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Effect of surface roughness on the image potential

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We have calculated the electrostatic potential of a point charge located near a rough dielectric-vacuum interface. The system consists of a vacuum in the region $x_3 > \zeta(\vec{x}_\parallel)$ and a dielectric characterized by an isotropic dielectric constant ϵ in the region $x_3 < \zeta(\vec{x}_\parallel)$. Here $\zeta(\vec{x}_\parallel)$ is a random function of $\vec{x}_\parallel = x_1\hat{x}_1 + x_2\hat{x}_2$ such that $\langle\zeta(\vec{x}_\parallel)\rangle = 0$, and $\langle\zeta(\vec{x}_\parallel)\zeta(\vec{x}'_\parallel)\rangle = \delta^2 W(\vec{x}_\parallel - \vec{x}'_\parallel)$, where δ is the root-mean-square deviation of the interface from flatness, and the angular brackets denote an average over the ensemble of realizations of $\zeta(\vec{x}_\parallel)$. We obtain the electrostatic potential of a point charge q, situated either in the vacuum or in the dielectric, at any point of the system by joining solutions of Poisson's equation above and below the interface at each point of the interface, and then averaging the result over the ensemble of realizations of the function $\zeta(\vec{x}_\parallel)$. Corrections to the results for a planar interface are obtained to $O(\delta^2)$. Analytic asymptotic expressions are presented for the averaged potential when the distance from the image charge to the point at which the potential is determined is small and large, respectively, compared with the average distance between consecutive peaks and valleys on the surface, for a Gaussian form of $W(\vec{x}_\parallel)$. These results are used to obtain the probability for electron-surface-plasmon scattering in the case of an electron moving along a specified trajectory above the rough surface. Although surface roughness increases the energy loss suffered by the electron, the effect is qualitatively different from that required to explain the results of a recent experiment by Lecante, Ballu, and Newns.

I. INTRODUCTION

When a point charge is situated in the vicinity of the plane interface between vacuum and a dielectric medium, characterized, for simplicity, by an isotropic dielectric tensor, the potential at any other point of this composite system can be expressed as the sum of the direct Coulomb potential of the point charge, and the Coulomb potential of an effective, fictitious charge situated at the position of the image (reflection) of the true charge in the interface. The latter potential is the well-known image potential.

This concept of the image potential can, of course, be generalized to the case in which the interface separates not a dielectric from vacuum, but separates two different dielectric media, each of which can be characterized by an anisotropic dielectric tensor, and/or to the case in which the interface is not planar but curved.

The image potential enters into any physical effect in which a charged particle, e.g., an electron or an ion, is situated in the vicinity of a solid surface under conditions when the discrete nature of the solid can be assimilated into a continuum. For example, the image potential is effective in binding electrons near the surface of liquid He,[1,2] and in the case of an inversion layer at a semiconductor-oxide interface, the image potential causes a shift in the electron energy levels.[3,4] An interesting experiment in which image potential effects play a role was carried out recently by Lecante, *et al.*,[5] who studied the inelastic scattering of an electron traveling along a parabolic trajectory just above a clean metal surface, and showed by direct measurement that the electrostatic potential of a surface plasmon does extend into the vacuum outside the metal, as predicted by theory.

In the majority of cases in which image-potential effects have been studied it has been assumed that the interface between the two dielectric media is planar. However, even with a great deal of effort, it is almost impossible to create a perfectly smooth surface. It is, therefore, interesting to determine the extent to which the image potential is affected by the roughness of the interface between two dielectric media, in one of which a point charge is located.

In this paper we present a calculation of the image potential associated with a system consisting of vacuum above the surface $x_3 = \zeta(\vec{x}_\parallel)$ and a dielectric, characterized by an isotropic dielectric tensor ϵ below this surface. The calculations are carried out for the two cases: (a) the point charge is situated in the vacuum $[x_3 > \zeta(\vec{x}_\parallel)]$; (b) the point charge is situated in the dielectric $[x_3 < \zeta(\vec{x}_\parallel)]$. The surface profile function $\zeta(\vec{x}_\parallel)$ is assumed to be a stationary stochastic function of $\vec{x}_\parallel = x_1\hat{x}_1 + x_2\hat{x}_2$, where $\hat{x}_1$ and $\hat{x}_2$ are unit vectors along perpendicular axes. It is characterized by the following two statistical properties:

$$\langle\zeta(\vec{x}_\parallel)\rangle = 0\,, \tag{1.1}$$

$$\langle\zeta(\vec{x}_\parallel)\zeta(\vec{x}'_\parallel)\rangle = \delta^2 W(\vec{x}_\parallel - \vec{x}'_\parallel)\,. \tag{1.2}$$

In these equations the angular brackets denote an average over the ensemble of realizations of the surface roughness, and $\delta^2 = \langle\zeta^2(\vec{x}_\parallel)\rangle$ is the mean-square deviation of the surface from flatness. In our calculations we will assume a Gaussian form for the correlation function $W(\vec{x}_{\parallel})$,

$$W(\vec{x}_{\parallel}) = \exp(-x_{\parallel}^2/a^2)\,. \tag{1.3}$$

The constant a appearing in this expression is called the transverse correlation length. It is a measure of the mean distance between consecutive peaks and valleys on the surface. The value of the image potential averaged over the ensemble of realizations of $\zeta(\vec{x}_{\parallel})$ will be obtained, and the influence of surface roughness on it determined.

We elaborate in Sec. II on the mathematical procedure that we have adopted to solve the Poisson equation for the region under consideration. In Sec. III we obtain the solutions for the coefficients that emerge in Sec. II and introduce the averaging over the ensemble of realization of $\zeta(\vec{x}_{\parallel})$. In Sec. IV the averaged image potential is obtained from the results of Sec. III, and analytic asymptotic expressions for it are derived in the limits that the distance between the image charge and the point at which the potential is determined is small and large compared with the transverse correlation length. The results of Sec. IV suggest a simple, three-layer model of surface roughness, that can reproduce the effects of roughness on the image potential. This model is described and its properties studied in Sec. V. Finally, in Sec. VI, we extend the analysis of Secs. II–V to calculate the dynamic energy loss by electrons moving in a parabolic path above a rough vacuum-dielectric interface. We find that, contrary to the proposition of Lecante *et al.*,[5] surface roughness does not explain the discrepancy between their theoretical and experimental results.

II. THE POISSON EQUATION

The electrostatic potential $\varphi(\vec{x}\,|\,\vec{x}')$ at the point $\vec{x}$ due to a point charge q at $\vec{x}'$ is the solution of Poisson's equation. This equation takes different forms depending on whether the charge is outside or inside the dielectric medium:

$$x_3' > \zeta(\vec{x}_{\parallel}'):\ \nabla^2\varphi(\vec{x}\,|\,\vec{x}') = \begin{cases} -4\pi q\,\delta(\vec{x}-\vec{x}'), & x_3 > \zeta(\vec{x}_{\parallel}) \\ 0, & x_3 < \zeta(\vec{x}_{\parallel})\,, \end{cases} \tag{2.1a}$$

$$x_3' < \zeta(\vec{x}_{\parallel}'):\ \nabla^2\varphi(\vec{x}\,|\,\vec{x}') = \begin{cases} 0, & x_3 > \zeta(\vec{x}_{\parallel}) \\ -\dfrac{4\pi q}{\epsilon}\,\delta(\vec{x}-\vec{x}'), & x_3 < \zeta(\vec{x}_{\parallel})\,. \end{cases} \tag{2.1b}$$

The boundary conditions on the scalar potential are its continuity across the surface $x_3 = \zeta(\vec{x}_{\parallel})$,

$$\varphi(\vec{x}\,|\,\vec{x}')\,\big|_{x_3=\zeta(\vec{x}_{\parallel})-} = \varphi(\vec{x}\,|\,\vec{x}')\,\big|_{x_3=\zeta(\vec{x}_{\parallel})+}\,, \tag{2.2a}$$

and the proper jump discontinuity in its normal derivative across this surface,

$$\epsilon\hat{n}\cdot\nabla\varphi(\vec{x}\,|\,\vec{x}')\,\big|_{x_3=\zeta(\vec{x}_{\parallel})-} = \hat{n}\cdot\nabla\varphi(\vec{x}\,|\,\vec{x}')\,\big|_{x_3=\zeta(\vec{x}_{\parallel})+}\,. \tag{2.2b}$$

In Eq. (2.2b) the unit vector normal to the surface $x_3 = \zeta(\vec{x}_{\parallel})$ at each point is

$$\hat{n} = \left(-\frac{\partial\zeta}{\partial x_1}\,,\,-\frac{\partial\zeta}{\partial x_2}\,,\,1\right)\left[1+\left(\frac{\partial\zeta}{\partial x_1}\right)^2+\left(\frac{\partial\zeta}{\partial x_2}\right)^2\right]^{-1/2}. \tag{2.3}$$

The solution of the partial differential equations (2.1) for the case of the external charge lying outside the dielectric medium $[x_3' > \zeta(\vec{x}_{\parallel}')]$ can be written as

$$\varphi(\vec{x}\,|\,\vec{x}') = \begin{cases} \displaystyle\int\frac{d^2k_{\parallel}}{(2\pi)^2}\exp[i\vec{k}_{\parallel}\cdot(\vec{x}_{\parallel}-\vec{x}_{\parallel}')]\left(\frac{2\pi q}{k_{\parallel}}\right)\exp(-k_{\parallel}|x_3-x_3'|) + \int\frac{d^2k_{\parallel}}{(2\pi)^2}A(\vec{k}_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel})\exp(-k_{\parallel}x_3)\,, & x_3 > \zeta(\vec{x}_{\parallel}) \quad (2.4a) \\ \displaystyle\int\frac{d^2k_{\parallel}}{(2\pi)^2}B(\vec{k}_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel})\exp(k_{\parallel}x_3)\,, & x_3 < \zeta(\vec{x}_{\parallel})\,. \quad (2.4b) \end{cases}$$

In these equations $\vec{k}_{\parallel} = \hat{x}_1k_1 + \hat{x}_2k_2$ is a two-dimensional wave vector parallel to the x_1x_2 plane. The first term on the right-hand side of Eq. (2.4a) is the particular integral of the first of Eqs. (2.1a), while the remaining terms are solutions of the corresponding homogeneous equation.

In a similar fashion, when the external charge is inside the dielectric medium $[x_3' < \zeta(\vec{x}_{\parallel}')]$, the scalar potential can be written in the form

$$\varphi(\vec{x}\,|\,\vec{x}') = \begin{cases} \displaystyle\int\frac{d^2k_{\parallel}}{(2\pi)^2}C(\vec{k}_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel} - k_{\parallel}x_3), & x_3 > \zeta(\vec{x}_{\parallel}) \quad (2.5a) \\ \displaystyle\int\frac{d^2k_{\parallel}}{(2\pi)^2}\exp[i\vec{k}_{\parallel}\cdot(\vec{x}_{\parallel}-\vec{x}_{\parallel}')]\left(\frac{2\pi q}{\epsilon k_{\parallel}}\right)\exp(-k_{\parallel}|x_3-x_3'|) + \int\frac{d^2k_{\parallel}}{(2\pi)^2}D(\vec{k}_{\parallel})\exp(i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel})\exp(k_{\parallel}x_3), & x_3 < \zeta(\vec{x}_{\parallel})\,. \quad (2.5b) \end{cases}$$

In Eqs. (2.4) and (2.5), $A(\vec{k}_{\parallel})$, $B(\vec{k}_{\parallel})$, $C(\vec{k}_{\parallel})$, and $D(\vec{k}_{\parallel})$ are unknown coefficients that are to be determined with the aid of the boundary conditions [Eqs. (2.7)]. The resulting equations for the coefficients $A(\vec{k}_{\parallel})$ and $B(\vec{k}_{\parallel})$ can be written in the following matrix form:

$$\begin{pmatrix} A(\vec{k}_{\parallel}) \\ B(\vec{k}_{\parallel}) \end{pmatrix} - \frac{1}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2} q_{\parallel}\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel}) \begin{pmatrix} \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}+\epsilon & -\epsilon(\hat{k}_{\parallel}\cdot\hat{q}_{\parallel}-1) \\ \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}-1 & -\epsilon\hat{k}_{\parallel}\cdot\hat{q}_{\parallel}-1 \end{pmatrix} \begin{pmatrix} A(\vec{q}_{\parallel}) \\ B(\vec{q}_{\parallel}) \end{pmatrix}$$

$$+\frac{1}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2}\int \frac{d^2Q_{\parallel}}{(2\pi)^2} q_{\parallel}^2\hat{\zeta}(\vec{Q}_{\parallel})\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel}-\vec{Q}_{\parallel}) \begin{pmatrix} \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})+\frac{1}{2}\epsilon & \frac{\epsilon}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})-\frac{1}{2}\epsilon \\ \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})-\frac{1}{2} & \frac{\epsilon}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})+\frac{1}{2} \end{pmatrix} \begin{pmatrix} A(\vec{q}_{\parallel}) \\ B(\vec{q}_{\parallel}) \end{pmatrix}$$

$$=\frac{2\pi q}{(\epsilon+1)k_{\parallel}}\exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(-k_{\parallel}x_3')\begin{pmatrix} 1-\epsilon \\ 2 \end{pmatrix} + \frac{2\pi q}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2}\exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel}')\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel})\exp(-q_{\parallel}x_3')\begin{pmatrix} \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}-\epsilon \\ \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}+1 \end{pmatrix}$$

$$+\frac{2\pi q}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2}\int \frac{d^2Q_{\parallel}}{(2\pi)^2} q_{\parallel}\exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(-q_{\parallel}x_3')\hat{\zeta}(\vec{Q}_{\parallel})\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel}-\vec{Q}_{\parallel}) \begin{pmatrix} \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})-\frac{1}{2}\epsilon \\ \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})+\frac{1}{2} \end{pmatrix}, \quad (2.6)$$

where $\hat{k}_{\parallel}$ and $\hat{q}_{\parallel}$ are unit vectors along the directions of $\vec{k}_{\parallel}$ and $\vec{q}_{\parallel}$, respectively.

The corresponding equation for $C(\vec{k}_{\parallel})$ and $D(\vec{k}_{\parallel})$, obtained in a similar fashion, is

$$\begin{pmatrix} C(\vec{k}_{\parallel}) \\ D(\vec{k}_{\parallel}) \end{pmatrix} - \frac{1}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2} q_{\parallel}\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel}) \begin{pmatrix} \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}+\epsilon & -\epsilon\hat{k}_{\parallel}\cdot\hat{q}_{\parallel}+\epsilon \\ \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}-1 & -\epsilon\hat{k}_{\parallel}\cdot\hat{q}_{\parallel}-1 \end{pmatrix} \begin{pmatrix} C(\vec{q}_{\parallel}) \\ D(\vec{q}_{\parallel}) \end{pmatrix}$$

$$+\frac{1}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2}\int \frac{d^2Q_{\parallel}}{(2\pi)^2} q_{\parallel}^2\hat{\zeta}(\vec{Q}_{\parallel})\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel}-\vec{Q}_{\parallel}) \begin{pmatrix} \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})+\frac{1}{2}\epsilon & \frac{\epsilon}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})-\frac{1}{2}\epsilon \\ \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})-\frac{1}{2} & \frac{\epsilon}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})+\frac{1}{2} \end{pmatrix} \begin{pmatrix} C(\vec{q}_{\parallel}) \\ D(\vec{q}_{\parallel}) \end{pmatrix}$$

$$=\frac{2\pi q}{(\epsilon+1)k_{\parallel}}\exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(k_{\parallel}x_3')\begin{pmatrix} 2 \\ 1-1/\epsilon \end{pmatrix} - \frac{2\pi q}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2}\exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(q_{\parallel}x_3')\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel})\begin{pmatrix} \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}+1 \\ \hat{k}_{\parallel}\cdot\hat{q}_{\parallel}-1/\epsilon \end{pmatrix}$$

$$+\frac{2\pi q}{\epsilon+1}\int \frac{d^2q_{\parallel}}{(2\pi)^2}\int \frac{d^2Q_{\parallel}}{(2\pi)^2} q_{\parallel}\exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(q_{\parallel}x_3')\hat{\zeta}(\vec{Q}_{\parallel})\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel}-\vec{Q}_{\parallel}) \begin{pmatrix} \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})+\frac{1}{2} \\ \frac{1}{k_{\parallel}}(\hat{q}_{\parallel}\cdot\vec{Q}_{\parallel}+\frac{1}{2}q_{\parallel})-\frac{1}{2\epsilon} \end{pmatrix}. \quad (2.7)$$

In obtaining Eqs. (2.6) and (2.7), we have assumed that the surface roughness can be treated as a small perturbation to the plane surface, and thus have retained only terms of up to $O(\zeta^2)$ in the expansion of the exponential functions $\exp[\pm k_{\parallel}\zeta(\vec{x}_{\parallel})]$ entering the boundary conditions. In addition, we have replaced the surface-roughness profile function by its Fourier integral representation

$$\zeta(\vec{x}_{\parallel}) = \int \frac{d^2Q_{\parallel}}{(2\pi)^2} \exp(i\vec{Q}_{\parallel}\cdot\vec{x}_{\parallel})\hat{\zeta}(\vec{Q}_{\parallel}) . \tag{2.8}$$

In Sec. III, we proceed to solve Eqs. (2.6) and (2.7) to obtain the coefficient functions $A(\vec{k}_{\parallel}), B(\vec{k}_{\parallel}), C(\vec{k}_{\parallel}), D(\vec{k}_{\parallel})$ averaged over the ensemble of realization of the surface roughness.

III. DETERMINATION OF THE COEFFICIENTS

The equations for the coefficients $A(\vec{k}_{\parallel}), B(\vec{k}_{\parallel})$, etc., obtained in Sec. II contain the Fourier coefficient of the surface-roughness-profile function $\zeta(\vec{x}_{\parallel})$. We do not know this function in any given case. The best we can do in this situation is to solve for these coefficients and then average the results over $\zeta(\vec{x}_{\parallel})$ or, more precisely, over the ensemble of realizations of its Fourier coefficient $\hat{\zeta}(\vec{k}_{\parallel})$. The latter is characterized by the properties

$$\langle \hat{\zeta}(\vec{k}_{\parallel})\rangle = 0 , \tag{3.1}$$

$$\langle \hat{\zeta}(\vec{k}_{\parallel})\hat{\zeta}(\vec{k}_{\parallel}')\rangle = \delta^2(2\pi)^2 g(k_{\parallel})\delta(\vec{k}_{\parallel}+\vec{k}_{\parallel}') , \tag{3.2}$$

which follow from Eqs. (1.1), (1.2), and (2.8). The surface structure function $g(k_{\parallel})$ is the Fourier transform of the correlation function $W(\vec{x}_{\parallel})$ and, in the present case, is given by

$$g(k_{\parallel}) = \pi a^2 \exp(-a^2k_{\parallel}^2/4) . \tag{3.3}$$

Averaging over the ensemble of realizations of the surface roughness in the way just described will be seen to restore infinitesimal translational invariance to the system we are studying, i.e., the averaged image potential will depend on the coordinates $\vec{x}_{\parallel}$ and $\vec{x}_{\parallel}'$ only through their difference.

In this section we solve for the averaged values of the coefficients $A(\vec{k}_{\parallel}), B(\vec{k}_{\parallel}), C(\vec{k}_{\parallel}), D(\vec{k}_{\parallel})$ by two different methods, the first perturbative, the second nonperturbative. The results of the first approach are particularly useful for obtaining the change due to surface roughness in the image potential caused by a static point charge. This case will be discussed in Sec. IV. The results of the nonperturbative approach are necessary for the discussion of the energy loss suffered by an electron moving along a prescribed trajectory above a rough metal surface that will be presented in Sec. VI. Although the perturbative results can be obtained from the nonperturbative results by expanding the latter in powers of the mean-square departure of the surface from flatness δ^2, we outline an independent calculation of the perturbative results. This is because results obtained at an intermediate stage of such a calculation have an independent interest in situations where the surface profile function $\zeta(\vec{x}_{\parallel})$ is a prescribed function rather than a random function characterized by the properties (1.1) and (1.2).

To obtain the perturbative solutions of Eq. (2.6) we expand $A(\vec{k}_{\parallel})$ and $B(\vec{k}_{\parallel})$ formally according to

$$A(\vec{k}_{\parallel}) = A^{(0)}(\vec{k}_{\parallel}) + A^{(1)}(\vec{k}_{\parallel}) + A^{(2)}(\vec{k}_{\parallel}) + \cdots , \tag{3.4a}$$

$$B(\vec{k}_{\parallel}) = B^{(0)}(\vec{k}_{\parallel}) + B^{(1)}(\vec{k}_{\parallel}) + B^{(2)}(\vec{k}_{\parallel}) + \cdots , \tag{3.4b}$$

where the superscript denotes the order of each term in $\hat{\zeta}(\vec{k}_{\parallel})$. When these expansions are substituted into Eq. (2.6), and terms of the same order in $\hat{\zeta}(\vec{k}_{\parallel})$ on both sides are equated, the solutions of the resulting equations are

$$\begin{pmatrix} A^{(0)}(\vec{k}_{\parallel}) \\ B^{(0)}(\vec{k}_{\parallel}) \end{pmatrix} = \frac{2\pi q}{k_{\parallel}} \frac{1}{(\epsilon+1)} \exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}') \exp(-k_{\parallel}x_3') \begin{pmatrix} 1-\epsilon \\ 2 \end{pmatrix} , \tag{3.5a}$$

$$\begin{pmatrix} A^{(1)}(\vec{k}_{\parallel}) \\ B^{(1)}(\vec{k}_{\parallel}) \end{pmatrix} = -4\pi q \frac{\epsilon-1}{(\epsilon+1)^2} \int \frac{d^2q_{\parallel}}{(2\pi)^2} \exp(-i\vec{q}_{\parallel}\cdot\vec{x}_{\parallel}') \exp(-q_{\parallel}x_3')\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel}) \begin{pmatrix} \epsilon+\hat{k}_{\parallel}\cdot\hat{q}_{\parallel} \\ -1+\hat{k}_{\parallel}\cdot q_{\parallel} \end{pmatrix} , \tag{3.5b}$$

$$\begin{aligned} \begin{pmatrix} A^{(2)}(\vec{k}_{\parallel}) \\ B^{(2)}(\vec{k}_{\parallel}) \end{pmatrix} = {} & -4\pi q \frac{\epsilon-1}{(\epsilon+1)^3} \int \frac{d^2q_{\parallel}}{(2\pi)^2} \int \frac{d^2Q_{\parallel}}{(2\pi)^2} \exp(-i\vec{Q}_{\parallel}\cdot\vec{x}_{\parallel}') \exp(-Q_{\parallel}x_3')q_{\parallel}\hat{\zeta}(\vec{k}_{\parallel}-\vec{q}_{\parallel})\hat{\zeta}(\vec{q}_{\parallel}-\vec{Q}_{\parallel}) \\ & \times \begin{pmatrix} \epsilon(\epsilon-1)+2\epsilon\hat{q}_{\parallel}\cdot(\hat{Q}_{\parallel}+\hat{k}_{\parallel}) - (\hat{k}_{\parallel}\cdot\hat{q}_{\parallel})(\hat{q}_{\parallel}\cdot\hat{Q}_{\parallel})(\epsilon-1) \\ -(\epsilon-1) - 2\hat{Q}_{\parallel}\cdot\hat{q}_{\parallel} + 2\epsilon(\hat{k}_{\parallel}\cdot\hat{q}) - (\hat{k}_{\parallel}\cdot\hat{q}_{\parallel})(\hat{q}_{\parallel}\cdot\hat{Q}_{\parallel})(\epsilon-1) \end{pmatrix} . \end{aligned} \tag{3.5c}$$

Evidently the results given by Eq. (3.5a), when substituted into Eqs. (2.4), yield the image potential associated with a planar vacuum-dielectric interface. As they stand, the coefficients $A^{(1,2)}(\vec{k}_\parallel)$ and $B^{(1,2)}(\vec{k}_\parallel)$ can be used with Eqs. (2.4) to yield the corrections to the planar-interface image potential in the case that the surface-profile function $\zeta(\vec{x}_\parallel)$ is a known function of $\vec{x}_\parallel$ and not a random function. This is the situation if, for example, $\zeta(\vec{x}_\parallel)$ is due to a grating ruled on the surface of the dielectric or to the passage of a Rayleigh wave along the surface of the dielectric.[6] Equations (3.5b) and (3.5c) can also be used to obtain the energy of interaction of an electron above the surface of liquid helium.[7]

The expressions for the averaged values of $A(\vec{k}_\parallel)$ and $B(\vec{k}_\parallel)$ obtained with the use of Eqs. (3.1)–(3.3) are

$$\langle A(\vec{k}_\parallel)\rangle = A^{(0)}(\vec{k}_\parallel) + \langle A^{(2)}(\vec{k}_\parallel)\rangle , \tag{3.6a}$$

$$\langle B(\vec{k}_\parallel)\rangle = B^{(0)}(\vec{k}_\parallel) + \langle B^{(2)}(\vec{k}_\parallel)\rangle , \tag{3.6b}$$

where

$$\begin{bmatrix} \langle A^{(2)}(\vec{k}_\parallel)\rangle \\ \\ \langle B^{(2)}(\vec{k}_\parallel)\rangle \end{bmatrix} = -16\pi q \frac{\delta^2}{a^4}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\exp(-i\vec{k}_\parallel\cdot\vec{x}'_\parallel)\frac{\exp(-k_\parallel x'_3)}{k_\parallel^3}\begin{bmatrix} (\epsilon-\frac{1}{2})\mathcal{J}_0(\xi)+\dfrac{4\epsilon}{\epsilon-1}\mathcal{J}_1(\xi)-\frac{1}{2}\mathcal{J}_2(\xi) \\ \\ -\frac{3}{2}\mathcal{J}_0(\xi)+2\mathcal{J}_1(\xi)-\frac{1}{2}\mathcal{J}_2(\xi) \end{bmatrix} . \tag{3.7}$$

The integrals $\mathcal{J}_n(\xi)$ appearing in these expressions are defined by

$$\mathcal{J}_n(\xi) = e^{-\xi^2/4}\int_0^\infty du\, e^{-u^2/\xi^2}u^2 I_n(u) , \tag{3.8}$$

$$= \tfrac{1}{16}\pi^{1/2}e^{-\xi^2/8}\xi^5\{I_{n/2-1}(\tfrac{1}{8}\xi^2) + [1+(4/\xi^2)-(4n/\xi^2)]I_{n/2}(\tfrac{1}{8}\xi^2)\} , \tag{3.9}$$

where

$$\xi = ak_\parallel , \tag{3.10}$$

and $I_n(u)$ is a modified Bessel function.

When the charge q is inside the dielectric medium, it is the coefficients $C(\vec{k}_\parallel)$ and $D(\vec{k}_\parallel)$ appearing in Eqs. (2.5) that are required. If we expand these coefficients formally in powers of $\hat{\zeta}(\vec{k}_\parallel)$, as was done in Eqs. (3.4), we find that the contributions to $C(\vec{k}_\parallel)$ and $D(\vec{k}_\parallel)$ of zeroth, first, and second order in $\hat{\zeta}(\vec{k}_\parallel)$ are

$$\begin{bmatrix} C^0(\vec{k}_\parallel) \\ \\ D^0(\vec{k}_\parallel) \end{bmatrix} = \frac{2\pi q}{k_\parallel}\frac{1}{(\epsilon+1)}\exp(-i\vec{k}_\parallel\cdot\vec{x}'_\parallel)\exp(k_\parallel x'_3)\begin{bmatrix} 2 \\ 1-1/\epsilon \end{bmatrix} , \tag{3.11a}$$

$$\begin{bmatrix} C^{(1)}(\vec{k}_\parallel) \\ \\ D^{(1)}(\vec{k}_\parallel) \end{bmatrix} = -4\pi q\frac{(\epsilon-1)}{(\epsilon+1)^2}\int\frac{d^2q_\parallel}{(2\pi)^2}\exp(-i\vec{q}_\parallel\cdot\vec{x}'_\parallel)\exp(q_\parallel x'_3)\hat{\zeta}(\vec{k}_\parallel-\vec{q}_\parallel)\begin{bmatrix} \hat{k}_\parallel\cdot\hat{q}_\parallel-1 \\ \\ \hat{k}_\parallel\cdot\hat{q}_\parallel+1/\epsilon \end{bmatrix} , \tag{3.11b}$$

$$\begin{bmatrix} C^{(2)}(\vec{k}_\parallel) \\ \\ D^{(2)}(\vec{k}_\parallel) \end{bmatrix} = 4\pi q\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\int\frac{d^2q_\parallel}{(2\pi)^2}\int\frac{d^2Q_\parallel}{(2\pi)^2}\hat{\zeta}(\vec{k}_\parallel-\vec{q}_\parallel)\hat{\zeta}(\vec{q}_\parallel-\vec{Q}_\parallel)q_\parallel\exp(-i\vec{Q}_\parallel\cdot\vec{x}'_\parallel)\exp(Q_\parallel x'_3)$$
$$\times\begin{bmatrix} -(\epsilon-1)+2\hat{q}_\parallel\cdot(\epsilon\hat{Q}_\parallel-\hat{k}_\parallel)-(\epsilon-1)(\hat{k}_\parallel\cdot\hat{q}_\parallel)(\hat{q}_\parallel\cdot\hat{Q}_\parallel) \\ \\ 1-1/\epsilon-2\hat{q}_\parallel\cdot(\hat{k}_\parallel+\hat{Q}_\parallel)-(\epsilon-1)(\hat{k}_\parallel\cdot\hat{q}_\parallel)(\hat{q}_\parallel\cdot\hat{Q}_\parallel) \end{bmatrix} . \tag{3.11c}$$

The values of $C(\vec{k}_\parallel)$ and $D(\vec{k}_\parallel)$ averaged over the ensemble of realizations of the surface roughness are

$$\langle C(\vec{k}_\parallel)\rangle = C^{(0)}(\vec{k}_\parallel) + \langle C^{(2)}(\vec{k}_\parallel)\rangle , \tag{3.12a}$$

$$\langle D(\vec{k}_\parallel)\rangle = D^{(0)}(\vec{k}_\parallel) + \langle D^{(2)}(\vec{k}_\parallel)\rangle , \tag{3.12b}$$

where

$$\begin{pmatrix} \langle C^{(2)}(\vec{k}_\parallel)\rangle \\ \langle D^{(2)}(\vec{k}_\parallel)\rangle \end{pmatrix} = 16\pi q \frac{\delta^2}{a^4}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\exp(-i\vec{k}_\parallel\cdot\vec{x}_\parallel')\frac{\exp(k_\parallel x_3')}{k_\parallel^3}\begin{pmatrix} \frac{3}{2}\mathcal{J}_0(\xi)-2\mathcal{J}_1(\xi)+\frac{1}{2}\mathcal{J}_2(\xi) \\ (\frac{1}{2}-1/\epsilon)\mathcal{J}_0(\xi)+4/(\epsilon-1)\mathcal{J}_1(\xi)+\frac{1}{2}\mathcal{J}_2(\xi) \end{pmatrix}. \tag{3.13}$$

In Sec. IV, we will use these perturbative results for the coefficients $A(\vec{k}_\parallel)$, $B(\vec{k}_\parallel)$, $C(\vec{k}_\parallel)$, and $D(\vec{k}_\parallel)$, in combination with Eqs. (2.4) and (2.5), to obtain the effect of surface roughness on the image potential to second order in the ratio δ/a. However, for some applications, particularly in the study of resonant phenomena (an example of one such application will be studied in Sec. VI), it is necessary to have nonperturbative expressions for the average values of the coefficients $A(\vec{k}_\parallel), B(\vec{k}_\parallel), C(\vec{k}_\parallel), D(\vec{k}_\parallel)$. We will conclude this section by showing how such expressions can be obtained for $\langle A(\vec{k}_\parallel)\rangle$ and $\langle B(\vec{k}_\parallel)\rangle$, and will simply state the corresponding results for $\langle C(\vec{k}_\parallel)\rangle$ and $\langle D(\vec{k}_\parallel)\rangle$.

We denote the column vector $[A(\vec{k}_\parallel), B(\vec{k}_\parallel)]$ by $\vec{V}(\vec{k}_\parallel)$, and write Eq. (2.6) schematically as

$$(\vec{I}+\vec{L})\vec{V}=\vec{f}, \tag{3.14}$$

where $\vec{f}$ is a (random) two-component column vector, $\vec{I}$ is the 2×2 unit matrix, and $\vec{L}$ is a (random) 2×2 matrix integral operator. We next introduce the averaging operator P,

$$P\vec{V}\equiv\langle\vec{V}\rangle, \tag{3.15}$$

and the operator $Q=1-P$. On applying both of these operators to Eq. (3.14) in turn we obtain the pair of equations

$$P\vec{V}+P\vec{L}\vec{V}=P\vec{f}, \tag{3.16}$$

$$Q\vec{V}+Q\vec{L}\vec{V}=Q\vec{f}. \tag{3.17}$$

Since the vector $\vec{V}$ can be written in the form

$$\vec{V}=P\vec{V}+Q\vec{V}, \tag{3.18}$$

we can rewrite Eq. (3.17) as

$$Q\vec{V}+Q\vec{L}Q\vec{V}=Q\vec{f}-Q\vec{L}P\vec{V}. \tag{3.19}$$

We solve this equation for $Q\vec{V}$,

$$Q\vec{V}=(\vec{I}+Q\vec{L})^{-1}Q\vec{f}-(\vec{I}+Q\vec{L})^{-1}Q\vec{L}P\vec{V}, \tag{3.20}$$

and substitute the solution into Eq. (3.16) to obtain the equation satisfied by $\langle\vec{V}\rangle$. We write this equation in the form

$$\vec{M}\langle\vec{V}\rangle=\vec{g}, \tag{3.21}$$

with the formal solution

$$\langle\vec{V}\rangle=\vec{M}^{-1}\vec{g}, \tag{3.22}$$

where

$$\vec{M}=\vec{I}+\langle\!\langle(\vec{I}+\vec{L}Q)^{-1}\vec{L}\rangle, \tag{3.23a}$$

$$\vec{g}=\langle\!\langle(\vec{I}+\vec{L}Q)^{-1}\vec{f}\rangle. \tag{3.23b}$$

Equation (3.21) is exact. It has something of the character of a Dyson equation, with $\langle\!\langle\vec{I}+\vec{L}Q)^{-1}\vec{L}\rangle$ playing the role of the proper self-energy. As with the Dyson equation, we can obtain a nonperturbative solution for $\langle\vec{V}\rangle$ by obtaining $\vec{M}$ and $\vec{g}$ in a perturbative fashion and substituting the resulting expressions into the solution (3.22).

In the context of Eq. (2.6) we can write

$$\vec{L}=\vec{L}_1+\vec{L}_2, \tag{3.24a}$$

$$\vec{f}=\vec{f}_0+\vec{f}_1+\vec{f}_2, \tag{3.24b}$$

where the subscript denotes the order of each term in $\hat{\xi}(\vec{k}_\parallel)$. From Eq. (3.1) it follows that $\langle\vec{L}_1\rangle=\langle\vec{f}_1\rangle=0$, so that to second order in $\hat{\xi}(\vec{k}_\parallel)$ the matrices $\vec{M}$ and $\vec{g}$ reduce to

$$\vec{M}=\vec{I}+\langle\vec{L}_2\rangle-\langle\vec{L}_1^2\rangle, \tag{3.25a}$$

$$\vec{g}=\vec{f}_0+\langle\vec{f}_2\rangle-\langle\vec{L}_1\vec{f}_1\rangle. \tag{3.25b}$$

The expressions for $\vec{L}_1, \vec{L}_2, \vec{f}_0, \vec{f}_1, \vec{f}_2$ are obtained by comparing Eqs. (3.14) and (3.24) with Eq. (2.6). The ensemble-averaged values of the combinations of these quantities appearing in Eqs. (3.25), obtained with the help of Eqs. (3.1) and (3.2), are

$$\langle\vec{L}_2\rangle=\frac{1}{2}\frac{\delta^2}{a^2}a^2k_\parallel^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \tag{3.26a}$$

$$\langle\vec{L}_1^2\rangle=4\frac{(\epsilon-1)}{(\epsilon+1)^2}\frac{\delta^2}{a^2}\frac{1}{a^2k_\parallel^2}\begin{pmatrix}(\epsilon-\frac{1}{2})\mathcal{J}_0+\frac{4\epsilon}{\epsilon-1}\mathcal{J}_1-\frac{1}{2}\mathcal{J}_2 & \epsilon(\frac{3}{2}\mathcal{J}_0-2\mathcal{J}_1+\frac{1}{2}\mathcal{J}_2)\\ -(\frac{3}{2}\mathcal{J}_0-2\mathcal{J}_1+\frac{1}{2}\mathcal{J}_2) & \frac{1}{2}(\epsilon-2)\mathcal{J}_0+\frac{4\epsilon}{\epsilon-1}\mathcal{J}_1+\frac{\epsilon}{2}\mathcal{J}_2\end{pmatrix}, \tag{3.26b}$$

$$\vec{f}_0=\frac{2\pi q}{(\epsilon+1)k_{\parallel}}\exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(-k_{\parallel}x_3')\begin{bmatrix}1-\epsilon\\ \\ 2\end{bmatrix}, \tag{3.27a}$$

$$\langle\vec{f}_2\rangle=\frac{\pi q}{(\epsilon+1)}\delta^2 k_{\parallel}\exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(-k_{\parallel}x_3')\begin{bmatrix}1-\epsilon\\ \\ 2\end{bmatrix}, \tag{3.27b}$$

and

$$\langle\vec{L}_1\vec{f}_1\rangle=\frac{4\pi q}{k_{\parallel}^3a^4}\delta^2\frac{(\epsilon-1)}{(\epsilon+1)^2}\exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(-k_{\parallel}x_3')\begin{bmatrix}\mathcal{J}_2+(2\epsilon+1)\mathcal{J}_0\\ \mathcal{J}_2+4\dfrac{(\epsilon+1)}{(\epsilon-1)}\mathcal{J}_1-\mathcal{J}_0\end{bmatrix}, \tag{3.27c}$$

where we have suppressed the argument ξ of the $\mathcal{J}_n$'s appearing in these expressions to simplify the notation.

We note from the results given by Eqs. (3.25)–(3.27) that although $\vec{L}$ is a matrix integral operator, $\overleftrightarrow{M}$ is simply a scalar matrix. The averaging operation has converted the integral equation (3.14) for $\vec{V}$ into an ordinary matrix equation for $\langle\vec{V}\rangle$, whose solution is simply obtained.

The ensemble-averaged forms of the coefficients $A(\vec{k}_{\parallel})$ and $B(\vec{k}_{\parallel})$ are now readily obtained from Eqs. (3.22) and (3.25)–(3.27). We find finally that

$$\langle A(\vec{k}_{\parallel})\rangle=\frac{2\pi q}{k_{\parallel}}\exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(-k_{\parallel}x_3')a(k_{\parallel}), \tag{3.28a}$$

$$\langle B(\vec{k}_{\parallel})\rangle=\frac{2\pi q}{k_{\parallel}}\exp(-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}')\exp(-k_{\parallel}x_3')b(k_{\parallel}), \tag{3.28b}$$

where

$$a(k_{\parallel})=\frac{1}{(\epsilon+1)}\frac{M_{22}(k_{\parallel})h_1(k_{\parallel})-M_{12}(k_{\parallel})h_2(k_{\parallel})}{|\overleftrightarrow{M}(k_{\parallel})|}, \tag{3.29a}$$

$$b(k_{\parallel})=\frac{1}{(\epsilon+1)}\frac{M_{11}(k_{\parallel})h_2(k_{\parallel})-M_{21}(k_{\parallel})h_1(k_{\parallel})}{|\overleftrightarrow{M}(k_{\parallel})|}. \tag{3.29b}$$

The functions $M_{ij}(k_{\parallel})$ and $h_i(k_{\parallel})$ appearing in these expressions are given by

$$M_{11}(k_{\parallel})=1+\frac{1}{2}\frac{\delta^2}{a^2}\xi^2-4\frac{\delta^2}{a^2}\frac{1}{\xi^2}\frac{\epsilon-1}{(\epsilon+1)^2}\times\left((\epsilon-\tfrac{1}{2})\mathcal{J}_0+\frac{4\epsilon}{\epsilon-1}\mathcal{J}_1-\tfrac{1}{2}\mathcal{J}_2\right), \tag{3.30a}$$

$$M_{12}(k_{\parallel})=-4\frac{\delta^2}{a^2}\frac{1}{\xi^2}\frac{\epsilon(\epsilon-1)}{(\epsilon+1)^2}(\tfrac{3}{2}\mathcal{J}_0-2\mathcal{J}_1+\tfrac{1}{2}\mathcal{J}_2), \tag{3.30b}$$

$$M_{21}(k_{\parallel})=4\frac{\delta^2}{a^2}\frac{1}{\xi^2}\frac{\epsilon-1}{(\epsilon+1)^2}(\tfrac{3}{2}\mathcal{J}_0-2\mathcal{J}_1+\tfrac{1}{2}\mathcal{J}_2), \tag{3.30c}$$

$$M_{22}(k_{\parallel})=1+\frac{1}{2}\frac{\delta^2}{a^2}\xi^2-4\frac{\delta^2}{a^2}\frac{1}{\xi^2}\frac{\epsilon-1}{(\epsilon+1)^2}\times\left(\tfrac{1}{2}(\epsilon-2)\mathcal{J}_0+\frac{4\epsilon}{\epsilon-1}\mathcal{J}_1+\tfrac{1}{2}\epsilon\mathcal{J}_2\right), \tag{3.30d}$$

and

$$h_1(k_{\parallel})=(1-\epsilon)\left(1+\frac{1}{2}\frac{\delta^2}{a^2}\xi^2+2\frac{\delta^2}{a^2}\frac{1}{\xi^2}\frac{1}{(\epsilon+1)}\times[\mathcal{J}_2+(2\epsilon+1)\mathcal{J}_0]\right) \tag{3.31a}$$

$$h_2(k_{\parallel})=2\left[1+\frac{1}{2}\frac{\delta^2}{a^2}\xi^2+\frac{\delta^2}{a^2}\frac{(1-\epsilon)}{(\epsilon+1)}\frac{1}{\xi^2}\left(\mathcal{J}_2+\frac{4(\epsilon+1)}{(\epsilon-1)}\mathcal{J}_1-\mathcal{J}_0\right)\right]. \tag{3.31b}$$

The ensemble-averaged forms of the coefficients $C(\vec{k}_{\parallel})$ and $D(\vec{k}_{\parallel})$, for the case when the charge q is located in the dielectric are obtained in a similar fashion with Eq. (2.7) as the starting equation. The resulting expressions are

$$\langle C(\vec{k}_{\parallel})\rangle=\frac{2\pi q}{k_{\parallel}}\exp(-ik_{\parallel}\cdot x_{\parallel}')\exp(k_{\parallel}x_3')c(k_{\parallel}), \tag{3.32a}$$

$$\langle D(\vec{k}_{\parallel})\rangle=\frac{2\pi q}{k_{\parallel}}\exp(-ik_{\parallel}\cdot x_{\parallel}')\exp(k_{\parallel}x_3')d(k_{\parallel}), \tag{3.32b}$$

where

$$c(k_{\parallel})=\frac{1}{\epsilon+1}\frac{M_{22}(k_{\parallel})h_1'(k_{\parallel})-M_{12}(k_{\parallel})h_2'(k_{\parallel})}{|\overleftrightarrow{M}(k_{\parallel})|}, \tag{3.33a}$$

$$d(k_{\parallel})=\frac{1}{\epsilon+1}\frac{M_{11}(k_{\parallel},\omega)h_2'(k_{\parallel})-M_{21}(k_{\parallel})h_1'(k_{\parallel})}{|\overleftrightarrow{M}(k_{\parallel})|}, \tag{3.33b}$$

and

$$h_1'(k_\parallel)=2\left[1+\frac{1}{2}\frac{\delta^2}{a^2}\xi^2 + \frac{\delta^2}{a^2}\frac{1}{\xi^2}\frac{\epsilon-1}{\epsilon+1}\left(\mathcal{J}_2-4\frac{(\epsilon+1)}{\epsilon-1}\mathcal{J}_1-\mathcal{J}_0\right)\right], \quad (3.34a)$$

$$h_2'(k_\parallel)=\frac{\epsilon-1}{\epsilon}\left[1+\frac{1}{2}\frac{\delta^2}{a^2}\xi^2 + 2\frac{\delta^2}{\xi^2}\frac{1}{\xi^2}\frac{\epsilon}{\epsilon+1}\left(\mathcal{J}_2+\frac{\epsilon+2}{\epsilon}\mathcal{J}_0\right)\right]. \quad (3.34b)$$

We note finally that the perturbative results for $\langle A(\vec{k}_\parallel)\rangle$, $\langle B(\vec{k}_\parallel)\rangle$, and $\langle C(\vec{k}_\parallel)\rangle$, $\langle D(\vec{k}_\parallel)\rangle$ given by Eqs. (3.5a), (3.6)–(3.7), and by Eqs. (3.11a), (3.12)–(3.13), respectively, can be obtained by expanding the results given by Eqs. (3.28)–(3.31) and by Eqs. (3.32)–(3.34), respectively, to the first nonvanishing order in (δ^2/a^2). However, as we have pointed out earlier, this way of obtaining the perturbative results does not yield the results given by Eqs. (3.5b)–(3.5c) and Eqs. (3.11b)–(3.11c), which are of interest in themselves.

IV. IMAGE POTENTIAL IN THE PRESENCE OF SURFACE ROUGHNESS

In Sec. III we have obtained the ensemble-averaged values of the coefficients $A(\vec{k}_\parallel)$, $B(\vec{k}_\parallel)$, $C(\vec{k}_\parallel)$, and $D(\vec{k}_\parallel)$ that determine the image potential in the four regions of (x_3, x_3') space defined by the possibilities $x_3 \gtrless 0$, $x_3' \gtrless 0$. To distinguish the different forms the electrostatic potential takes in these regions we introduce the definitions

$$\langle\varphi(\vec{x}\,|\,\vec{x}')\rangle \equiv \varphi_{\rm I}(\vec{x}\,|\,\vec{x}'),\ x_3>0,\ x_3'>0 \quad (4.1a)$$

$$\equiv \varphi_{\rm II}(\vec{x}\,|\,\vec{x}'),\ x_3<0,\ x_3'>0 \quad (4.1b)$$

$$\equiv \varphi_{\rm III}(\vec{x}\,|\,\vec{x}'),\ x_3>0,\ x_3'<0 \quad (4.1c)$$

$$\equiv \varphi_{\rm IV}(\vec{x}\,|\,\vec{x}'),\ x_3<0,\ x_3'<0. \quad (4.1d)$$

When we substitute the results given by Eqs. (3.5a), (3.6)–(3.7), and (3.11a), (3.12)–(3.13), into Eqs. (2.4a), (2.4b), (2.5a), (2.5b), respectively, we obtain for these four potentials the following expressions to $O(\delta^2/a^2)$:

$$\varphi_{\rm I}(\vec{x}\,|\,\vec{x}')=\frac{q}{a}\frac{1}{(\rho^2+d^2)^{1/2}}-\frac{q}{a}\left(\frac{\epsilon-1}{\epsilon+1}\right)\frac{1}{(\rho^2+z^2)^{1/2}} - 8\frac{q}{a}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\mathcal{G}_{\rm I}(z,\rho), \quad (4.2a)$$

$$\varphi_{\rm II}(\vec{x}\,|\,\vec{x}')=\frac{q}{a}\frac{2}{\epsilon+1}\frac{1}{(\rho^2+z^2)^{1/2}}+8\frac{q}{a}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\mathcal{G}_{\rm II}(z,\rho) = \varphi_{\rm III}(\vec{x}\,|\,\vec{x}'), \quad (4.2b)$$

$$\varphi_{\rm IV}(\vec{x}\,|\,\vec{x}')=\frac{q}{a}\frac{1}{\epsilon}\frac{1}{(\rho^2+d^2)^{1/2}}+\frac{q}{a}\frac{(\epsilon-1)}{\epsilon(\epsilon+1)}\frac{1}{(\rho^2+z^2)^{1/2}} + 8\frac{q}{a}\frac{1}{\epsilon}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\mathcal{G}_{\rm IV}(z,\rho), \quad (4.2c)$$

where

$$\mathcal{G}_{\rm I}(z,\rho)=\int_0^\infty d\xi\, J_0(\xi\rho)\frac{e^{-\xi z}}{\xi^2} \times\left((\epsilon-\tfrac{1}{2})\mathcal{J}_0(\xi)+\frac{4\epsilon}{\epsilon-1}\mathcal{J}_1(\xi)-\tfrac{1}{2}\mathcal{J}_2(\xi)\right), \quad (4.3a)$$

$$\mathcal{G}_{\rm II}(z,\rho)=\int_0^\infty d\xi\, J_0(\xi\rho)\frac{e^{-\xi z}}{\xi^2} \times\left[\tfrac{3}{2}\mathcal{J}_0(\xi)-2\mathcal{J}_1(\xi)+\tfrac{1}{2}\mathcal{J}_2(\xi)\right], \quad (4.3b)$$

$$\mathcal{G}_{\rm IV}(z,\rho)=\int_0^\infty d\xi\, J_0(\xi\rho)\frac{e^{-\xi z}}{\xi^2} \times\left((\tfrac{1}{2}\epsilon-1)\mathcal{J}_0(\xi)+\frac{4\epsilon}{\epsilon-1}\mathcal{J}_1(\xi)+\frac{\epsilon}{2}\mathcal{J}_2(\xi)\right). \quad (4.3c)$$

In Eqs. (4.3) $J_0(\xi\rho)$ is a Bessel function, and we have introduced the following dimensionless variables:

$$d=|x_3-x_3'|/a, \quad (4.4a)$$

$$z=(|x_3|+|x_3'|)/a, \quad (4.4b)$$

$$\rho=|\vec{x}_\parallel-\vec{x}_\parallel'|/a. \quad (4.4c)$$

The expression given by the first line of each of Eqs. (4.2) is the direct Coulomb potential of the charge q and/or the image potential associated with a flat dielectric-vacuum interface. The expression given by the second line of each of these equations is the contribution to the image potential due to the roughness of that interface, to $O(\delta^2/a^2)$.

Thus the contribution to the image potential from the surface roughness depends on the functions $\mathcal{G}_{\rm I}(z,\rho)-\mathcal{G}_{\rm IV}(z,\rho)$ defined by Eqs. (4.3). In general, the evaluation of these integrals as functions of the two variables z and ρ must be carried out numerically.

However, in certain limiting cases it is possible to obtain the asymptotic forms of these integrals. One such case is that for $\rho=0$, which arises, for example, in obtaining the effect of surface roughness on the energies of the electric subbands in an inversion layer at a semiconductor surface.[8] In this case it is possible to obtain the leading terms in the asymptotic expansions of $\mathcal{G}_{\rm I}(z,0)-\mathcal{G}_{\rm IV}(z,0)$ for both $z\ll 1$ and $z\gg 1$. We now turn to a determination of these expansions.

The integrals $\mathcal{G}_{\mathrm{I}}(z,\rho)-\mathcal{G}_{\mathrm{IV}}(z,\rho)$ contain the functions $\mathcal{G}_n(\xi)$ in their integrands. These functions are defined by Eqs. (3.8)–(3.9). Their asymptotic forms in the limits of large and small ξ are needed for the analysis that follows and are obtained from those of the modified Bessel functions.[9] Thus, we have that for case (a), where $\xi \gg 1$:

$$\mathcal{G}_0(\xi) \sim \tfrac{1}{4}\xi^4+\tfrac{1}{4}\xi^2+\tfrac{1}{8}+\tfrac{3}{8}\,1/\xi^2+O(\xi^{-4}), \qquad (4.5a)$$

$$\mathcal{G}_1(\xi)=\tfrac{1}{4}\xi^4, \qquad (4.5b)$$

$$\mathcal{G}_2(\xi) \sim \tfrac{1}{4}\xi^4-\tfrac{3}{4}\xi^2+\tfrac{9}{8}+\tfrac{15}{8}\,1/\xi^2+O(\xi^{-4}). \qquad (4.5c)$$

For case (b), where $\xi \ll 1$:

$$\mathcal{G}_0(\xi) \sim \pi^{1/2}\left[\tfrac{1}{4}\xi^3+\tfrac{1}{32}\xi^5-\tfrac{1}{1024}\xi^7+O(\xi^9)\right], \qquad (4.6a)$$

$$\mathcal{G}_1(\xi)=\tfrac{1}{4}\xi^4, \qquad (4.6b)$$

$$\mathcal{G}_2(\xi) \sim \pi^{1/2}\left[\tfrac{3}{64}\xi^5-\tfrac{1}{512}\xi^7+O(\xi^9)\right]. \qquad (4.6c)$$

We now proceed to calculate the asymptotic forms of the functions $\mathcal{G}_{\mathrm{I}}(z,0)$, $\mathcal{G}_{\mathrm{II}}(z,0)$, and $\mathcal{G}_{\mathrm{IV}}(z,0)$ for large and small values of the parameter z.

A. Large z

Recall that z is defined as the ratio $(|x_3|+|x_3'|)/a$, where the magnitudes $|x_3|$ and $|x_3'|$ indicate roughly the distance from the surface at which the potential is measured and that at which the point charge is located, respectively, and a is the rough-surface transverse-correlation length. In the limit $z \gg 1$ one is therefore obtaining the image potential far from the surface.

It is clear from the form of the functions $\mathcal{G}(z,0)$ given by Eqs. (4.3) that for large z ($z \gg 1$) only small values of ξ can contribute significantly to the integral. We can therefore use the asymptotic forms in Eq. (4.6) for $\mathcal{G}_n(\xi)$ to obtain the following result:

$$\mathcal{G}_{\mathrm{I}}(z,0) \sim \int_0^\infty d\xi\, \frac{e^{-\xi z}}{\xi^2}\left(\frac{\pi^{1/2}}{8}(2\epsilon-1)\xi^3+\frac{\epsilon}{\epsilon-1}\xi^4 + \frac{\pi^{1/2}}{128}(2\epsilon-5)\xi^5+\cdots\right)$$
$$=\frac{\pi^{1/2}}{8}(2\epsilon-1)\frac{1}{z^2}+\frac{2\epsilon}{\epsilon-1}\frac{1}{z^3} + \frac{3\pi^{1/2}}{64}(2\epsilon-5)\frac{1}{z^4}+\cdots . \qquad (4.7a)$$

The asymptotic expansions for $\mathcal{G}_{\mathrm{II}}(z,0)$ and $\mathcal{G}_{\mathrm{IV}}(z,0)$ in the limit of large z are obtained in the same way with the results that

$$\mathcal{G}_{\mathrm{II}}(z,0) \sim \tfrac{3}{8}\pi^{1/2}\frac{1}{z^2}-\frac{1}{z^3}+\tfrac{27}{64}\pi^{1/2}\frac{1}{z^4}+\cdots, \qquad (4.7b)$$

$$\mathcal{G}_{\mathrm{IV}}(z,0) \sim \tfrac{1}{8}\pi^{1/2}(\epsilon-2)\frac{1}{z^2}+\frac{\epsilon}{\epsilon-1}(3\epsilon-1)\frac{1}{z^3} + \tfrac{3}{64}\pi^{1/2}(5\epsilon-4)\frac{1}{z^4}+\cdots . \qquad (4.7c)$$

B. Small z

For completeness we present here an outline of the derivation of the forms of the integrals $\mathcal{G}_{\mathrm{I}}(z,0)$–$\mathcal{G}_{\mathrm{IV}}(z,0)$ in the limit that $(|x_3|+|x_3'|)\ll a$, although the results may have only a limited significance. This is because in obtaining the equations for the coefficients $A(\vec{k}_\parallel),\ldots,D(\vec{k}_\parallel)$, Eqs. (2.6)–(2.7), we expanded exponentials of the type of $\exp[\pm k_\parallel \zeta(\vec{x}_\parallel)]$ in powers of $k_\parallel\zeta(\vec{x}_\parallel)$ up to second-order terms. This presupposes that $k_\parallel\zeta(\vec{x}_\parallel)$ is small, of the order of, or smaller, than unity. This in turn means that $k_\parallel$ is of the order of, or smaller, than $[\zeta(\vec{x}_\parallel)]^{-1}$, and, as an order-of-magnitude estimate of this inequality, we can say that the expansion is valid for $k_\parallel<\delta^{-1}$. Now, the small-$k_\parallel$ behavior of a function determines the large-z behavior of its Laplace transform, which is the form of the integrals (4.3) defining the functions $\mathcal{G}_{\mathrm{I}}(z,0)$–$\mathcal{G}_{\mathrm{IV}}(z,0)$ when $\rho=0$. Consequently, it is only the large-z behavior of these integrals that we can hope to obtain accurately by our procedures. In particular we expect the preceding analysis to be valid when $(|x_3|+|x_3'|)>\delta$, i.e., when $z>\delta/a$. The requirement that z be much smaller than unity means that $|x_3|$ and $|x_3'|$ each have to be smaller than a. Consequently, the results to be obtained in this subsection are expected to hold only for values of $|x_3|$ and $|x_3'|$ satisfying the inequalities $\delta<x_3,x_3'<a$.

We begin the derivation by breaking up the range of integration in the integral for $\mathcal{G}_{\mathrm{I}}(z,0)$ into two parts according to

$$\mathcal{G}_{\mathrm{I}}(z,0)=\int_0^1 d\xi e^{-\xi z}f_{\mathrm{I}}(\xi)+\int_1^\infty d\xi e^{-\xi z}f_{\mathrm{I}}(\xi), \qquad (4.8)$$

where

$$f_{\mathrm{I}}(\xi)=\frac{1}{\xi^2}\left((\epsilon-\tfrac{1}{2})\mathcal{G}_1(\xi)+\frac{4\epsilon}{\epsilon-1}\mathcal{G}_1(\xi)-\tfrac{1}{2}\mathcal{G}_2(\xi)\right). \qquad (4.9)$$

In the first integral the exponential factor can be expanded in powers of z and the series integrated term by term, to yield the formal result that

$$\mathcal{G}_{\mathrm{I}}^{(1)}(z,0)=\int_0^1 d\xi f_{\mathrm{I}}(\xi)-z\int_0^1 d\xi\,\xi f_{\mathrm{I}}(\xi) +\tfrac{1}{2}z^2\int_0^1 d\xi\,\xi^2 f_{\mathrm{I}}(\xi)-\cdots . \qquad (4.10)$$

In the second integral we use the large ξ expansion for $f_{\mathrm{I}}(\xi)$ to obtain

$$\mathcal{G}_{\mathrm{I}}^{(2)}(z,0)=\int_1^\infty d\xi\, e^{-\xi z}\left(\frac{(\epsilon+1)^2}{4(\epsilon-1)}\xi^2+\tfrac{1}{4}(\epsilon+1) +\tfrac{1}{8}(\epsilon-5)\frac{1}{\xi^2}+\cdots\right). \qquad (4.11)$$

If we define the integral

$$F_n(z)=\int_1^\infty d\xi\,\xi^n e^{-\xi z},$$

that satisfies the recurrence relation

$$F_n(z)=F_0(z)+(n/z)F_{n-1}(z)\,,$$

with

$$F_0(z)=e^{-z}/z$$
$$=1/z-1+\tfrac{1}{2}z-\tfrac{1}{6}z^2+\tfrac{1}{24}z^3+\cdots\,,\quad 0<z<1$$
$$F_{-1}(z)=E_1(z)$$
$$=-\ln z-\gamma+z-\tfrac{1}{4}z^2+\tfrac{1}{18}z^3-\cdots\,,\quad 0<z<1\,,$$

where $E_1(z)$ is the exponential integral and $\gamma=0.577216$ is Euler's constant, the small-z form of the integral $\mathcal{G}_{\rm I}^{(2)}(z,0)$ is readily obtained. We find that

$$\mathcal{G}_{\rm I}^{(2)}(z,0)\sim\frac{(\epsilon+1)^2}{2(\epsilon-1)}\frac{1}{z^3}+\tfrac{1}{4}(\epsilon+1)\frac{1}{z}+\mathcal{C}+\tfrac{1}{8}(\epsilon-5)z\ln z+O(z)\,,\qquad(4.12)$$

where the constant $\mathcal{C}$ is given by

$$\mathcal{C}=-\frac{(\epsilon+1)^2}{12(\epsilon-1)}-\tfrac{1}{4}(\epsilon+1)+\int_1^\infty d\xi\left(f_{\rm I}(\xi)-\frac{(\epsilon+1)^2}{4(\epsilon-1)}\xi^2-\tfrac{1}{4}(\epsilon+1)\right).\qquad(4.13)$$

It follows from Eqs. (4.8), (4.10), and (4.12) that the leading terms in the small-z expansion of $\mathcal{G}_{\rm I}(z,0)$ are

$$\mathcal{G}_{\rm I}(z,0)\sim\frac{(\epsilon+1)^2}{2(\epsilon-1)}\frac{1}{z^3}+\tfrac{1}{4}(\epsilon+1)\frac{1}{z}+O(z^0)\,.\qquad(4.14)$$

In a similar way the leading terms in the small-z expansion of the function $\mathcal{G}_{\rm IV}(z,0)$ are found to be

$$\mathcal{G}_{\rm IV}(z,0)\sim\frac{(\epsilon+1)^2}{2(\epsilon-1)}\frac{1}{z^3}-\tfrac{1}{4}(\epsilon+1)\frac{1}{z}+O(z^0)\,.\qquad(4.15)$$

In contrast the function $\mathcal{G}_{\rm II}(z,0)$ is found to approach a constant value as z tends to zero. The leading two terms in the small-z expansion of this integral are

$$\mathcal{G}_{\rm II}(z,0)\sim\int_0^\infty d\xi\, f_{\rm II}(\xi)+\tfrac{3}{4}z\ln z+O(z)\,,\qquad(4.16)$$

where

$$f_{\rm II}(\xi)=\frac{1}{\xi^2}\left[\tfrac{3}{2}\mathcal{J}_0(\xi)-2\mathcal{J}_1(\xi)+\tfrac{1}{2}\mathcal{J}_2(\xi)\right].\qquad(4.17)$$

The value of the integral is readily obtained if the integral representation in Eq. (3.8) for $\mathcal{J}_n(\xi)$ is used in Eq. (4.16) and the orders of integration are interchanged. In this way we obtain finally

$$\mathcal{G}_{\rm II}(z,0)\sim\frac{15\pi^{1/2}}{32}+\tfrac{3}{4}z\ln z+O(z)\,.\qquad(4.18)$$

Thus, in the two limits of large and small values of the parameter z, the expressions for the scalar potential in the case that $\rho=0$ are as summarized below. For case (i), where $z\gg1$:

$$\Phi_{\rm I}(x_3|x_3')\approx\frac{(q/a)}{d}-\frac{(\epsilon-1)}{(\epsilon+1)}\frac{(q/a)}{z}-8\frac{q}{a}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\left(\frac{\pi^{1/2}}{8}(2\epsilon-1)\frac{1}{z^2}+\frac{2\epsilon}{\epsilon-1}\frac{1}{z^3}+\frac{3\pi^{1/2}}{64}(2\epsilon-5)\frac{1}{z^4}+\cdots\right),\qquad(4.19)$$

$$\Phi_{\rm II}(x_3|x_3')\approx\frac{2(q/a)}{\epsilon+1}\frac{1}{z}+8\frac{q}{a}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\left(\frac{3\pi^{1/2}}{8}\frac{1}{z^2}-\frac{1}{z^3}+\frac{27\pi^{1/2}}{64}\frac{1}{z^4}+\cdots\right)=\Phi_{\rm III}(x_3|x_3')\,,\qquad(4.20)$$

$$\Phi_{\rm IV}(x_3|x_3')\approx\frac{(q/a)}{\epsilon d}+\left(\frac{\epsilon-1}{\epsilon+1}\right)\frac{q/a}{\epsilon z}+\frac{8(q/a)}{\epsilon}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\left(\frac{\pi^{1/2}}{8}(\epsilon-2)\frac{1}{z^2}+\frac{\epsilon(3\epsilon-1)}{\epsilon-1}\frac{1}{z^3}+\frac{3\pi^{1/2}}{64}(5\epsilon-4)\frac{1}{z^4}+\cdots\right).\qquad(4.21)$$

We note that the first term in the expansion of $\Phi_{\rm I}$ and $\Phi_{\rm IV}$ is the direct potential term while the rest of the terms constitute the image potential. Of course, there are no direct potential terms for $\Phi_{\rm II}$ and $\Phi_{\rm III}$. Also note that these expansions have the form of the terms in the multipole expansion (dipole, quadrupole, etc.) of the potential of a charge distribution. It is as if the surface roughness has smeared the image monopole into an extended charge distribution.

The results for case (ii), where $z\ll1$, can be summarized as follows:

$$\Phi_{\rm I}(x_3|x_3')\approx\frac{(q/a)}{d}-\left(\frac{\epsilon-1}{\epsilon+1}\right)\frac{(q/a)}{z}-8\frac{q}{a}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\left(\frac{(\epsilon+1)^2}{2(\epsilon-1)}\frac{1}{z^3}+\tfrac{1}{4}(\epsilon+1)\frac{1}{z}+\cdots\right),\qquad(4.22)$$

$$\Phi_{\rm II}(x_3|x_3')\approx\frac{2(q/a)}{(\epsilon+1)}\frac{1}{z}+8\frac{q}{a}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\left(\frac{15\pi^{1/2}}{32}+z\ln z+\cdots\right)\qquad(4.23)$$

$$=\Phi_{\rm III}(x_3|x_3')\,,\qquad(4.24)$$

$$\Phi_{\rm IV}(x_3|x_3')\approx\frac{(q/a)}{\epsilon d}+\frac{(q/a)}{\epsilon}\left(\frac{\epsilon-1}{\epsilon+1}\right)\frac{1}{z}+8\frac{(q/a)}{\epsilon}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{\delta^2}{a^2}\left(\frac{(\epsilon+1)^2}{2(\epsilon-1)}\frac{1}{z^3}-\tfrac{1}{4}(\epsilon+1)\frac{1}{z}+\cdots\right).\qquad(4.25)$$

In Figs. 1 and 2 we have plotted $\Phi_{\rm I}(x_3|x_3')$ when $z\gg1$ and $z\ll1$, respectively.

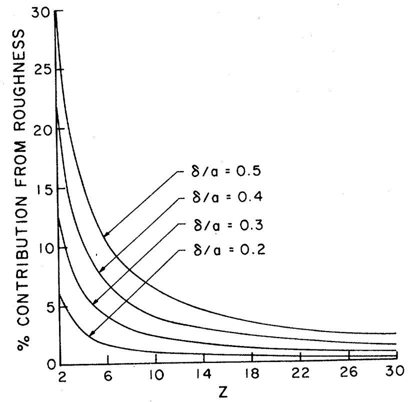

FIG. 1. The variation of the surface-roughness contribution to the image potential z, for large z, plotted for different values of δ/a. Here $\rho=0$.

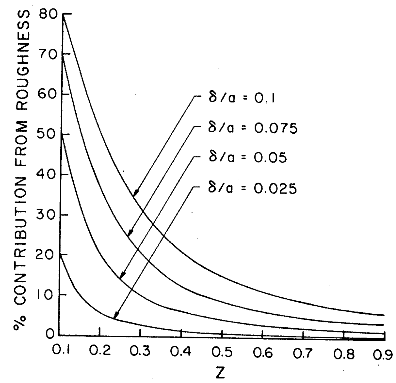

FIG. 2. The variation of the surface-roughness contribution to the image potential with z, for small z, plotted for various δ/a values. Here $\rho=0$.

V. A SIMPLE MODEL OF SURFACE ROUGHNESS

We see from the result given by Eq. (4.19) that one consequence of surface roughness for the image potential is to make it more attractive, when both x_3 and x_3' are outside the dielectric medium. A simple physical model of surface roughness that helps to explain this result and those obtained for the remaining three potentials $\varphi_{II}(x_3|x_3')$, $\varphi_{III}(x_3|x_3')$, $\varphi_{IV}(x_3|x_3')$ is the following. The region of our physical system in which the roughness is confined is defined by the inequalities $\zeta(\vec{x}_\parallel)_{\min}<x_3<\zeta(\vec{x}_\parallel)_{\max}$. In view of the assumption that $\langle\zeta(\vec{x}_\parallel)\rangle=0$, we have that half of this region is filled with the dielectric whose dielectric constant is ϵ, while the remaining half is occupied by vacuum. We therefore represent this region by a film of thickness L, straddling the plane $x_3=0$, whose dielectric constant ϵ_s is intermediate between 1 and ϵ. In particular, we assume that the film occupies the region $-\alpha L<x_3<(1-\alpha)L$, where $0<\alpha<1$, and the appropriate values of L, α, and ϵ_s will be obtained below. The space above this film $[x_3>(1-\alpha)L]$ is occupied by vacuum, and the space below it $(x_3<-\alpha L)$ is filled with the dielectric whose dielectric constant is ϵ. If now a charge q is placed at a point $\vec{x}'$ in the vacuum, and the electrostatic potential at a point $\vec{x}$, either in the vacuum or in the dielectric, is sought, the results can be expressed in the forms

$$\varphi_I(\vec{x}|\vec{x}')=\int\frac{d^2k_\parallel}{(2\pi)^2}\exp[i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')]\frac{2\pi q}{k_\parallel}\{\exp(-k_\parallel|x_3-x_3'|)+a(k_\parallel)\exp[-k_\parallel(x_3+x_3')]\},\quad x_3>(1-\alpha)L,\ x_3'>(1-\alpha)L \tag{5.1a}$$

$$\varphi_{II}(\vec{x}|\vec{x}')=\int\frac{d^2k_\parallel}{(2\pi)^2}\exp[i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')]\frac{2\pi q}{k_\parallel}b(k_\parallel)\exp[k_\parallel(x_3-x_3')],\quad x_3<-\alpha L,\ x_3'>(1-\alpha)L, \tag{5.1b}$$

where

$$a(k_\parallel)=\exp(-2k_\parallel\alpha L)\frac{(1+\epsilon_s)(\epsilon_s-\epsilon)+(1-\epsilon_s)(\epsilon_s+\epsilon)\exp(2k_\parallel L)}{(\epsilon+\epsilon_s)(\epsilon_s+1)+(\epsilon-\epsilon_s)(\epsilon_s-1)\exp(-2k_\parallel L)}, \tag{5.2a}$$

$$b(k_\parallel)=\frac{4\epsilon_s}{(\epsilon+\epsilon_s)(\epsilon_s+1)+(\epsilon-\epsilon_s)(\epsilon_s-1)\exp(-2k_\parallel L)}. \tag{5.2b}$$

In a similar fashion, when the charge is in the dielectric $(x_3'<-\alpha L)$, the potentials to which it gives rise in the vacuum and in the dielectric are given by

$$\varphi_{III}(\vec{x}|\vec{x}')=\int\frac{d^2k_\parallel}{(2\pi)^2}\exp[i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')]\frac{2\pi q}{k_\parallel}c(k_\parallel)\exp[-k_\parallel(x_3-x_3')],\quad x_3>(1-\alpha)L,\ x_3'<-\alpha L \tag{5.3a}$$

$$\varphi_{IV}(\vec{x}|\vec{x}')=\int\frac{d^2k_\parallel}{(2\pi)^2}\exp[i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')]\frac{2\pi q}{\epsilon k_\parallel}\{\exp(-k_\parallel|x_3-x_3'|)+d(k_\parallel)\exp[k_\parallel(x_3+x_3')]\},\quad x_3<-\alpha L,\ x_3'<-\alpha L, \tag{5.3b}$$

where

$$c(k_{\parallel})=\frac{4\epsilon_s}{(\epsilon+\epsilon_s)(\epsilon_s+1)+(\epsilon-\epsilon_s)(\epsilon_s-1)\exp(-2k_{\parallel}L)}, \tag{5.4a}$$

$$d(k_{\parallel})=\exp(2k_{\parallel}\alpha L)\frac{(\epsilon-\epsilon_s)(\epsilon_s+1)+(\epsilon+\epsilon_s)(\epsilon_s-1)\exp(-2k_{\parallel}L)}{(\epsilon+\epsilon_s)(\epsilon_s+1)+(\epsilon-\epsilon_s)(\epsilon_s-1)\exp(-2k_{\parallel}L)}. \tag{5.4b}$$

In the limit that $(|x_3|+|x_3'|)$ is large, only small values of $k_{\parallel}$ contribute significantly to that part of each of the integrals in Eqs. (5.1) and (5.3) that yields the image potential. Alternatively, we can assume that the thickness L of the layer whose dielectric constant is ϵ_s is small, and that the image potential can be expanded in powers of L. In either case we have to expand the coefficients $a(k_{\parallel}), b(k_{\parallel}), c(k_{\parallel}), d(k_{\parallel})$ in powers of L. To first order in L we find that

$$a(k_{\parallel})=-\frac{\epsilon-1}{\epsilon+1}-2k_{\parallel}L\frac{1}{\epsilon_s(\epsilon+1)^2}\times[(\epsilon_s-1)(\epsilon^2+\epsilon_s)+\alpha\epsilon_s(\epsilon^2-1)]+O(L^2), \tag{5.5a}$$

$$b(k_{\parallel})=\frac{2}{\epsilon+1}+2k_{\parallel}L\frac{(\epsilon-\epsilon_s)(\epsilon_s-1)}{\epsilon_s(\epsilon+1)^2}+O(L^2)=c(k_{\parallel}), \tag{5.5b}$$

$$d(k_{\parallel})=\frac{\epsilon-1}{\epsilon+1}+2k_{\parallel}L\frac{1}{\epsilon_s(\epsilon+1)^2}\times[\alpha\epsilon_s(\epsilon^2-1)-\epsilon(\epsilon_s^2-1)]+O(L^2). \tag{5.5c}$$

The electrostatic potentials that follow from these results, in the case that $\vec{x}_{\parallel}=\vec{x}_{\parallel}'$, are given by

$$\varphi_{\mathrm{I}}(x_3|x_3')=\frac{(q/a)}{d}-\frac{q}{a}\frac{\epsilon-1}{\epsilon+1}\frac{1}{z}-2\frac{q}{a}\frac{L}{a}\times\frac{[(\epsilon_s-1)(\epsilon^2+\epsilon_s)-\alpha\epsilon_s(\epsilon^2-1)]}{\epsilon_s(\epsilon+1)^2}\frac{1}{z^2}+\cdots, \tag{5.6a}$$

$$\varphi_{\mathrm{II}}(x_3|x_3')=\frac{2(q/a)}{\epsilon+1}\frac{1}{z}+2\frac{q}{a}\frac{L}{a}\frac{(\epsilon-\epsilon_s)(\epsilon_s-1)}{\epsilon_s(\epsilon+1)^2}\frac{1}{z^2}+\cdots=\varphi_{\mathrm{III}}(x_3|x_3'), \tag{5.6b}$$

$$\varphi_{\mathrm{IV}}(x_3|x_3')=\frac{(q/a)}{\epsilon d}+\frac{(q/a)}{\epsilon}\frac{\epsilon-1}{\epsilon+1}\frac{1}{z}+\frac{2(q/a)}{\epsilon}\frac{L}{a}\frac{[\alpha\epsilon_s(\epsilon^2-1)-\epsilon(\epsilon_s^2-1)]}{\epsilon_s(\epsilon+1)^2}\frac{1}{z^2}+\cdots, \tag{5.6c}$$

where we have used the variables defined in Eqs. (4.4).

We now have to specify ϵ_s and L. The dielectric constant ϵ of the substrate can be expressed as

$$\epsilon=1+4\pi\chi, \tag{5.7}$$

so that the susceptibility χ is given by

$$\chi=(\epsilon-1)/4\pi. \tag{5.8}$$

It is χ that characterizes the dielectric medium from a microscopic standpoint. Consequently, since the layer of thickness L and dielectric constant ϵ_s is a model for the region to which the surface roughness is confined, and which is only half-filled with dielectric, we must have that

$$\epsilon_s=1+4\pi\chi_s=1+4\pi(\tfrac{1}{2}\chi)=\tfrac{1}{2}(\epsilon+1). \tag{5.9}$$

We see from Eq. (5.6b) that $\varphi_{\mathrm{II}}(x_3|x_3')=\varphi_{\mathrm{III}}(x_3|x_3')$ is independent of the parameter α. Thus, when we substitute Eq. (5.9) into Eq. (5.6b), we find that

$$\varphi_{\mathrm{II}}(x_3|x_3')=\frac{2(q/a)}{\epsilon+1}\frac{1}{z}+\frac{q}{a}\frac{L}{a}\frac{(\epsilon-1)^2}{(\epsilon+1)^3}\frac{1}{z^2}+\cdots=\varphi_{\mathrm{III}}(x_3|x_3'). \tag{5.10}$$

When we compare this expression with the one given by Eq. (4.20), we see that they agree completely to this order in z^{-1} if we take L to be

$$L=3\pi^{1/2}\delta(\delta/a). \tag{5.11}$$

We have been unable to devise an independent argument that yields this value of L.

When Eqs. (5.9) and (5.11) are substituted into Eqs. (5.6a) and (5.6c), we obtain the results that

$$\varphi_{\mathrm{I}}(x_3|x_3')=\frac{(q/a)}{d}-\frac{q}{a}\frac{\epsilon-1}{\epsilon+1}\frac{1}{z}-3\frac{q}{a}\pi^{1/2}\frac{\delta^2}{a^2}\times\frac{(\epsilon-1)[2\epsilon^2+\epsilon+1-2\alpha(\epsilon+1)^2]}{(\epsilon+1)^3}\frac{1}{z^2}+\cdots, \tag{5.12a}$$

$$\varphi_{\mathrm{IV}}(x_3|x_3')=\frac{(q/a)}{\epsilon d}+\frac{(q/a)}{\epsilon}\frac{\epsilon-1}{\epsilon+1}\frac{1}{z}+3\frac{(q/a)}{\epsilon}\pi^{1/2}\frac{\delta^2}{a^2}\times\frac{(\epsilon-1)[2\alpha(\epsilon+1)^2-\epsilon(\epsilon+3)]}{(\epsilon+1)^3}\frac{1}{z^2}+\cdots. \tag{5.12b}$$

It follows from a comparison of these results with those given by Eqs. (4.19) and (4.21) that the choice $\alpha=\frac{2}{3}$ yields agreement between the two sets of results for the roughness contribution to the image potential to leading order in ϵ in the limit of large ϵ. With this choice of α, Eqs. (5.12) become

$$\varphi_{\rm I}(x_3\,|x_3') = \frac{(q/a)}{d} - \frac{q}{a}\frac{\epsilon-1}{\epsilon+1}\frac{1}{z} - \frac{q}{a}\pi^{1/2}\frac{\delta^2}{a^2}\frac{(\epsilon-1)(2\epsilon^2-5\epsilon-1)}{(\epsilon+1)^3}\frac{1}{z^2}+\cdots\,, \tag{5.13a}$$

$$\varphi_{\rm IV}(x_3\,|x_3') = \frac{(q/a)}{\epsilon d} + \frac{(q/a)}{\epsilon}\frac{\epsilon-1}{\epsilon+1}\frac{1}{z} + \frac{(q/a)}{\epsilon}\pi^{1/2}\frac{\delta^2}{a^2}\frac{(\epsilon-1)(\epsilon^2-\epsilon+4)}{(\epsilon+1)^3}\frac{1}{z^2}+\cdots\,. \tag{5.13b}$$

We can improve this model by letting α be a function of ϵ. For example, by choosing $\alpha=(2/3)-[1/(3\epsilon)]$ we can make Eqs. (5.12) agree with the exact results (4.19) and (4.21) through the first two terms in the large-ϵ form of the roughness contribution to the image potential. However, such refinements seem to us to be asking a simple model to carry more weight than is warranted by that simplicity.

Thus, we see that the introduction of a thin layer of a dielectric material, whose dielectric constant $\epsilon_s=\frac{1}{2}(\epsilon+1)$ is the mean of that of the substrate ϵ and that of the vacuum above it, into the region $-\frac{2}{3}L<x_3<\frac{1}{3}L$, makes the image potential in region I more attractive, and the image potentials in regions II, III, IV more repulsive. The addition of this dielectric layer can be said to "stiffen" the dielectric constant of the vacuum because it corresponds to replacing the layer of vacuum $0<x_3<\frac{1}{3}L$, whose dielectric constant is unity, with a layer of dielectric whose dielectric constant ϵ_s is greater than unity. At the same time the dielectric constant of the substrate is "softened," because the layer $-\frac{2}{3}L<x_3<0$, whose dielectric constant is ϵ, is replaced by material whose dielectric constant ϵ_s is smaller than ϵ. Because the latter layer is twice as thick as the former, the net effect of introducing the layer of dielectric constant ϵ_s is to soften the dielectric constant of our vacuum-dielectric system.

A second effect of this layer can be described by saying that it moves into the vacuum by a distance $z_0\approx\frac{3}{2}\pi^{1/2}(\delta^2/a^2)(\epsilon-1)^2/(\epsilon+1)^2$ the surface with respect to which the image potential is measured. This is because the results given by Eqs. (5.10) and (5.13) can be obtained to a reasonable approximation by replacing z with $(z-z_0)$ in the expressions for the image potential associated with a flat surface at $x_3=0$. Since the new surface relative to which the image potential is measured is in the vacuum and not in the dielectric substrate, an implication of this result is that it is the stiffening of the dielectric constant of the vacuum by the thick layer of dielectric constant ϵ_s that determines the position of this surface, rather than the softening of the dielectric substrate.

These results suggest that the reason that surface roughness makes the image potential more attractive in region I and more repulsive in regions II, III, IV is that by partially filling the region $\zeta(\vec{x}_\parallel)_{\min}<x_3<\zeta(\vec{x}_\parallel)_{\max}$ above the substrate of dielectric constant ϵ with some of the same material it moves out into the vacuum the reference plane with respect to which the image potential is determined.

It appears to us that the simple three-layer model just described can be used to mimic the effects of surface roughness at vacuum-dielectric interfaces whenever the fact that it is an intrinsically translationally invariant model is not important and when the distances from the surface where these effects are determined are large compared with $\delta(\delta/a)$. Thus, while it can be used to describe image-potential effects, it cannot be used to provide the angular distribution of the intensity of electromagnetic radiation scattered away from the specular direction by a rough surface, since this model would predict only specular reflection.

Finally, the results of this section also help us to understand why the effects of surface roughness are as small as they are. For it might be thought that the thickness L of the dielectric slab mimicking the surface roughness should be of the order of δ, the root-mean-square deviation of the surface from flatness. In this case the correction to the image potential from surface roughness would be of the order of $\delta/(x_3+x_3')$, returning to dimensional variables. Thus if δ were of the order of 25 Å and x_3 and x_3' were each of the order of 50 Å, surface roughness would give rise to a 25% correction to the flat surface value of the image potential. In fact, as we have just seen, the thickness of this layer is the generally much smaller quantity $\delta(\delta/a)$, so that the roughness induced correction to the image potential is only of the order of $\delta(\delta/a)/(x_3+x_3')$. This is clearly seen when we rewrite Eq. (4.19) in the form

$$\varphi_{\rm I}(x_3\,|x_3') = \frac{q}{|x_3-x_3'|} - q\left(\frac{\epsilon-1}{\epsilon+1}\right)\frac{1}{x_3+x_3'} \times\left(1+\pi^{1/2}\frac{(\epsilon-1)(2\epsilon-1)}{(\epsilon+1)^2}\frac{\delta}{a}\frac{\delta}{x_3+x_3'}+\cdots\right). \tag{5.14}$$

VI. APPLICATION TO ELECTRONS MOVING IN A PARABOLIC TRAJECTORY OVER A ROUGH SURFACE

In Secs. II–IV we have concentrated on the static situation of a fixed charge located in either the vacuum or the dielectric. We shall now extend the technique developed therein to study the dynamic situation of a beam of electrons moving over a rough surface in a prescribed trajectory. This application has been inspired by the experiment of Lecante *et al.*,[5] in which the energy loss from a beam of electrons moving in a parabolic trajectory over a metallic surface is measured. They suggest that surface roughness may be responsible for the larger shift in the peak frequency of the energy-loss function, with changes in the energy of the incident electrons, as compared with the semiclassical calculations of Muscat.[10] In this section we extend Muscat's calculations to the case of a rough vacuum-dielectric-metal interface. We proceed as follows.

In the presence of a time-dependent charge density in the region $x_3' > \zeta(\vec{x}_\parallel')$ Eq. (2.1) is replaced by

$$\nabla^2\varphi(\vec{x},\omega) = \begin{cases} -4\pi\rho(\vec{x},\omega), & x_3 > \zeta(\vec{x}_\parallel) \quad (6.1a) \\ 0, & x_3 < \zeta(\vec{x}_\parallel), \quad (6.1b) \end{cases}$$

where

$$\varphi(\vec{x},\omega) = \int_{-\infty}^{\infty} dt\, \varphi(\vec{x},t) e^{i\omega t}, \tag{6.2a}$$

$$\rho(\vec{x},\omega) = \int_{-\infty}^{\infty} dt\, \rho(\vec{x},t) e^{i\omega t}, \tag{6.2b}$$

are the Fourier transforms of the electrostatic potential and of the charge density that establishes it, respectively. The solution of Eqs. (6.1) can be written as

$$\varphi(\vec{x},\omega) = \int G(\vec{x},\vec{x}'\,|\,\omega)\rho(\vec{x}',\omega)\, d^3x', \tag{6.3}$$

where the Green's function $G(\vec{x},\vec{x}'\,|\,\omega)$ satisfies the following equations:

$$\nabla^2 G(\vec{x},\vec{x}'\,|\,\omega) = \begin{cases} -4\pi\delta(\vec{x}-\vec{x}'), & x_3 > \zeta(\vec{x}_\parallel),\ x_3' > \zeta(\vec{x}_\parallel') \\ 0, & x_3 < \zeta(\vec{x}_\parallel),\ x_3' > \zeta(\vec{x}_\parallel'), \end{cases} \tag{6.4}$$

together with the boundary conditions

$$G(\vec{x},\vec{x}'\,|\,\omega)\big|_{x_3=\zeta(\vec{x}_\parallel)-} = G(\vec{x},\vec{x}'\,|\,\omega)\big|_{x_3=\zeta(\vec{x}_\parallel)+} \tag{6.5a}$$

and

$$\epsilon(\omega)\hat{n}\cdot\nabla G(\vec{x},\vec{x}'\,|\,\omega)\big|_{x_3=\zeta(\vec{x}_\parallel)-} = \hat{n}\cdot\nabla G(\vec{x},\vec{x}'\,|\,\omega)\big|_{x_3=\zeta(\vec{x}_\parallel)+}, \tag{6.5b}$$

where $\epsilon(\omega)$ is the frequency-dependent dielectric constant of the medium in the region $x_3 < \zeta(\vec{x}_\parallel)$. The Fourier component $G(\vec{x},\vec{x}'\,|\,\omega)$ is then equivalent to $\varphi(\vec{x}\,|\,\vec{x}')$ in Eqs. (2.1) with $q=1$, $\epsilon \to \epsilon(\omega)$, and hence is directly obtainable from Eq. (2.4) with $A(\vec{k}_\parallel)$ and $B(\vec{k}_\parallel)$ satisfying Eq. (2.6).

We need here only the coefficient $A(\vec{k}_\parallel)$, since the beam of electrons is in the region above the dielectric and the image potential that comes into play is that calculated at the location of the electron itself.

The external charge density resulting from an electron moving in a parabolic trajectory is now a function of both space and time and can be written as

$$\rho(\vec{x},t) = -e\delta[x_3 - r(t)]\,\delta(\vec{x}_\parallel - \vec{V}_\parallel t), \tag{6.6a}$$

where $\vec{V}_\parallel$ is the horizontal velocity, and

$$r(t) = x_{03} + \tfrac{1}{2}(F/m)t^2. \tag{6.6b}$$

In the above equations e and m are, respectively, the magnitude of the charge and the mass of the electron, x_{03} is the classical turning point of the orbit and F is the magnitude of the vertical force on the electron that keeps it in parabolic motion. We assume that the maximum height of the surface profile function is smaller than x_{03}. This assures that the electrons will not penetrate the dielectric medium.

We refer the reader to Muscat[10] for a detailed derivation of the probability $P(\vec{k}_\parallel,\omega)$ that an electron is scattered into a unit volume of $\vec{k}_\parallel$, ω space about $(\vec{k}_\parallel,\omega)$, where $\hbar\vec{k}_\parallel$ is the momentum of the electron parallel to the surface, and $\hbar\omega$ is the energy loss of the scattered particle. Here, we present only the essential steps.

The rate at which a charge density $\rho(\vec{x},t)$ does work in the presence of a time varying external electric field $\vec{E}(\vec{x},t)$ is given by the classical expression

$$\dot{W} = \int d^3x\, \rho(\vec{x},t)\vec{V}(\vec{x},t)\cdot\vec{E}(\vec{x},t), \tag{6.7}$$

where $\vec{V}(\vec{x},t)$ is the velocity of the charged particle. With the help of Green's theorem and the continuity equation this equation can be rewritten in the following form

$$\dot{W} = -\int d^3x\, \varphi(\vec{x},t)\dot{\rho}(\vec{x},t). \tag{6.8}$$

The work done by the charge density is obtained by integrating Eq. (6.8) over all times so that

$$W = -i\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\omega \int d^3x \int d^3x'\, G(\vec{x},\vec{x}'\,|\,\omega) \times \rho(\vec{x}',\omega)\rho(\vec{x},-\omega), \tag{6.9}$$

where we have used Eq. (6.3) for $\varphi(\vec{x},\omega)$.

Before we proceed to calculate the probability $P(\vec{k}_\parallel,\omega)$ for the energy loss suffered by electrons moving in a parabolic trajectory over the surface of a metal, we should point out that our main interest lies in estimating the effect of surface roughness on this energy loss. Since we do not know the exact profile of the rough surface, we shall assume it to be randomly rough. Thus all quantities that we calculate will be averaged over the ensemble of realizations of the surface roughness profile function. The function $G(\vec{x},\vec{x}'|\omega)$ in Eq. (6.9) is therefore to be replaced by its ensemble-averaged value, denoted by $\langle G(\vec{x},\vec{x}'|\omega)\rangle$.

We obtain the expression for the probability $P(k_\parallel,\omega)$ by comparing the ensemble-averaged form of Eq. (6.9) with the quantum-mechanical expression for the quantum mean-energy loss of a particle[11]

$$W=\hbar\int_0^\infty \omega\, d\omega \int d^2k_\parallel P(\vec{k}_\parallel,\omega). \tag{6.10}$$

Thus, with the help of Eq. (6.5), we have

$$P(\vec{k}_\parallel,\omega)=\frac{\mathrm{Im}}{4\pi^3\hbar}\int_{x_{03}}^\infty dx_3\int_{x_{03}}^\infty dx_3' g(k_\parallel,\omega|x_3,x_3') \times\rho(-\vec{k}_\parallel,-\omega|x_3)\rho(\vec{k}_\parallel,\omega|x_3'), \tag{6.11}$$

where we have used the following Fourier transforms:

$$\langle G(\vec{x},\vec{x}'|\omega)\rangle=\int\frac{d^2k_\parallel}{(2\pi)^2}\exp[i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')] \times g(k_\parallel,\omega|x_3,x_3'), \tag{6.12}$$

$$\rho(\vec{k}_\parallel,\omega|x_3)=\int d^2x_\parallel \exp(-i\vec{k}_\parallel\cdot\vec{x}_\parallel)\rho(\vec{x},\omega). \tag{6.13}$$

It follows from earlier remarks that the expression for the ensemble-averaged quantity $\langle G(\vec{x},\vec{x}'|\omega)\rangle$ can be obtained from Eq. (2.4) with the replacements $q=1$ and $\epsilon=\epsilon(\omega)$, and the substitution of the ensemble-averaged value of the coefficient $A(\vec{k}_\parallel)$. Whether $\langle A(\vec{k}_\parallel)\rangle$ is obtained perturbatively or nonperturbatively the Fourier coefficient $g(k_\parallel\omega|x_3x_3')$ can be written formally as

$$g(k_\parallel\omega|x_3x_3')=\frac{2\pi}{k_\parallel}(\exp(-k_\parallel|x_3-x_3'|) + a(k_\parallel,\omega)\exp[-k_\parallel(x_3+x_3')]). \tag{6.14}$$

Note that here we show an explicit dependence on the frequency ω for all quantities that involve the dielectric constant $\epsilon(\omega)$. This is because we are now dealing with a dynamic phenomenon, in contrast with the situation considered in Sec. III.

For the form of the external charge density given by Eq. (6.5) the Fourier transform $\rho(\vec{k}_\parallel,\omega|x_3)$ is given by

$$\rho(\vec{k}_\parallel,\omega|x_3)=-e\left(\frac{2m}{F(x_3-x_{03})}\right)^{1/2} \times\cos\left[(\omega+\vec{k}_\parallel\cdot\vec{V}_\parallel)\left(\frac{2m}{F}(x_3-x_{03})\right)^{1/2}\right]. \tag{6.15}$$

The probability $P(k_\parallel,\omega)$ for the energy loss from the moving electron is then obtained by substituting Eqs. (6.14) and (6.15) in Eq. (6.11). Thus, we obtain the result that

$$P(\vec{k}_\parallel,\omega)=\frac{e^2m}{\pi F\hbar}\frac{\exp(-2k_\parallel x_{03})}{k_\parallel^2} \times\exp[-(\omega+\vec{k}_\parallel\cdot\vec{V}_\parallel)^2mF/k_\parallel]\,\mathrm{Im}a(k_\parallel,\omega). \tag{6.16}$$

When the metal surface is flat we see from either Eq. (3.5a) or Eq. (3.29) that

$$a(k_\parallel,\omega)=\frac{1-\epsilon(\omega)}{\epsilon(\omega)+1}, \tag{6.17}$$

and Eq. (6.16) becomes the expression for $P(\vec{k}_\parallel,\omega)$ obtained in this case by Muscat.[10] It follows that for a flat surface

$$-\mathrm{Im}a(k_\parallel,\omega)=\frac{2\epsilon_2(\omega)}{[\epsilon_1(\omega)+1]^2+\epsilon_2^2(\omega)}, \tag{6.18}$$

where $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are the real and imaginary parts of $\epsilon(\omega)$, respectively. We see from the result given by Eq. (6.18) that $-\mathrm{Im}a(k_\parallel,\omega)$ has a resonant-type peak at a frequency close to that at which $\epsilon_1(\omega)+1=0$. This is essentially the frequency of the surface plasmon in the metal. [Strictly speaking, the surface plasmon frequency is the complex root of the equation $\epsilon(\omega)+1=0$, the real part of which is well approximated by the root of $\epsilon_1(\omega)+1$ when the damping described by $\epsilon_2(\omega)$ is small.] This means that in obtaining $a(k_\parallel,\omega)$ for a rough surface we must use the nonperturbative expression for $\langle A(\vec{k}_\parallel)\rangle$ given by Eqs. (3.28)–(3.29). This is because in the perturbation series for $\langle A(\vec{k}_\parallel)\rangle$ each succeeding term has one higher power of $[\epsilon(\omega)+1]$ in the denominator. This means that in each order of the perturbation theory the resulting expression for $a(k_\parallel,\omega)$ will have a pole at the same frequency as in the case of a flat surface, but of increasing order. We expect on physical grounds, however, that one of the effects of surface roughness on $a(k_\parallel,\omega)$ will be to renormalize the resonant frequency but to retain the simple pole structure of $a(k_\parallel,\omega)$, now at the renormalized frequency, and with a renormalized residue. The nonperturbative approach to obtaining $\langle A(\vec{k}_\parallel)\rangle$ sums the perturbation series to all orders, but keeps only the lowest order (in δ/a) approximation to what we have called the analog of the proper self-energy in Sec. III. In this way the resonant structure of $-\mathrm{Im}a(k_\parallel,\omega)$ in the presence of surface roughness is preserved. Thus, in what follows we will use the result for $a(k_\parallel,\omega)$ obtained from Eq. (3.29a).

Lecante *et al.* make contact between the theoretical and experimental results by defining an integrated probability, or rather a differential linear cross section, according to

$$\frac{d\lambda}{d(\hbar\omega)} \equiv \frac{1}{\hbar}\int_{z_m}^{\infty} dx_{03} \int d^2k_{\parallel} P(k_{\parallel}, \omega) . \qquad (6.19)$$

Here z_m is the vertical distance above the metal surface at which the potential felt by the electron is a maximum. In writing Eq. (6.19) it has been assumed that all trajectories with $x_{03} \geq z_m$ are equally probable. Thus, with the further assumption that the Gaussian in Eq. (6.16) can be replaced by a δ function, we find that

$$\frac{d\lambda}{d(\hbar\omega)} = -\frac{e^2}{\hbar}\left(\frac{m}{\pi F}\right)^{1/2} \int_{\omega/V_{\parallel}}^{\infty} dk_{\parallel} \frac{\exp(-2k_{\parallel} z_m)}{k_{\parallel}^{3/2}(k_{\parallel}^2 V_{\parallel}^2 - \omega^2)^{1/2}} \times \mathrm{Im}\, a(k_{\parallel}, \omega) . \qquad (6.20)$$

The exact evaluation of the integral in Eq. (6.20) is not trivial. We therefore use numerical methods to compute the quantity $d\lambda/d(\hbar\omega)$ for electrons traveling in a parabolic trajectory over a molybdenum plate.[5] A beam of electrons of kinetic energy $2E_0$ is incident at 45° at an aperture in the upper plate of a capacitor whose plates are separated by a distance D and have a potential difference of E_0 volts. The electrons leave the condenser at 45° through another aperture on the upper plate.

In Figs. 3–6, we plot the differential linear cross section for the energy loss suffered by these electrons, as a function of $\hbar\omega$, for various values of E_0 and the surface-roughness parameters δ and a. We take D to be 0.1 cm and use the values of the dielectric function for Mo from optical-reflection data.[12] We calculate the vertical distance z_m from the maximum of the potential $V(x_3)$ given by

$$V(x_3) = -Fx_3 - \tfrac{1}{2}\Phi_I(x_3 \,|\, x_3, \rho = 0) , \qquad (6.21)$$

where the image potential Φ_I is given by Eq. (4.18). Thus

$$z_m = q/4F + \pi^{1/2}(\delta^2/a) . \qquad (6.22)$$

The correction term $\pi^{1/2}\delta^2/a$ in Eq. (6.22) has very little quantitative influence on our calculated results. For δ = 10 Å, and a = 500 Å, this correction term shifts z_m only by 0.4 Å, while $q/4F$ is roughly 150 Å for the parameters relevant to the experiment. Thus, while one might wish to improve the roughness induced shift in z_m through resort to a more sophisticated calculation, the results will surely not change meaningfully.

VII. CONCLUSIONS

We find the effect of surface roughness on the image potential to be significant (see Figs. 1 and 2). The effect is most pronounced when $z \ll 1$ (Fig. 2) because the roughness parameters are now com-

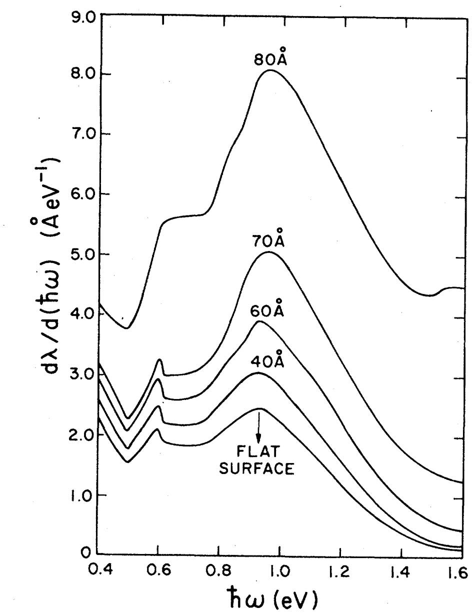

FIG. 3. The differential linear cross section for energy loss by 800-eV electrons moving in a parabolic trajectory above a rough Mo surface. Here a = 200 Å and the curves are labeled by the value of δ.

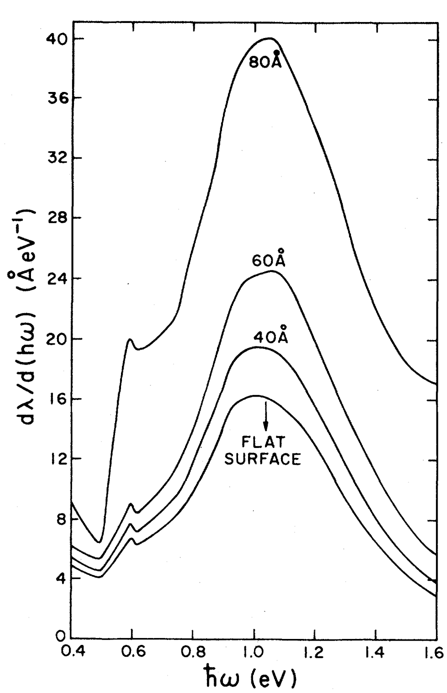

FIG. 4. The differential linear cross section for energy loss by 1600-eV electrons moving in a parabolic trajectory above a rough Mo surface. Here a = 200 Å and the curves are labeled by the value of δ.

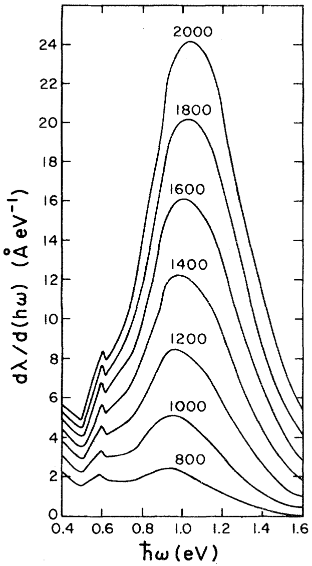

FIG. 5. The differential linear cross section for energy loss by electrons moving over a perfectly flat surface. The curves are labeled with values of the energy of the incident electrons (in eV).

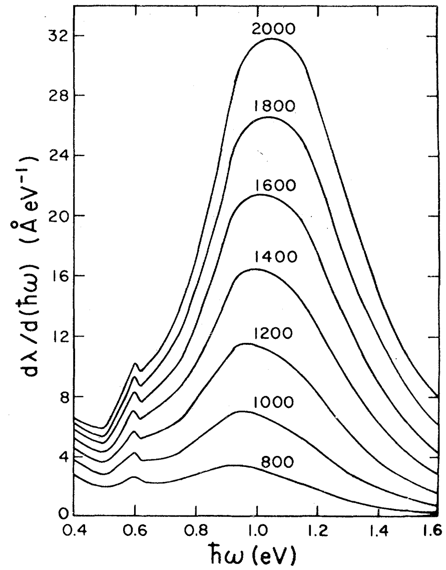

FIG. 6. The differential linear cross section for energy loss by electrons moving over a rough Mo surface. Here $\delta = 50$ Å and $a = 200$ Å. The curves are labeled with the value of the incident energy of the electrons (in eV).

parable to the distance between the location of the charge q and the point at which the potential is calculated. In the other limit, when $z \gg 1$ (Fig. 1), the contribution to the image potential from roughness can still be as high as 30%. As is expected the effect is greatest at points near the location of the charge and decreases as one moves away from this point. Moreover, the image potential for a rough surface is more attractive than that for a flat surface.

We have also presented a simple, phenomenological model of a rough surface that is capable of reproducing qualitatively and semiquantitatively the forms of the image potential obtained from our detailed calculations for a rough surface, in the limit of large z. We feel that this model should be useful in providing useful information simply and quickly about the effects of surface roughness on a number of other physical properties of solids.

Surface roughness has a quantitative and a qualitative effect on the dynamic energy loss from electrons moving in a parabolic trajectory over a metal surface. As is expected, the energy loss increases as the ratio δ/a is increased. For example, in Fig. 3, the peak of the energy loss cross section enhances from 2.467 (Å eV^{-1}) for flat surface to 3.059 (Å eV^{-1}) when δ is changed to 40 Å, with a further increase to 3.897 (Å eV^{-1}) for $\delta = 60$ Å. A similar trend is observed in Fig. 4, where the incidence energy of the electrons is 1600 eV. In this case, the magnitude of the energy loss at a given frequency is larger than that for the 800-eV electrons, for same values of δ and a. Thus, the energy loss is enhanced when either the incident electron energy is increased or the ratio δ/a is made larger.

We also find that with either the increase of the electron energy or of the roughness ratio δ/a the peak of the energy-loss spectrum shifts towards higher frequency. However, this shift is not sufficiently pronounced to explain the data of Lecante *et al.*[5] What is interesting is that even for the perfectly flat surface our calculations (Fig. 5) do not predict as large a shift in the energy at which the differential linear cross section is a maximum as is obtained by Lecante *et al.*[5] Also, our use of a realistic dielectric function, which departs dramatically from the free-electron model, gives rise to more structure in the curves than in Fig. 2 of Ref. 5. It is unclear to us how the latter has been calculated.

We are thus led to conclude that by increasing δ from 0 to 60 Å for a fixed energy of the incident electrons and $a = 200$ Å, the magnitude of the dynamic energy loss suffered by the electrons is enhanced significantly but there is no pronounced effect on the frequency at which the energy loss is maximum. If in the samples used by Lecante *et al.*[5] the ratio δ/a is of the order of that considered here, then, contrary to their suggestion, we can conclude that surface roughness cannot explain the large shift in frequency observed by them when the energy of the incident electrons is changed slightly. On the other hand, if δ/a is much larger for their samples, the conclusions reached here do not apply and we cannot comment on the effect of surface roughness on their results.

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