Self-energy of a charged particle placed in a gap between two metal surfaces and near a metallic slab

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We derive general expressions for the self-energy of a charged particle placed in the gap between two metal surfaces and near a metallic slab. Treating the electron gas in the metal within the hydrodynamic approximation, the self-energy of a charged particle is obtained, taking into account the dispersion of the surface plasmons and the effect of the recoil of the charged particle. We show that the self-energy saturates to a finite negative value at the metal surface and inclusion of recoil and dispersion reduces the magnitude of the self-energy.

I. INTRODUCTION

The study of the interaction between an external charged particle and polarization modes of metallic surfaces has been of considerable interest in view of its various applications.[1] For example, the knowledge of the interaction potential is useful in the interpretation of reflection electron-energy-loss experiments, low-energy electron diffraction, and reflection of high-energy electrons by metal surfaces. The energy loss by a charged particle interacting with a metal surface has been determined in experiments with scanning transmission electron microscopy. The interaction of a charged particle with a metal surface is important in the study of thin films by means of particle beam spectroscopies. The image potential experienced by a tunneling electron is also of importance in the study of the *I-V* response of a metal-insulator or metal-semiconductor junction or interface.

Recently, Sols and Ritchie[2] have studied the interaction between a charge particle and the polarization modes of a metallic slab and of two coupled metal surfaces. These authors have not considered the dispersion of the surface plasmons in their calculations. In the present paper, we have extended the results of Sols and Ritchie[2] by including the effect of the dispersion. We have derived general expressions for the self-energy of the charged particle using the formalism of Manson and Ritchie.[3] The calculations are restricted to speeds of the charged particle below the threshold speeds above which excitations of real plasmons may occur. The unperturbed state of the electron is described by a plane wave.

The paper is organized as follows: In Sec. II, we present the theoretical formulation. Numerical results are presented and discussed in Sec. III. The summary of the results is given in Sec. IV.

II. THEORETICAL FORMALISM

We consider a particle with charge Q and mass M interacting with two plane parallel metal surfaces or with a metallic slab. In order to obtain the interaction Hamiltonian for these systems, we start with the linearized hydrodynamic equation and solve the Poisson and Laplace equations in all of space. The solutions give us the normal modes of the systems. Application of the boundary conditions on the normal modes of the displacement and velocity vectors yields the dispersion relations for the surface and bulk plasmons. These normal modes are quantized and used to express the interaction Hamiltonian for a charged particle interacting with the two systems.

The total Hamiltonian for the systems can be expressed as

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

where the first term is the kinetic energy of the charged particle, and $H_{\rm metal}$, the Hamiltonian representing the metal electrons, is given by

$$H_{\rm metal}=\sum_{\mathbf{k},\alpha}\hbar\omega_{s\alpha}[a^{\dagger}_{\mathbf{k},\alpha}a_{\mathbf{k},\alpha}+\tfrac{1}{2}]\ . \tag{2}$$

In Eq. (2), $\omega_{s,\alpha}$ represents the surface-plasmon frequency for symmetric and antisymmetric modes which are designated by $\alpha=\pm1$, respectively; $a_{\mathbf{k},\alpha}$ and $a^{\dagger}_{\mathbf{k},\alpha}$ are, respectively, the annihilaton and creation operators for surface plasmon with wave vector $\mathbf{k}$ parallel with the surface. The expressions for the normal mode of these systems are given separately for the case of a charged particle placed in a gap[4,5] and near a metal slab.[6] $H_{\rm int}$ is obtained in the following.

A. Interaction Hamiltonian for a charged particle located in a gap between two metal surfaces

The interaction Hamiltonian for this case is given by

$$H_{\rm int}=Q\sum_{\mathbf{k},\alpha}(a_{\mathbf{k},\alpha}+a^{\dagger}_{-\mathbf{k},\alpha})e^{i\mathbf{k}\cdot\mathbf{R}}N_{k,\alpha}g_{k,\alpha}(Z)\ . \tag{3}$$

In Eq. (3) $N_{k,\alpha}$ and $g_{k,\alpha}$ are defined as follows:

$$
g_{\mathbf{k},\alpha}=\begin{cases}\omega_{s\alpha}^2\gamma_\alpha e^{k(Z+a)}-kw_p^2 e^{\gamma_\alpha(Z+a)}, & Z<-a\\[4pt] \dfrac{(\omega_{s\alpha}^2\gamma_\alpha-k\omega_p^2)(e^{-kZ}+\alpha e^{+kZ})}{e^{ka}+\alpha e^{-ka}}, & |Z|<a\\[4pt] \alpha(\omega_{s\alpha}^2\gamma_\alpha e^{-k(Z-a)}-k\omega_p^2 e^{-\gamma_\alpha(Z-a)}), & Z>a\end{cases} \tag{4}
$$

and

$$
N_{k,\alpha}^2=\left[\frac{\omega_p^2(1-\alpha e^{-2ka})(2\omega_{s\alpha}^2-\omega_p^2-\alpha e^{-2ka})^2 m\hbar}{16\pi^2 ne^2k^3A(\omega_{s\alpha}^2-\omega_p^2)^2\omega_{s\alpha}[3\omega_p^2(1-\alpha e^{-2ka})+2(\omega_{s\alpha}^2-\omega_p^2)]}\right]. \tag{5}
$$

The squared normal mode frequency $\omega_{s\alpha}^2$ is found to be[4,5,7]

$$
\omega_{s\alpha}^2=(\tfrac{1}{2})\{\omega_p^2(1+\alpha e^{-2ka})+\beta^2k^2+\beta k[\beta^2k^2+2\omega_p^2(1-\alpha e^{-2ka})]^{1/2}\}\ , \tag{6}
$$

where β^2 is the dispersion parameter and is chosen to be $(3/5)v_F^2$ corresponding to random-phase approximation and γ_α is found from

$$
\gamma_\alpha^2=k^2+(\omega_p^2-\omega_{s\alpha}^2)/\beta^2\ . \tag{7}
$$

B. Interaction Hamiltonian for a charged particle near a metallic slab

The form of the interaction Hamiltonian for this case is similar to Eq. (3), but $g_{k,\alpha}$ and $N_{k,\alpha}$ are different. Here again $\alpha=1$ corresponds to the symmetric modes and $\alpha=-1$ corresponds to the antisymmetric modes. The explicit expression for $g_{k,\alpha}$ is given by

$$
g_{k_+}(Z)=\begin{cases}[\omega_s^2\cosh(ka)-(k/\gamma)w_p^2\sinh(ka)\coth(\gamma a)]e^{k(Z+a)}, & Z<-a\\[4pt] \omega_s^2\cosh(kZ)-\dfrac{k\omega_p^2\sinh(ka)}{\gamma\sinh(\gamma a)}\cosh(\gamma Z), & |Z|<a\\[4pt] [\omega_s^2\cosh(ka)-(k/\gamma)\omega_p^2\sinh(ka)\coth(\gamma a)e^{-k(Z-a)}, & Z>a\ ;\end{cases} \tag{8a}
$$

and

$$
g_{k_-}(Z)=\begin{cases}-[\omega_s^2\sinh(ka)-(k/\gamma)\omega_p^2\cosh(ka)\tanh(\gamma a)]e^{k(Z+a)}, & Z<-a\\[4pt] \omega_s^2\sinh(kZ)-\dfrac{k\omega_p^2\cosh(ka)}{\gamma\cosh(\gamma a)}\sinh(\gamma Z), & |Z|<a\\[4pt] [\omega_s^2\sinh(ka)-(k/\gamma)\omega_p^2\cosh(ka)\tanh(\gamma a)]e^{-k(Z-a)}, & Z>a\ .\end{cases} \tag{8b}
$$

The normalization coefficients for the symmetric and antisymmetric modes, denoted by N_{k_+} and N_{k_-}, are expressed by

$$
N_{k_+}^2=\frac{m\gamma^3\hbar}{e^2 2Akn\omega_{s_+}d_1\sinh^2(ka)}\ , \tag{9a}
$$

where

$$
d_1=\{2\gamma^2[\gamma\coth(ka)-k\coth(\gamma a)]+k(k^2-\gamma^2)\coth(\gamma a)+(k^2-\gamma^2)k\gamma a\times[1+\coth^2(\gamma a)]\} \tag{9b}
$$

and

$$
N_{k_-}^2=\frac{m\gamma^3\hbar}{e^2 2Akn\omega_{s_-}d_2\cosh^2(ka)}\ , \tag{9c}
$$

where

$$
d_2=\{2\gamma^2[\gamma\tanh(ka)-k\tanh(\gamma a)]+k(k^2-\gamma^2)\tanh(\gamma a)+(k^2-\gamma^2)k\gamma a[1+\tanh^2(\gamma a)]\}\ . \tag{9d}
$$

The quantity γ occurring in Eqs. (8a)–(9d) is obtained by solving the transcendental equation

$$
\omega_p^2+\beta^2(k^2-\gamma^2)=(\omega_p^2/2)(1-\alpha e^{-2ka})\times\{1+(k/\gamma)[\coth(\gamma a)]^\alpha\}\ . \tag{10}
$$

With the value of γ obtained from Eq. (10), we find the surface-plasmon frequencies for symmetric and antisymmetric modes using the equation

$$
\omega_{s\alpha}^2=\omega_p^2+\beta^2(k^2-\gamma^2)\ . \tag{11}
$$

The numerical solutions for the surface-plasmon frequencies obtained from Eqs. (10) and (11) are discussed in a separate paper.[6]

C. Expressions for the self-energy of a charged particle

1. *Self-energy of a charged particle in a gap between two metal surfaces*

According to the formalism proposed by Manson and Ritchie,[3] the self-energy $\Sigma(Z)$ of a charged particle is

$$\Sigma(Z)=-\sum_{\mathbf{K},\alpha}\frac{\langle \mathbf{r}|\mathbf{K}\rangle}{\langle r|\mathbf{K}_0\rangle}\frac{\langle 0|H_{\rm int}|\mathbf{K}_0\rangle\langle n,\mathbf{K}|H_{\rm int}|0,\mathbf{K}_0\rangle}{\varepsilon_{\mathbf{K}}-\varepsilon_0+\varepsilon_n-i\delta}\ . \tag{12}$$

In Eq. (12), $|\mathbf{K}_0\rangle$ and $|\mathbf{K}\rangle$ represent the initial and intermediate states of the charged particle having momentum $\hbar\mathbf{K}_0$ and $\hbar\mathbf{K}$, respectively. $\mathbf{K}_0=(\mathbf{k}_0,q_0)$ where $\mathbf{k}_0$ and q_0 are parallel and perpendicular to the metal surface, respectively, and, similarly, $\mathbf{K}=(\mathbf{k},k_3)$. $\varepsilon_{\mathbf{K}}$ and ε_0 are the intermediate and initial of the charged particle. ε_n is the energy of the plasmon field in its nth excited state. We now substitute the interaction Hamiltonian given by Eq. (3) into Eq. (12). We perform the summation over the intermediate states and over the parallel component of the surface plasmons. The integration over k_3 is accomplished by using the methods of the contour integration and choosing the contour in the upper and lower half of the complex plane, depending on the sign of Z. These intergrations are lengthy but reasonably straightforward. The self-energy can now be expressed as an integral over k which cannot be evaluated analytically. Restricting to the initial speeds of the charged particle to values below the threshold value by imposing the requirement that $\mu_{s\alpha}^2>0$, where

$$\mu_{s\alpha}^2=(k-k_0)^2+(2M\omega_{s\alpha}/\hbar)-K_0^2\ , \tag{13}$$

we are able to write the self-energy according to

$$\begin{aligned}\Sigma(|Z|<a)=&-Q^2(M/4\hbar)\sum_\alpha\int_0^\infty\frac{dk}{k^2}\frac{(1-\alpha e^{-2ka})}{(e^{ka}+\alpha e^{-ka})^2}(\omega_{s\alpha}^2\gamma_\alpha-k\omega_p^2)\frac{[2\omega_{s\alpha}^2-\omega_p^2-\alpha\omega_p^2e^{-2ka}]^2[e^{-kZ}+\alpha e^{kZ}]}{(\omega_{s\alpha}^2-\omega_p^2)^2[3\omega_p^2(1-\alpha e^{-2ka})+2(\omega_{s\alpha}^2-\omega_p^2)]\omega_{s\alpha}}\\
&\times\left[\frac{e^{-(\mu_{s\alpha}+iq_0)(Z+a)}}{\mu_{s\alpha}}\left[\frac{2k\omega_{s\alpha}\gamma_\alpha e^{ka}}{k^2+(q_0-i\mu_{s\alpha})^2}-\frac{k\omega_p^2(e^{ka}+\alpha e^{-ka})}{\gamma_\alpha+\mu_{s\alpha}+iq_0}\right.\right.\\
&\left.+\frac{k\omega_p^2e^{ka}}{\mu_{s\alpha}-k+iq_0}+\frac{\alpha k\omega_p^2e^{-ka}}{k+\mu_{s\alpha}+iq_0}\right]+\frac{2(\omega_{s\alpha}^2\gamma_\alpha-k\omega_p^2)e^{-kZ}}{(q_0+ik)^2+\mu_{s\alpha}^2}\\
&+\frac{e^{(\mu_{s\alpha}-iq)(Z-a)}}{\mu_{s\alpha}}\left[\frac{2k\alpha\omega_{s\alpha}^2\gamma_\alpha e^{ka}}{k^2+(q_0+i\mu_{s\alpha})^2}-\frac{k\omega_p^2(e^{-ka}+\alpha e^{ka})}{\gamma_\alpha+\mu_{s\alpha}-iq_0}+\frac{k\omega_p^2e^{-ka}}{\mu_{s\alpha}+k-iq_0}\right.\\
&\left.\left.-\frac{\alpha k\omega_p^2e^{ka}}{k-\mu_{s\alpha}+iq_0}\right]+\frac{2\alpha(\omega_{s\alpha}^2\gamma_\alpha-k\omega_p^2)e^{kZ}}{(q_0-ik)^2+\mu_{s\alpha}^2}\right]\ .\end{aligned} \tag{14}$$

Equation (14) represents the self-energy of a charged particle for all speeds below the threshold value and includes the effects of plasmon dispersion. By choosing values of $\mathbf{k}_0$ and q_0, the particle may make any arbitrary angle to the surfaces. The contribution to the self-energy due to the bulk-plasmon modes is not significant[8] and is not considered in this paper. To obtain the self-energy in which the effect of the dispersion is removed, we substitute $\beta=0$ in Eq. (14). The result for the dispersionless case which agrees with the work of Sols and Ritchie[2] is then given by

$$\begin{aligned}\Sigma(|Z|<a)=&-Q^2(M/2\hbar)\sum_\alpha\int_0^\infty dk\frac{\omega_{s\alpha}e^{-2ka}(e^{-kZ}+\alpha e^{kZ})}{(1+\alpha e^{-2ka})}\\
&\times\left[\frac{e^{-kZ}}{(q_0+ik)^2+\mu_{s\alpha}^2}+\alpha\frac{e^{kZ}}{(q_0-ik)^2+\mu_{s\alpha}^2}\right.\\
&\left.+\left[\frac{k}{\mu_{s\alpha}}\right]e^{ka}\left\{\frac{e^{-i(Z+a)(q_0-i\mu_{s\alpha})}}{k^2+(q_0-i\mu_{s\alpha})^2}+\alpha\frac{e^{-i(Z-a)(q_0+i\mu_{s\alpha})}}{k^2+(q_0+i\mu_{s\alpha})^2}\right\}\right]\ .\end{aligned} \tag{15}$$

In Eq. (15), $\mu_{s\alpha}^2$ is the same as defined earlier but $\omega_{s\alpha}^2$ occurring in its definition is given by $\omega_{s\alpha}^2=(\omega_p^2/2)(1+\alpha e^{-2ka})$.

2. *Self-energy of a charged particle near a metallic slab*

Substituting the interaction Hamiltonian obtained in *B*, corresponding to the present case, into Eq. (12) and following the same procedure as in the previous section, we obtain

$$
\begin{aligned}
\Sigma(z)=-\frac{MQ^2A}{4\pi^2\hbar^2}\sum_k\Bigg[&g_{k_+}(Z>a)N_{k_+}^2\Bigg\{\frac{e^{-iZ(q_0-i\mu_s)}}{\mu_s}\\
&\times\Bigg\{\frac{\omega_s^2ke^{ka}(e^{ia(q_0-\mu_s)}+e^{-ia(q_0-i\mu_s)})}{k^2+(q_0-i\mu_s)^2}-\frac{k}{\gamma}\sinh(ka)\coth(\gamma a)\omega_p^2\Bigg[\frac{e^{-ia(q_0-\mu_s)}}{\mu_s+k+iq_0}-\frac{e^{ia(q_0-i\mu_s)}}{\mu_s-k+iq_0}\Bigg]\\
&-\frac{k\omega_p^2\sinh(ka)}{2\gamma\sinh(\gamma a)}\Bigg[\frac{e^{a(\mu_s+\gamma+iq_0)}-e^{-a(\mu_s+\gamma+iq_0)}}{\mu_s+\gamma+iq_0}-\frac{e^{a(-\mu_s+\gamma-iq_0)}-e^{a(\mu_s-\gamma+iq_0)}}{\mu_s-\gamma+iq_0}\Bigg]\Bigg\}\\
&+\frac{2\omega_s^2e^{(-kZ+ka)}\cosh(ka)}{\mu_s^2+(q_0+ik)^2}-\frac{2k\omega_p^2\sinh(ka)\coth(\gamma a)e^{(-kZ+ka)}}{\mu_s^2+(q_0+ik)^2}\Bigg\}\\
+&g_{k_-}(Z>a)N_{k_-}^2\Bigg\{\frac{e^{-i(q-i\mu_s)Z}}{\mu_s}\Bigg\{\frac{\omega_s^2ke^{ka}(e^{ia(q_0-i\mu_s)}-e^{-ia(q_0-i\mu_s)})}{k^2+(q_0-i\mu_s)^2}\\
&+\frac{k}{\gamma}\cosh(ka)\omega_p^2\tanh(\gamma a)\Bigg[\frac{e^{ia(q_0-i\mu_s)}}{\mu_s-k+iq_0}+\frac{e^{-ia(q_0-i\mu_s)}}{\mu_s+k+iq_0}\Bigg]\\
&-\frac{k\omega_p^2\cosh(ka)}{2\gamma\cosh(\gamma a)}\Bigg[\frac{e^{a(\mu_s+\gamma+iq_0)}-e^{-a(\mu_s+\gamma+iq_0)}}{\mu_s+\gamma+iq_0}\\
&-\frac{e^{a(\mu_s-\gamma+iq_0)}-e^{a(\gamma-\mu_s-iq_0)}}{\mu_s-\gamma+iq_0}\Bigg]\Bigg\}\\
&+\frac{2\omega_s^2e^{(-kZ+ka)}\sinh(ka)}{\mu_s^2+(q_0+ik)^2}-\frac{2k\omega_p^2\cosh(ka)\tanh(\gamma a)e^{(-kZ+ka)}}{\mu_s^2+(q_0+ik)^2}\Bigg\}\Bigg]\,.
\end{aligned}
\tag{16}
$$

Here, $\mu_{s\alpha}^2$ is given by (13) with $\omega_{s\alpha}$ determined by Eqs. (10) and (11) and γ obtained from Eq. (10). Equation (16) is valid for all speeds of the particle below the threshold speed. It includes the effects of the recoil associated with the mass of the particle and the dispersion. The effect of dispersion is removed by putting $\beta=0$ in Eq. (16). For the dispersionless case, the self-energy for zero speed, i.e., $\mathbf{K}=0$, is given by

$$
\begin{aligned}
\Sigma(Z)=\frac{-Q^2}{4|Z-a|}+\frac{Q^2}{4}\int_0^\infty\sum_\alpha dk(k/\mu_{s\alpha})e^{-k(Z-a)}\\
\times[e^{-\mu_{s\alpha}(Z-a)}\\
+\alpha e^{-\mu_{s\alpha}(Z+a)}]\,,
\end{aligned}
\tag{17}
$$

where $\omega_{s\alpha}^2=(\omega_p^2/2)(1-\alpha e^{-2ka})$ is substituted in the definition of $\mu_{s\alpha}$. The expression (17) agrees with the result obtained by Sols and Ritchie.[2]

III. NUMERICAL RESULTS AND DISCUSSION

We present numerical results for the self-energy of an electron at zero speed (i.e., $\mathbf{K}=0$) located within the gap between two metal surfaces when the dispersion effects are included as well as not included [Eqs. (14) and (15), respectively]. We take $Q=-e$, the charge of the electron. The self-energy is expressed in Rydberg units and the distance between the metal surfaces in units of Bohr radius a_0. The numerical calculations are done for several values of the electron density parameter r_s.

In Fig. 1, we plot the self-energy of an electron as a function of its position within the gap formed by two surfaces for $r_s=2.1$ and for the separation $D=3.89a_0$. The solid and the dashed curves give the self-energy of the electron when dispersion is included and not included, respectively. Since the self-energy is symmetric with respect to the center point of the gap, we therefore give the results for $+ve$ values of Z only. The first two terms inside the squared bracket in Eq. (15) correspond to the classical image potential ($Q^2/4|Z-a|$) which gives a finite value at the center and goes to infinity at the surface. When recoil effects are included, Eq. (15) gives the numerical values for the self-energy equal to -0.329 Ry at the center and -0.88 Ry at the surface. These values reduce to -0.194 Ry at the center and -0.329 Ry at the metal surface when dispersion is considered. The decrease in the self-energy occurs due to the screening effects of the metal electrons. In Figs. 2 and 3, we have plotted the self-energy of the electron when the dispersion is included and omitted for $r_s=4.0$ and 6.0. Comparison of Figs. 1, 2, and 3 shows that the self-energy decreases with the increase in the value of r_s. The variations of the self-energy with distance are more pro-

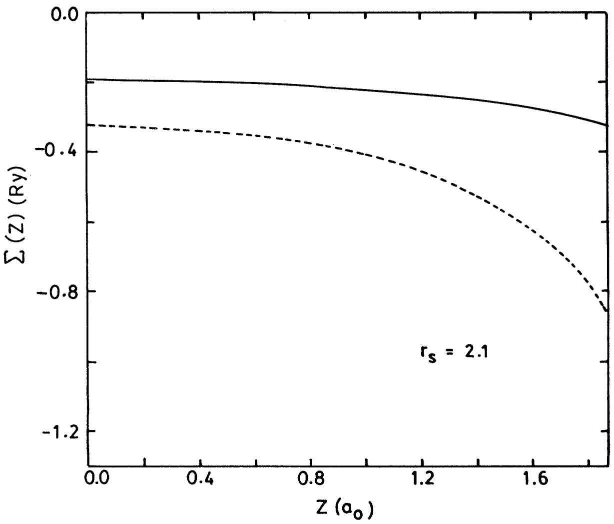

FIG. 1. Self-energy of an electron with zero speed as a function of distance between the gap of two metal surfaces for $r_s = 2.1$. The solid and the dashed curves are with dispersion included and excluded, respectively.

nounced as we approach the surface.

In Figs. 4 and 5, we have plotted the self-energy at the center of the gap as a function of the gap width with and without the dispersion. We notice that the dispersion effects are not important for the width $D = 10a_0$ when the values of the self-energy with and without dispersion become equal. The values of the self-energy at $D = 0$ correspond to the values when the electron is placed inside the bulk of the metal with and without dispersion, respectively. It is also observed that for a given r_s value, the self-energy decreases as the gap width is increased.

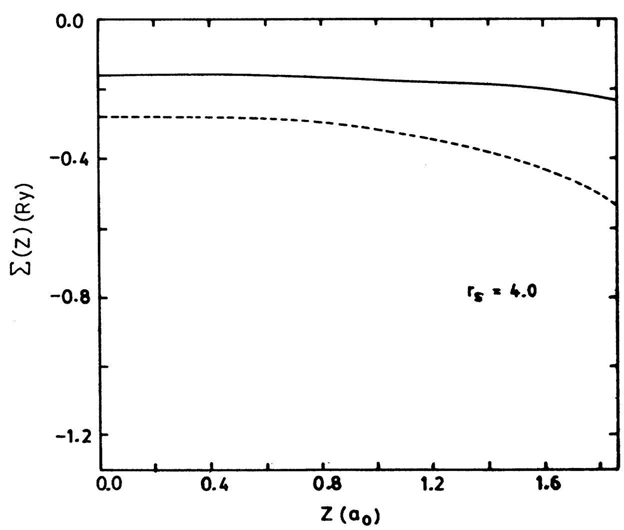

FIG. 2. Self-energy of an electron with zero speed as a function of distance between the gap of two metal surfaces for $r_s = 4.0$. The solid and the dashed curves are with dispersion included and excluded, respectively.

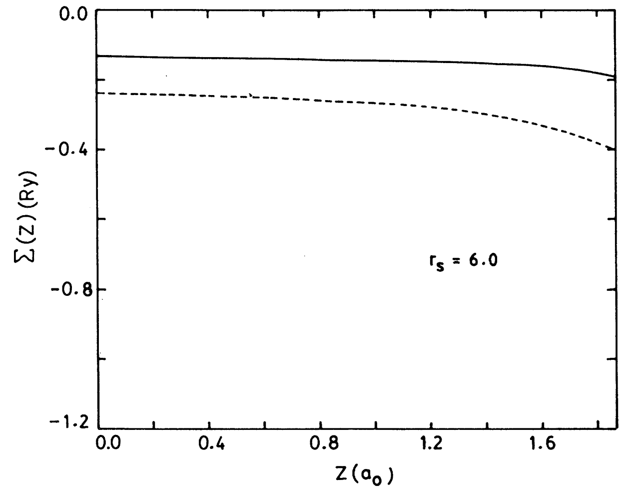

FIG. 3. Self-energy of an electron with zero speed as a function of distance between the gap of two metal surfaces for $r_s = 6.0$. The solid and the dashed curves are with dispersion included and excluded, respectively.

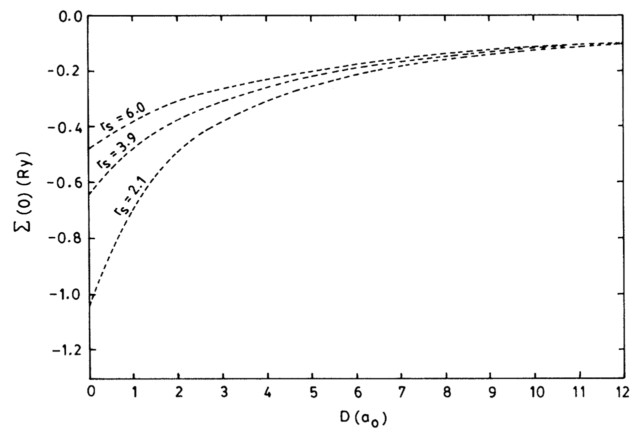

FIG. 4. Self-energy of an electron at zero speed placed at the center between two metal surfaces as a function of gap width with dispersion effects excluded.

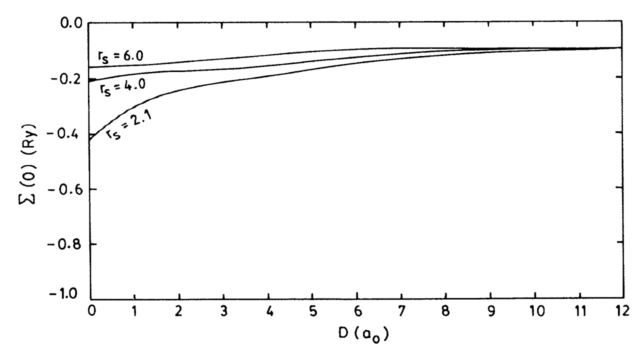

FIG. 5. Self-energy of an electron at zero speed placed at the center between two metal surfaces as a function of gap width with dispersion effects included.

IV. SUMMARY AND CONCLUSIONS

In this paper, we have obtained the general expressions for the self-energy of a moving charged particle located inside the gap of two similar metal surfaces and near a metal slab. The results are obtained within the hydrodynamic model for the metal electrons. The unperturbed state of the electron is described by a plane-wave state propagating in an arbitrary direction, but the speed of the particle is below the threshold speed. The interaction of the charged particle with the metal electrons is treated as perturbation. The self-energy is obtained by using the formalism of Manson and Ritchie.[3] The numerical results are presented for the self-energy of the electron at zero speed for the metallic density parameter $r_s = 2.1$, 4.0, and 6.0. The range of r_s covers most of the metals. The effects of the recoil of the electron and dispersion of plasmons are included in the calculation of the electron self-energy. It is found that both these effects are important near the surface and lead to the saturation of the self-energy as we approach the surface.

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