0\rangle}\right]\langle\mathbf{r}|\mathbf{k}_0\rangle\ . \tag{7}$$

Here a mixed representation $|n,\mathbf{k}\rangle\equiv|n\rangle|\mathbf{k}\rangle$ is used, $|n\rangle$ referring to the plasmons and $|\mathbf{k}\rangle$ to the particle. Comparing Eq. (7) with (6) we get

$$E(\mathbf{r})=\int d^3r'\left\langle n\left|\sum_{n,\mathbf{k}}{}'\frac{\langle 0|V|n,\mathbf{k}\rangle\langle n,\mathbf{k}|V|0\rangle}{E_{0,\mathbf{k}_0}-E_{n,\mathbf{k}}+i\delta}\right|\mathbf{r}'\right\rangle\frac{\langle \mathbf{r}'|\mathbf{k}_0\rangle}{\langle \mathbf{r}|\mathbf{k}_0\rangle}$$

$$=\left\langle \mathbf{r}\left|\sum_{n,\mathbf{k}}{}'\frac{\langle 0|V|n,\mathbf{k}\rangle\langle n,\mathbf{k}|V|0,\mathbf{k}_0\rangle}{E_{0,\mathbf{k}_0}-E_{n,\mathbf{k}}+i\delta}\right|\mathbf{r}\right\rangle\frac{1}{\langle \mathbf{r}|\mathbf{k}_0\rangle}=\sum_{n,\mathbf{k}}{}'\frac{\langle 0|V(\mathbf{r})|n\rangle\langle n,\mathbf{k}|V|0,\mathbf{k}_0\rangle}{E_{0,\mathbf{k}_0}-E_{n,\mathbf{k}}+i\delta}\frac{\langle \mathbf{r}|\mathbf{k}\rangle}{\langle \mathbf{r}|\mathbf{k}_0\rangle}\ . \tag{8}$$

The last part of Eq. (8) follows from the fact that

$$\langle \mathbf{r}|\ \langle 0|V|n,\mathbf{k}\rangle=\left\langle 0\left|\int d^3r'\langle \mathbf{r}|V|\mathbf{r}'\rangle\langle \mathbf{r}'|\mathbf{k}\rangle\right|n\right\rangle$$

$$=\left\langle 0\left|\int d^3r'V(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\langle r'|\mathbf{k}\rangle\right|n\right\rangle=\langle 0|V(\mathbf{r})|n\rangle\langle \mathbf{r}|\mathbf{k}\rangle\ . \tag{9}$$

Substituting Eq. (3) into (8) we may obtain $E(\mathbf{r})$ by two methods: either by evaluating the matrix elements first and then completing the summation over the intermediate states or by reversing this order. The final result is the same. If we follow the second method we express the result of the summation over n and $\mathbf{k}$ by the Green's functions

$$G\left[\mathbf{r}-\mathbf{r}';\frac{\hbar^2k_0^2}{2M}-\hbar\omega_\lambda\right]=-\frac{M}{2\pi\hbar^2|\mathbf{r}-\mathbf{r}'|}\exp[-|\mathbf{r}-\mathbf{r}'|(k_\lambda^2-k_0^2)^{1/2}]\ \text{ for } k_0^2<k_\lambda^2,\ k_\lambda^2=\frac{2m\omega_\lambda}{\hbar} \tag{10a}$$

and

$$G\left[\mathbf{r}-\mathbf{r}';\frac{\hbar^2k_0^2}{2M}-\hbar\omega_\lambda\right]=-\frac{M}{2\pi\hbar^2|\mathbf{r}-\mathbf{r}'|}\exp[i|\mathbf{r}-\mathbf{r}'|(k_0^2-k_\lambda^2)^{1/2}]\ \text{ for } k_0^2>k_\lambda^2\ . \tag{10b}$$

The resulting expressions $E_s(\mathbf{r})$ due to the interaction of the particle with the surface plasmons when the energy of the particle is less than the energy of the surface plasmon (i.e., below threshold) and for $E_B(\mathbf{r})$ due to the interaction of the particle with the bulk plasmon when the energy of the particle is below the threshold energy for the bulk plasmons, are as follows:

$$E_s(z)=-Q^2\left[\frac{m}{e}\right]^2\frac{M}{\hbar^2}\sum_{\kappa}\frac{|N_\kappa|^2}{\alpha}(\omega_p^2\kappa-\omega_s^2\gamma)\exp(-\kappa z)$$
$$\times\left[(\omega_p^2\kappa-\omega_s^2\gamma)\left[\frac{\exp(-\kappa z)-\exp[-(\alpha+iq_0)z]}{\alpha-\kappa+iq_0}+\frac{\exp(-\kappa z)}{\alpha+\kappa-iq_0}\right]\right.$$
$$\left.+\left[\frac{\omega_p^2\kappa}{\alpha+\gamma+iq_0}-\frac{\omega_s^2\gamma}{\alpha+\kappa+iq_0}\right]\exp[-(\alpha+iq_0)z]\right],\ \ z>0 \tag{11a}$$

$$=-Q^2\left[\frac{m}{e}\right]^2\frac{M}{\hbar^2}\sum_{\kappa}\frac{|N_\kappa|^2}{\alpha}[\omega_p^2\kappa\exp(-\gamma|z|)-\omega_s^2\gamma\exp(-\kappa|z|)]$$
$$\times\left[(\omega_p^2\omega-\kappa_s^2\gamma)\frac{\exp[-(\alpha-iq_0)|z|]}{\kappa+\alpha-iq_0}+\left[\omega_p^2\kappa\frac{\exp(-\gamma|z|)-\exp[-(\alpha-iq_0)|z|]}{\alpha-\gamma-iq_0}\right.\right.$$
$$\left.-\omega_s^2\gamma\frac{\exp(-\kappa|z|)-\exp[-(\alpha-iq_0)|z|]}{\alpha-\kappa-iq_0}\right]$$
$$\left.+\frac{\omega_p^2\kappa\exp(-\gamma|z|)}{\alpha+\gamma+iq_0}-\omega_s^2\gamma\frac{\exp(-\kappa|z|)}{\alpha+\kappa+iq_0}\right],\ \ z<0\ . \tag{11b}$$

Here $\alpha^2=(\boldsymbol{\kappa}_0-\boldsymbol{\kappa})^2+k_s^2-k_0^2$, $k_s^2=2M\omega_s/\hbar$, and q_0 is the z component of $\mathbf{k}_0\equiv(\boldsymbol{\kappa}_0,q_0)$.

With $\eta^2=(\boldsymbol{\kappa}_0-\boldsymbol{\kappa})^2+k_B^2-k_0^2$ and $k_B^2=2M\omega_B/\hbar$, the bulk part is

$$E_B(z)=-Q^2\left[\frac{m}{e}\right]^2\frac{M}{\hbar^2}\sum_{\kappa,q}\frac{|M_{\kappa q}|^2}{\eta}\frac{\omega_p^2(\omega_B^2-\omega_p^2)\exp(-\kappa z)}{2\omega_B^2-\omega_p^2}$$

$$\times\left[\frac{\omega_p^2(\omega_B^2-\omega_p^2)}{2\omega_B^2-\omega_p^2}\left[\frac{\exp(-\kappa z)-\exp[-(\eta+iq_0)z]}{\eta-\kappa+iq_0}+\frac{\exp(-\kappa z)}{\eta+\kappa-iq_0}\right]\right.$$

$$+\left[\frac{\omega_p^2(\eta+iq_0)}{q^2+(\eta+iq_0)^2}-\frac{\kappa\omega_p^4}{(2\omega_B^2-\omega_p^2)[q^2+(\eta+iq_0)^2]}\right.$$

$$\left.\left.-\frac{\omega_B^2\omega_p^2}{(2\omega_B^2-\omega_p^2)(\kappa+\eta+iq_0)}\right]\exp[-(\eta+iq_0)z]\right],\quad z>0 \tag{12a}$$

$$=-Q^2\left[\frac{m}{e}\right]^2\frac{M}{\hbar^2}\sum_{\kappa,q}\frac{|M_{\kappa q}|^2}{\eta}\omega_p^4\left[\cos(q|z|)-\frac{\kappa\omega_p^2\sin(q|z|)}{q(2\omega_B^2-\omega_p^2)}-\frac{\omega_B^2\exp(-\kappa|z|)}{2\omega_B^2-\omega_p^2}\right]$$

$$\times\left[\frac{(\eta-iq_0)\cos(q|z|)+q\sin(q|z|)-(\eta-iq_0)\exp[-(\eta-iq_0)|z|]}{(\eta-iq_0)^2+q^2}\right.$$

$$+\frac{\omega_B^2-\omega_p^2}{2\omega_B^2-\omega_p^2}\frac{\exp[(-\eta+iq_0)|z|]}{k+\eta-iq_0}+\frac{(\eta+iq_0)\cos(q|z|)-q\sin(q|z|)}{(\eta+iq_0)^2+q^2}$$

$$-\frac{\kappa\omega_p^2}{q(2\omega_B^2-\omega_p^2)}\left[\frac{(\eta-iq_0)\sin(q|z|)-q\cos(q|z|)+q\exp[-(\eta-iq_0)|z|]}{(\eta-iq_0)^2+q^2}\right.$$

$$\left.+\frac{(\eta+iq_0)\sin(q|z|)+q\cos(q|z|)}{(\eta+iq_0)^2+q^2}\right]-\frac{\omega_B^2}{2\omega_B^2-\omega_p^2}$$

$$\left.\times\left[\frac{\exp(-\kappa|z|)}{\eta+\kappa+iq_0}+\frac{\exp(-\kappa|z|)-\exp[-(\eta-iq_0)|z|]}{\eta-iq_0-\kappa}\right]\right],\quad z<0\,. \tag{12b}$$

The corresponding results above threshold with dispersion included are complicated. If the dispersion of the plasmons is neglected the results are relatively simpler and are given as follows:

$$E_s(z)=-\frac{k_s^2Q^2}{4\pi}\sum_{\kappa}\frac{1}{\kappa}\exp(-\kappa z)\left[\Theta[(k_0^2-k_s^2)^{1/2}-|\boldsymbol{\kappa}+\boldsymbol{\kappa}_0|]\left[-\frac{\exp(-\kappa z)}{(\kappa+iq_0)^2+(\mu_s)^2}+\frac{i\kappa}{\mu_s}\frac{\exp[i(q_0+\mu_s)z]}{\kappa^2+(q_0+\mu_s)^2}\right]\right.$$

$$\left.+\Theta[|\boldsymbol{\kappa}+\boldsymbol{\kappa}_0|-(k_0^2-k_s^2)^{1/2}]\left[-\frac{\exp(-\kappa z)}{(\kappa+iq_0)^2-\nu_s^2}+\frac{\kappa}{\nu_s}\frac{\exp[(iq_0-\nu_s)z]}{k^2+(q_0+i\nu_s)^2}\right]\right]\quad\text{for } z>0 \tag{13a}$$

and

$$E_s(z)=-\frac{k_s^2Q^2}{4\pi}\sum_{\kappa}\frac{1}{\kappa}\exp(-\kappa z)\left[\Theta[(k_0^2-k_p^2)^{1/2}-|\boldsymbol{\kappa}+\boldsymbol{\kappa}_0|]\left[\frac{-\exp(-\kappa|z|)}{(\kappa-iq_0)^2+(\mu_s)^2}+\frac{i\kappa}{\mu_s}\frac{\exp[-i(q_0-\mu_s)|z|]}{\kappa^2+(q_0-\mu_s)^2}\right]\right.$$

$$+\Theta[|\boldsymbol{\kappa}+\boldsymbol{\kappa}_0|-(k_0^2-k_s^2)^{1/2}]$$

$$\left.\times\left[\frac{-\exp(-\kappa|z|)}{(\kappa-iq_0)^2-(\nu_s)^2}+\frac{\kappa}{\nu_s}\frac{\exp[-(iq_0-\nu_s)|z|]}{\kappa^2+(q_0-i\nu_s)^2}\right]\right]\quad\text{for } z<0\,, \tag{13b}$$

where

$$\mu_s=[k_0^2-k_s^2-(\boldsymbol{\kappa}+\boldsymbol{\kappa}_0)^2]^{1/2}\,,\quad \nu_s=[(\boldsymbol{\kappa}+\boldsymbol{\kappa}_0)^2-k_0^2+k_s^2]^{1/2},\quad\text{and } k_s^2=(2)^{1/2}\frac{M\omega_p}{\hbar}$$

$$E_B(z)=-\frac{Q^2k_p^2}{\pi^2}\sum_{\kappa,q}\frac{q^2}{(\kappa^2+q^2)^2}\left[\exp(-\kappa|z|)-\cos(q|z|)+\frac{\kappa}{q}\sin(q|z|)\right]$$

$$\times\Bigg[\Theta[(k_0^2-k_p^2)^{1/2}-|\kappa_0+\kappa|]\Bigg\{\frac{\exp(-\kappa|z|)}{(i\kappa+q_0)^2-(\mu_B)^2}-\frac{\exp(iq|z|)(\frac{1}{2}+i\kappa/2q)}{(q+q_0)^2-(\mu_B)^2-i\delta}$$

$$-\frac{\exp(-iq|z|)(\frac{1}{2}-i\kappa/2q)}{(-q+q_0)^2-(\mu_B)^2-i\delta}+\frac{1}{2\mu_B}\exp[-i(q_0-\mu_B)|z|]$$

$$\times\left[\frac{i}{\kappa-iq_0+i\mu_B}-\left[\frac{1}{2}+\frac{i\kappa}{2q}\right]\frac{1}{-q_0+\mu_B-q-i\delta}-\left[\frac{1}{2}-\frac{i\kappa}{2q}\right]\frac{1}{-q_0+\mu_B+q-i\delta}\right]\Bigg\}$$

$$+\Theta[|\kappa+\kappa_0|-(k_0^2-k_p^2)^{1/2}]\Bigg\{\frac{\exp(-\kappa|z|)}{(i\kappa+q_0)^2+(\nu_B)^2}-\frac{\exp(iq|z|)(\frac{1}{2}+i\kappa/2q)}{(q+q_0)^2+(\nu_B)^2}-\frac{\exp(-iq|z|)(\frac{1}{2}-i\kappa/2q)}{(-q+q_0)^2+(\nu_B)^2}$$

$$+\frac{1}{2\nu_B}\exp(-iq_0|z|-\nu_B|z|)$$

$$\times\left[\frac{1}{\kappa-iq_0-\nu_B}+\left[\frac{1}{2}+\frac{i\kappa}{2q}\right]\frac{i}{-q_0+i\nu_B-q}+\left[\frac{1}{2}-\frac{i\kappa}{2q}\right]\frac{i}{-q_0+i\nu_B+q}\right]\Bigg\}\Bigg]\quad\text{for } z<0\,, \tag{14a}$$

where

$$\mu_B=[k_0^2-k_p^2-(\kappa+\kappa_0)^2]^{1/2}\,,\quad \nu_B=[(\kappa+\kappa_0)^2-(k_0^2-k_p^2)]^{1/2},\quad\text{and } k_p^2=2M\omega_p/\hbar\,.$$

Therefore,

$$E_B(z)=0\ \text{for } z>0\,. \tag{14b}$$

In Eqs. (13) and (14), $\Theta(x)=1$ for $x>0$ and zero otherwise.

C. Limiting values of $E(z)$

The summations in Eqs. (8)–(11) can be performed analytically in certain limiting cases. The values of $E(\mathbf{r})$ in such cases are useful for their direct physical interpretation and also for their use in experimental comparisons. Such analytical expressions also provide a test for numerical work.

In the limit $z\to-\infty$ and $k_0\to 0$ the self-energy is obtained from (12b) and is given by

$$E_B(z\to-\infty,k_0=0)=-\frac{Q^2}{2}\frac{2k_p}{\pi}\frac{1}{(A^2+4)^{1/2}}\left[(2a_+)^{1/2}\tan^{-1}\left[\frac{(2a_+A)^{1/2}}{2-a_+}\right]+\frac{(2a_-)^{1/2}}{2}\ln\left[\frac{|(2a_-A)^{1/2}+a_-+2|}{|(2a_-A)^{1/2}-a_--2|}\right]\right], \tag{15}$$

where $A=k_p^2\beta^2/\omega_p^2$ and $a_\pm^2=(A^2+4)^{1/2}\pm A$. For a dispersionless plasmon $\beta=0$ or $A=0$, Eq. (12) reduces to

$$E_B(z\to-\infty,\,k_0=0)=-\frac{Q^2}{2}k_p\,, \tag{16}$$

and for the case of infinite mass of the particle $M\to\infty$ or $A\to\infty$,

$$E_B(z\to-\infty,\,k_0=0)=-\frac{Q^2}{2}\frac{\omega_p}{\beta} \tag{17}$$

If we neglect dispersion (i.e., $\beta=0$) the self-energy for all energies of the particle can be obtained either from Eq. (12b) or (14a). It is given by

$$E_B(z\to-\infty,k_0)=-\frac{Q^2k_p}{4\pi k_0}\int_0^\infty\frac{dk}{k}\ln\left[\frac{k^2+k_p^2+2kk_0}{k^2+k_p^2-2kk_0}\right]. \quad (18)$$

It can easily be shown that the imaginary part of (18) is

$$E_B''(z\to-\infty,k_0)=-\frac{Q^2k_p^2}{4k_0}\ln\left[\frac{k_0+(k_0^2-k_p^2)^{1/2}}{k_0-(k_0^2-k_p^2)^{1/2}}\right] \quad \text{for } k_0>k_p\,,$$

$$=0 \quad \text{for } k_0<k_p\,. \quad (19)$$

E_B'' is the nonconservative imaginary part of the self-energy and is zero for all energies of the particle below threshold. The real part of (18) is given by the same equation, but now the principal value of the logarithm should be taken. The real part of the surface contributions to the self-energy for $|z|\to\infty$ varies as $-Q^2/4|z|$, a behavior which is well known. For energies well below threshold the self-energy at the surface can be obtained from Eqs. (11) and (12) to be

$$E(z=0,k_0\to 0)=-\frac{Q^2}{3}\frac{\omega_p}{\beta}\,, \quad (20)$$

when the particle mass $M\to\infty$ (i.e., semiclassical limit). On the other hand, it reduces to

$$E(z=0,k_0\to 0)=\frac{-Q^2k_p}{(2)^{5/4}}\,, \quad (21)$$

in the limit of dispersionless plasmons (i.e., $\beta\to 0$).

The real and imaginary parts of the self-energy at the surface due to surface-plasmon contribution, for the above threshold case ($k_0>k_s$), can easily be worked out from Eqs. (13). The results are

$$E_s'(0^\pm)=-\frac{\pi}{4}\frac{Q^2k_s^2}{k_0}\,, \quad (22a)$$

$$E_{sc}''(0^\pm)=\mp\frac{k_s^2Q^2}{4k_0}\ln\left[\frac{2k_0^2-k_s^2}{k_s^2}\right], \quad (22b)$$

$$E_{sn}''(0^\pm)=\mp\frac{k_s^2Q^2}{4k_0}\ln\left[1\pm\frac{2k_0(k_0^2-k_s^2)^{1/2}}{2k_0^2-k_s^2}\right]. \quad (22c)$$

Equation (22c) represents the nonconservative imaginary part of the self-energy arising from the poles of energy denominator of Eq. (8), whereas (22b) is the conservative part of the self-energy which tends to zero away from the surface. Equations (22a) and (22c) have also been obtained by Manson and Ritchie.[1]

III. CALCULATION AND RESULTS

We now proceed to the numerical evaluation of expressions given in Sec. II. For a unit volume (or area) replacing

$$\sum_{\kappa,q}\to\int d^2\kappa\int_0^\infty dq \quad\text{and}\quad \sum_{\kappa}\to\int d^2\kappa\,,$$

the problem reduces to numerical integration. The real and imaginary parts of the self-energy can be easily

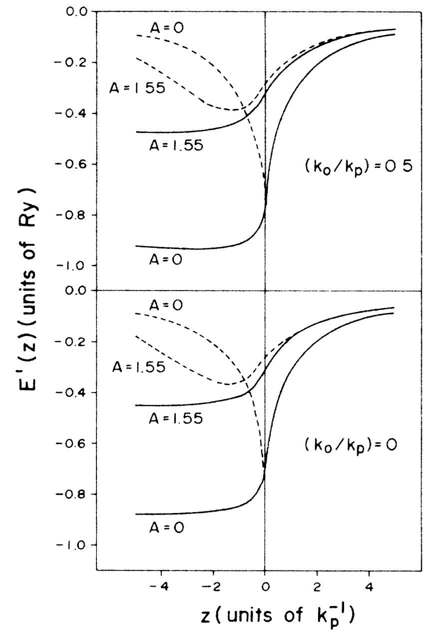

FIG. 1. Real part of self-energy $E'(z)$ as a function of z, below the threshold speeds. Dashed curves are the contributions due to surface plasmons. Solid curves denote the total (surface plus bulk) contributions.

separated far below the threshold case. In this case the real and imaginary parts are even and odd functions of k_0, respectively. For the terms with poles on real axis above the threshold, the real and imaginary parts are obtained using the identity

$$\frac{1}{x+i\delta}=\mathrm{P}\frac{1}{x}-i\pi\delta(x)\,, \quad (23)$$

where P stands for the principal value. The real and imaginary parts arising from (23) do not have a fixed parity with k_0. The imaginary part is then the nonconservative component which decreases slowly away from the surface. The surface contribution goes to zero while the bulk contribution saturates to a finite value. The conser-

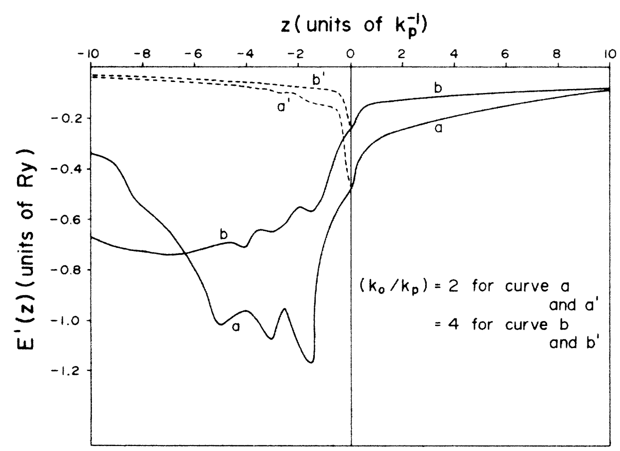

FIG. 2. Real part of the self-energy $E'(z)$ far above the threshold speeds. Curves a,a' and b,b' are for particle speeds 2 and 4, respectively. Here again, dashed and solid curves represent the surface and total contributions, respectively.

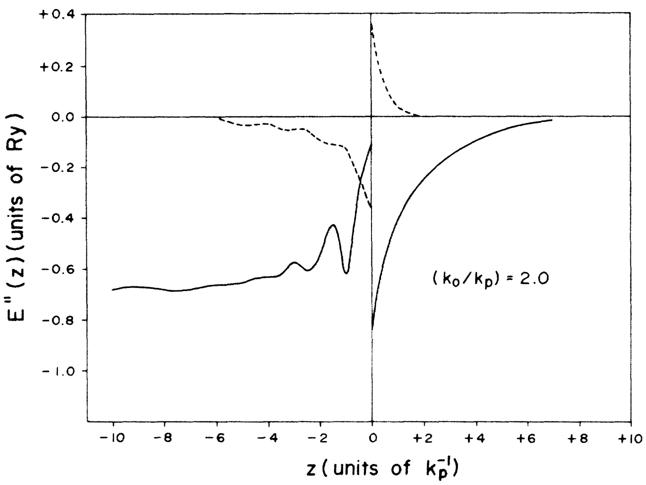

FIG. 3. Imaginary part of the self-energy far above the threshold speed of 2. The solid and dashed curves are the nonconservative and conservative (total) imaginary parts, respectively.

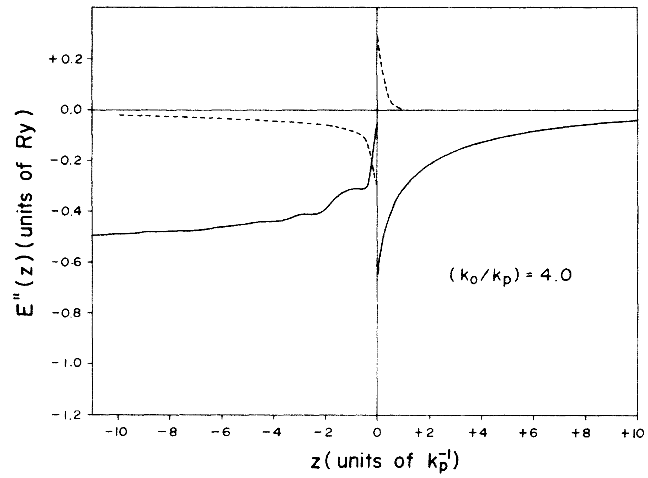

FIG. 4. Same as Fig. 3, but for incident-particle speed of 4.

vative imaginary part does not represent dissipation and is associated with those energy losses which are recovered as the particle leaves the surface.[1,10] It decreases quickly away from the surface.

The semiclassical limit of our expressions (11) and (12) which ignores the plasma-exchange processes is obtained in the limit M/m tending to infinity. Our results then reduce to the expected behavior of a moving charge particle in a dispersive semi-infinite medium.[3] The results in the absence of plasma dispersion are obtained in the limit $\beta \to 0$. In this limit Eq. (11) naturally reduces to the form given by Manson and Ritchie.[1]

For the surface contribution above the threshold our expression (13) can be easily cast to the form[11] given by Manson and Ritchie.[1] However, we make explicit calculations of the conservative and nonconservative parts of the imaginary parts of the self-energy.

The real and imaginary parts of the self-energy have been calculated for two normal-incidence ($\kappa_0 = 0$) speeds. In Fig. 1 we plot the real part far below threshold speeds. The surface contributions are shown separately. In Fig. 1, for A we take the value corresponding to metallic copper ($r_s = 2.7$) and $A = 0$. It is found that at zero speed the ratio of the inner potential to the potential at the boundary is 0.84, when the exchange of plasmons without dispersion is considered, and the same ratio becomes 0.71 when the dispersion effects are included. The experimentally found ratio is about 0.5. If may be noted that the saturation of the potential at $z = 0$ arises due to both the plasma-dispersion and the plasmon-exchange processes. In the limit $k_0 = 0$, i.e., for a stationary charged particle, the self-energy is real. For nonvanishing speed the imaginary part is an order of magnitude smaller than the real part and is therefore not plotted.

In Fig. 2 the real part of the self-energy far above the threshold case is plotted as a function of z for two speeds $k_0/k = 2.0$ and 4.0. The surface contribution is shown by the dashed curve while the total (bulk plus surface) self-energy is drawn by the solid curve. The bulk-plasmon contribution derived neglecting dispersion is zero outside the metal. It is clear from the figure that the potential saturates to a finite value at the surface. Inside the metal it oscillates and the amplitude of the oscillations decreases with increasing speed of the particle. The oscillatory behavior of the self-energy which has been demonstrated also by Manson and Ritchie,[1] in their dispersionless surface-plasmon model, is a feature of the quantum nature of the interaction. It is analogous to the similar behavior[12] of the generalized pair-distribution function of Van Hove used in the neutron scattering theory. For large z inside the metal the potential attains a velocity-dependent inner-potential value given by the real part of Eq. (18). In Figs. 3 and 4 we plot the conservative and the nonconservative imaginary parts of the self-energy by the dashed and the solid curves, respectively. Asymmetry in the conservative part is due to the bulk plasmons. The conservative part is sizable near the surface. The nonconservative part inside the metal for large z approaches a constant value given by Eq. (19).

We wish to point out that the accuracy of our numerical integration is better than 5%. Our computed results for the real and imaginary parts of the self-energy at $z = 0^{\pm}$ and $|z| \to \infty$ agree extremely well within our accuracy with the corresponding analytical results given in Sec. II C. Preliminary results of this paper have appeared in an earlier publication.[13]

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