Inverse dielectric function of a bounded solid-state plasma

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We examine here the inverse dielectric function of a slab of nonlocal, dynamic solid-state plasma having planar bounding surfaces, and determine explicit analytic results for the thick semi-infinite limit. This constitutes a closed form solution of the random-phase-approximation integral equation for the thick-slab limit. In this we employ potential solutions obtained earlier by D. M. Newns, and present the solution in terms of quadratures involving the free-electron (noninteracting) density-perturbation response function of the bounded plasma in the infinite-barrier model.

The longitudinal electrostatic response properties of a bounded solid-state plasma (with or without a magnetic field) are subsumed in the concept of an inverse dielectric function $\kappa(1,2)$ (Ref. 1) which describes dynamic and nonlocal screening phenomena, including image potentials in the vicinity of a surface. Thus the inverse dielectric function is of central importance in all electrostatic interaction problems at surfaces (as well as in bulk), including van der Waals attraction of an adatom to a solid surface and self-interaction energy of plasma electrons near a surface, as well as surface normal modes such as surface plasmons and/or polaritons marked by resonances of the response function $\kappa(1,2)$. With this in view, it is most desirable to obtain an explicit evaluation of the inverse dielectric function, which is defined by the relations

$$V(1)=\int d(2)\kappa(1,2)U(2) \quad \text{or} \quad \kappa(1,2)=\delta V(1)/\delta U(2)\ , \tag{1}$$

where $U(2)$ is the impressed potential at space-time point 2 and $V(1)$ is the effective potential it generates at space-time point 1. If $v(1-3)$ is the Coulomb interaction potential and $\rho(1)$ is the density, it is well known that the random-phase-approximation (RPA) integral equation for the inverse dielectric function $\kappa(1,2)$ has the form

$$\kappa(1,2)=\delta(1-2)+\int d(3)\int d(4)v(1-3)R(3,4)\kappa(4,2)\ , \tag{2}$$

and for the direct dielectric function, one has, explicitly,

$$\begin{aligned}\epsilon(1,2)&=\delta(1-2)-\int d(3)v(1-3)R(3,2)\\ &=\delta(1-2)+4\pi\alpha_0(1,2)\ ,\end{aligned} \tag{3}$$

where $4\pi\alpha_0(1,2)$ is the free-electron (noninteracting) polarizability. In these equations,

$$\int d(3)\kappa(1,3)\epsilon(3,2)=\delta(1-2)\ , \tag{4}$$

and $R(1,2)$ is the RPA density-perturbation response function

$$R(1,2)=-i\overline{G}_1(1,2)\overline{G}_1(2,1^+)\ , \tag{5}$$

where $\overline{G}_1(1,2)$ is the one-electron thermodynamic Green's function.[1] Although the direct dielectric function is given explicitly by Eq. (3) and is thus straightforward to evaluate, even for a planar boundary with a normal magnetic field, the more important inverse dielectric response function $\kappa(1,2)$ is harder to obtain because of the nontrivial problem of inverting the matrix $\epsilon(1,2)$ for a bounded plasma [which lacks translational invariance, so that the positional dependence of $\epsilon(1,2)$ is not just on $\mathbf{r}_1-\mathbf{r}_2$, but it also involves $\mathbf{r}_1+\mathbf{r}_2$], which is to say, equivalently, that the RPA integral equation (2) for $\kappa(1,2)$ is not to be solved by translationally invariant Fourier-transform techniques in the presence of a boundary (although it is thus solved in the bulk case).

Our object here is to develop an explicit solution for $\kappa(1,2)$ for a plane-bounded solid-state plasma using the potential solutions for a slab plasma developed by Newns in the infinite-barrier model. In his very useful paper, Newns[2] determines the effective potential $V(1)$ for an arbitrary impressed potential $U(2)$, and our point is that these results yield $\kappa(1,2)$ directly upon choosing $U(2)=\delta(2-1')$ as a mathematical model potential, for then we have

$$\begin{aligned}V_{1'}(1)&=\int d(2)\kappa(1,2)U(2)\\ &=\int d(2)\kappa(1,2)\delta(2-1')=\kappa(1,1')\end{aligned} \tag{6}$$

as an explicit solution of the RPA integral equation for $\kappa(1,1')$. It should be pointed out that an alternative procedure for determining $\kappa(1,2)$ explicitly was attempted by Bechstedt, Enderlein, and Reichardt[3] by calculating the dynamic nonlocal screening of the Coulomb interaction potential v,

$$\mathscr{V}(\mathbf{r},\mathbf{r}';\omega)=\int d\mathbf{r}''\,\kappa(\mathbf{r},\mathbf{r}'';\omega)v(\mathbf{r}''-\mathbf{r}')\ . \tag{7}$$

and evaluating the Laplacian

$$\begin{aligned}\nabla_{\mathbf{r}'}^2\mathscr{V}(\mathbf{r},\mathbf{r}';\omega)&=\int d\mathbf{r}''\,\kappa(\mathbf{r},\mathbf{r}'',\omega)\nabla_{\mathbf{r}'}^2 v(\mathbf{r}''-\mathbf{r}')\\ &=-4\pi e^2\kappa(\mathbf{r},\mathbf{r}',\omega)\ ,\end{aligned} \tag{8}$$

which yields $\kappa(\mathbf{r},\mathbf{r}';\omega)$ since

$$\nabla^2_{\mathbf{r}'} v(\mathbf{r}''-\mathbf{r}') = -4\pi e^2 \delta(\mathbf{r}''-\mathbf{r}') \,.$$

Unfortunately, Bechstedt's interesting calculation for $\kappa(\mathbf{r},\mathbf{r}';\omega)$ has a printing error (at the very end), as one can see from his local result

$$\kappa(\overline{Q}\to 0, z,z';\omega) \Longrightarrow \delta(z-z')[\eta_+(-z)+\eta_+(z)/\epsilon(\omega)]$$

[$\epsilon(\omega)$ is the local bulk dielectric function of the thick-slab plasma, and $\overline{Q}$ is wave-vector transform variable conjugate to $\overline{r}-\overline{r}'=(x-x',y-y')$; also $\eta_+(z)$ is the Heaviside step function and $z=0$ is the boundary plane], which is incapable of describing an image field as part of the dynamically screened Coulomb potential. Our considerations below will address this problem.

In considering $\kappa(1,1')$ for a thick slab of plasma with planar boundaries, we wish to employ Newns's calculation of effective potential $V(1)$ generated by the mathematical model potential $U(2)=\delta(2-1')$ with the associated source $\nabla_2^2 U(2)=4\pi S(2)$ [observe that Newns's convention $\nabla_2^2 U(2)\to 4\pi S(2)$ employed here differs from the usual one in the sign of $S(2)$]. In this we note that Newns's calculation[2] of potentials $V^{(A,S)}$, which are antisymmetric or symmetric, across the midplane of the slab defined by $z=d/2$ (d denotes slab thickness), yields results in a mixed $(z,\overline{Q})$ and ω representation given as follows for the regions $z\le 0$ and $0\le z\le d$:

$$V_Q^{(A,S)}(z,\omega)=\eta_+(-z)\{e^{Qz}[V_Q^{(A,S)}(0,\omega)-U_Q^{I(A,S)}(0,\omega)]+U_Q^{I(A,S)}(z,\omega)\} + \eta_+(z)\eta_+(d-z)\left[\left[-\frac{4}{d}\right]\sum_{q(A,S)}\sum_{q'(A,S)}\cos qz E^{-1}_{Qqq'}[2\pi S_{Qq'}^{(A,S)}(\omega)+QV_Q^{(A,S)}(0,\omega)-2QU_Q^{I(A,S)}(0,\omega)]\right], \tag{9}$$

where

$$U_Q^{I(A,S)}(z,z',\omega)=-\frac{2\pi}{Q}\int_{-\infty}^{0} dz'\, e^{-Q|z-z'|}S_Q^{(A,S)}(z',\omega) \quad \text{for } z<0 \,, \tag{10}$$

and

$$V_Q^{(A,S)}(0,\omega)=(1+\epsilon_Q^{(A,S)})^{-1}\left[2U_Q^{I(A,S)}(0,\omega)-\frac{8\pi}{d}\epsilon_Q^{(A,S)}\sum_{q(A,S)}\sum_{q'(A,S)}E^{-1}_{Qqq'}S_{Qq'}^{(A,S)}(\omega)\right] \tag{11}$$

and

$$\epsilon_Q^{(A,S)}\equiv\epsilon_Q^{(A,S)}(\omega)=\left[\frac{4Q}{d}\sum_{q(A,S)}\sum_{q'(A,S)}E^{-1}_{Qqq'}\right]^{-1}. \tag{12}$$

In the equations above we have

$$E_{Qqq'}\equiv E_{Qqq'}(\omega)=(Q^2+q^2)\delta_{qq'}/\eta_q+4\pi R_{Qqq'} \tag{13}$$

$$=4\pi(\Delta_{Qq}\delta_{qq'}/\eta_q-A_{Qqq'}) \,, \tag{14}$$

with

$$R_{Qqq'}=D_{Qq}\delta_{qq'}/\eta_q-A_{Qqq'} \tag{15}$$

as the density-perturbation response function $R(1,2)=\delta\rho(1)/\delta V(2)$ having a "diagonal" part D and an "off-diagonal" part $-A$. [In this, $\Delta_{Qq}=(4\pi)^{-1}(Q^2+q^2)+D_{Qq}$.] The notations (A,S) refer to antisymmetric or symmetric potentials and sources, and for the antisymmetric case, $q^{(A)},q'^{(A)}=(2n+1)\pi/d$, $n=0,1,2,\ldots,\infty$ and $\eta_q\equiv 1$, whereas for the symmetric case, $q^{(S)},q'^{(S)}=2n\pi/d$, $n=0,1,2,\ldots,\infty$ and $\eta_q=1$ for $q>0$, but $n_q=\frac{1}{2}$ for $q=0$. The transforms employed here are defined following Newns in accordance with [$\mathbf{r}=(\overline{R},z)$ and $\mathbf{q}=(\overline{Q},q)$]

$$f^{(A,S)}(\overline{R},z)=\frac{2}{d}\sum_{q(A,S)}\eta_q\int\frac{d^2\overline{Q}}{(2\pi)^2}e^{i\overline{Q}\cdot\overline{R}}\cos(qz)f_{Qq}^{(A,S)} \tag{16a}$$

and

$$f_{Qq}^{(A,S)}=\int_0^d dz\int d^2\overline{R}\, e^{-i\overline{Q}\cdot\overline{R}}\cos(qz)f^{(A,S)}(\overline{R},z) \,. \tag{16b}$$

It is to be noted that in region III, $z>d$, these solutions are continued antisymmetrically and/or symmetrically, having associated nonvanishing charge distributions in region III that are pushed away infinitely far as the slab becomes thick, $d\to\infty$. It is clear that an appropriate model of a thick semi-infinite slab must be devoid of such charge distributions in region III, albeit far away. (It should be borne in mind that even faraway charge distributions can influence fields at finite points, particularly in planar geometries, such as the case of a uniform plane sheet of charge producing a uniform field at all points by Gauss's law.) Such a model may be constructed by considering two continuations of the actual potential $V_Q(z,\omega)$, one antisymmetric continuation and one symmetric continuation, and averaging them with equal weight to get a continuation having *no* charge distributed in region III, while having its proper form at all finite points in the thick-slab semi-infinite limit as $d\to\infty$ (see Fig. 1). Indeed, the antisymmetric and symmetric continuations are closely related in the thick-slab limit, except for the $q=0$ term of the symmetric case, which yields a term having no antisymmetric counterpart. In order to examine the thick-slab semi-infinite limit, we note that for $d\to\infty$, and $q^{(A)}=(2n+1)\pi/d$ and $q^{(S)}=2n\pi/d$, and $\eta_q=1-\frac{1}{2}\delta_{q0}\delta((A,S)-S)$, where

$$\delta((A,S)-S)=\begin{cases}1 & \text{for } (A,S)\to S\,,\\ 0 & \text{for } (A,S)\to A\,,\end{cases}$$

so that

$$\sum_{q(A,S)} \eta_q \rightarrow \sum_{q(A,S)} -\tfrac{1}{2}(q=0 \text{ term})\delta((A,S)-S)$$
$$\rightarrow \frac{d}{2\pi}\int_0^\infty dq - \tfrac{1}{2}(q=0 \text{ term})\delta((A,S)-S)\,, \tag{17}$$

and $\delta_{qq'} \rightarrow (2\pi/d)\delta(q-q')$. Moreover, by the construction of the antisymmetric, symmetric, and average continuations discussed above, when $d\rightarrow\infty$ for the thick-slab limit, we have, at all *finite points,*

$$U^{(A)}(z,\omega)=U^{(S)}(z,\omega)=U^{\text{average}}(z,\omega)\equiv U(z,\omega)$$

with a corresponding statement for sources. Thus we have the actual potential $V_Q(z,\omega)$ of the semi-infinite thick-slab limit given by

$$V_Q(z,\omega)=\tfrac{1}{2}[V_Q^{(A)}(z,\omega)+V_Q^{(S)}(z,\omega)]$$
$$=\tfrac{1}{2}\sum_{A+S} V_Q^{(A,S)}(z,\omega) \quad \text{for } d\rightarrow\infty\ . \tag{18}$$

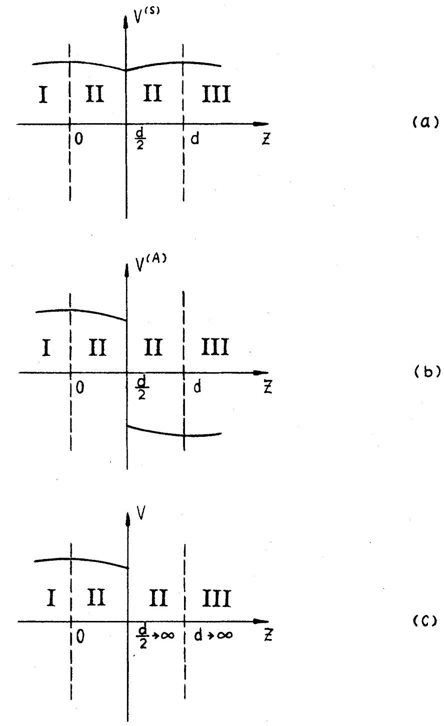

FIG. 1. (a) $V^{(S)}$ symmetrically continued potential. (b) $V^{(A)}$ antisymmetrically continued potential. (c) V average of the symmetric potential $V^{(S)}$ and antisymmetric potential $V^{(A)}$ with equal weight as $d\rightarrow\infty$ $(d/2\rightarrow\infty)$.

Employing the notation $\widetilde{E}_{Qqq'}=\eta_q E_{Qqq'}$, we have [henceforth the semi-infinite thick-slab $d\rightarrow\infty$ continuum limit will be understood, $\sum_{q(A,S)}\rightarrow(d/2\pi)\int_0^\infty dq$]

$$V_Q(z,\omega)=\tfrac{1}{2}\eta_+(-z)\left[e^{Qz}\left[\sum_{A+S}V_Q^{(A,S)}(0,\omega)-2U_Q^I(0,\omega)\right]+2U_Q^I(z,\omega)\right]$$
$$-\tfrac{1}{2}\eta_+(z)\left[\sum_{A+S}\left[\frac{4}{d}\right]\sum_{q(A,S)}\sum_{q'(A,S)}\cos qz\,\widetilde{E}^{\,-1}_{Qqq'}[2\pi S_{Qq'}^{(A,s)}(\omega)+QV_Q^{(A,S)}(0,\omega)-2QU_Q^I(0,\omega)]\right]$$
$$+\tfrac{1}{4}\eta_+(z)\left[\left[\frac{4}{d}\right]\sum_{q'(S)}\widetilde{E}^{\,-1}_{Q0q'}[2\pi S_{Qq'}^{(S)}(\omega)+QV_Q^{(S)}(0,\omega)-2QU_Q^I(0,\omega)]\right]\,, \tag{19}$$

where

$$V_Q^{(A,S)}(0,\omega)=[1+\epsilon_Q^{(A,S)}]^{-1}\left[2U_Q^I(0,\omega)-\frac{8\pi}{d}\epsilon_Q^{(A,S)}\sum_{q(A,S)}\sum_{q'(A,S)}\widetilde{E}^{\,-1}_{Qqq'}S_{Qq'}^{(A,S)}(\omega)+\frac{4\pi}{d}\epsilon_Q^{(S)}\sum_{q'(S)}\widetilde{E}^{\,-1}_{Q0q'}S_{Qq'}^{(S)}(\omega)\delta((A,S)-S)\right] \tag{20}$$

and

$$(\epsilon_Q^{(A,S)})^{-1}=\frac{4Q}{d}\left[\sum_{q(A,S)}\sum_{q'(A,S)}\widetilde{E}^{\,-1}_{Qqq'}-\tfrac{1}{2}\sum_{q'(S)}\widetilde{E}^{\,-1}_{Q0q'}\delta((A,S)-S)\right]\,. \tag{21}$$

It should be noted that

$$\widetilde{E}^{\,-1}_{Q0q'}\Big/\sum_q \widetilde{E}^{\,-1}_{Qqq'}\sim\frac{1}{d}$$

since $\sum_q(d/2\pi)\int_0^\infty dq$, and Eqs. (19)–(21) therefore provide thickness corrections in all orders of $1/d^n$ for the thick semi-infinite limit. We shall ignore such corrections, but it should be pointed out that some of them are important, even for the semi-infinite limit $d\rightarrow\infty$, for example, in the calculation of the surface self-energy which involves knowledge of the terms of order $O(1/d)$. Neglecting all such terms leads to revisions of Eqs. (19)–(21) as follows:

$$V_Q(z,\omega)=\tfrac{1}{2}\eta_+(-z)\left[e^{Qz}\left[\sum_{A+S}V_Q^{(A,S)}(0,\omega)-2U_Q^I(0,\omega)\right]+2U_Q^I(z,\omega)\right]$$
$$-\tfrac{1}{2}\eta_+(z)\left[\sum_{A+S}\left[\frac{4}{d}\right]\sum_{q(A,S)}\sum_{q'(A,S)}\cos(qz)\widetilde{E}\,{}^{-1}_{Qqq'}[2\pi S_{Qq'}^{(A,S)}(\omega)+QV_Q^{(A,S)}(0,\omega)-2QU_Q^I(0,\omega)]\right], \quad (19')$$

where

$$V_Q^{(A,S)}(0,\omega)=(1+\epsilon_Q^{(A,S)})^{-1}\left[2U_Q^I(0,\omega)-\frac{8\pi}{d}\epsilon_Q^{(A,S)}\sum_{q(A,S)}\sum_{q'(A,S)}\widetilde{E}\,{}^{-1}_{Qqq'}S_{Qq'}^{(A,S)}(\omega)\right] \quad (20')$$

and

$$(\epsilon_Q^{(A,S)})^{-1}=\frac{4Q}{d}\sum_{q(A,S)}\sum_{q'(A,S)}\widetilde{E}\,{}^{-1}_{Qqq'} . \quad (21')$$

Our choice of the mathematical model potential as a four-dimensional Dirac δ function $U(1)\rightarrow\delta(1-1')$ would correspond to the impressed source in the thick-slab region II as follows:

$$S_{Qq}=\frac{1}{4\pi}\int_0^\infty dz\cos qz\left[\frac{d^2}{dz^2}-Q^2\right]\delta(z-z')$$
$$=-\frac{Q^2}{4\pi}\cos(qz')\eta_+(z')+\frac{1}{4\pi}\int_0^\infty dz\cos(qz)\delta''(z-z')$$
$$=-\frac{q^2+Q^2}{4\pi}\cos(qz')\eta_+(z')+\frac{1}{4\pi}\delta'(z') \quad (22)$$

(where we have integrated by parts twice). However, one must note that our formulas above are predicated on using potentials and corresponding sources which are antisymmetrically or symmetrically continued across the slab. Therefore the mathematical model potential and its sources must be likewise continued, and it is readily shown that the source in the thick-slab region II for an antisymmetrically or symmetrically continued $\delta(1-1')$ $\rightarrow\delta(1-1')\mp\delta(\tilde{1}-1')$ potential is given by $S_{Qq}^{(A,S)}=2S_{Qq}$ ($\tilde{1}$ refers to the point 1 reflected across the midplane of the slab). Next, considering $U_Q^I(zz'\omega)$ as the potential due to that part of the impressed source of $U(1)\rightarrow\delta(1-1')$, which is located to the left of the slab in region I (note that the reflected point $\tilde{1}$ in region III cannot contribute here) and defining $\Theta(z)=\eta_+(z)-\eta_+(-z)$ and $\delta'(z)=d\delta(z)/dz$, we have

$$U_Q^I(z,z';\omega)=-\frac{2\pi}{Q}\int_{-\infty}^{0}dz''e^{-Q|z-z''|}\frac{1}{4\pi}\left[\frac{d^2}{dz''^2}-Q^2\right]\delta(z''-z')$$
$$=\frac{1}{2Q}\delta'(z')e^{-Q|z-z'|}+\delta(z')\Theta(z)e^{-Q|z|}+\eta_+(-z')\delta(z-z')$$
$$=\frac{1}{2Q}\delta'(z')e^{-Q|z|}+\tfrac{1}{2}\delta(z')\Theta(z)e^{-Q|z|}+\eta_+(-z')\delta(z-z') \quad (23a)$$

and

$$U_Q^I(0,z';\omega)=\frac{1}{2Q}\delta'(z')+\tfrac{1}{2}\delta(z') . \quad (23b)$$

In Eq. (23a) we employed the easily verified identity

$$\delta'(z')g(z')=\delta'(z')g(0)-g'(0)\delta(z')$$

for any reasonable function $g(z')$. To this, we may add Eq. (20′) in the form

$$V_Q^{(A,S)}(0,\omega)=(1+\epsilon_Q^{(A,S)})^{-1}\left\{Q^{-1}\delta'(z')+\delta(z')-\frac{8\pi}{d}\epsilon_Q^{(A,S)}\sum_{q(A,S)}\sum_{q'(A,S)}\widetilde{E}\,{}^{-1}_{Qqq'}\left[\frac{1}{2\pi}\delta'(z')-\left[\frac{q'^2+Q^2}{2\pi}\right]\cos(q'z')\eta_+(z')\right]\right\}, \quad (24)$$

and our solution for $\kappa(1,1')=V_{1'}(1)$ employing the impressed δ-function—model potential [neglecting terms of order $O(1/d)$] may be written in a mixed representation as follows:

$$\kappa(Q,z,z';\omega)=V_{1'Q}(z;\omega)\equiv V_Q(z,z',\omega)\ ,$$
$$\kappa(Q,z,z';\omega)=\tfrac{1}{2}\eta_+(-z)\left[e^{Qz}\left[\sum_{A+S}V_Q^{(A,S)}(0,\omega)-Q^{-1}\delta'(z')-\delta(z')\right]+Q^{-1}\delta'(z')e^{-Q|z|}+\delta(z')\Theta(z)e^{-Q|z|}+2\eta_+(-z')\delta(z-z')\right]$$
$$-\tfrac{1}{2}\eta_+(z)\sum_{A+S}\left[\frac{4}{d}\right]\sum_{q(A,S)}\sum_{q'(A,S)}\cos(qz)\widetilde{E}^{-1}_{Qqq'}[QV_Q^{(A,S)}(0,\omega)-(q'^2+Q^2)\cos(q'z')\eta_+(z')-Q\delta(z')]\ . \tag{25}$$

This result [Eqs. (25), (24), and (21′)] still permits, in principle, the inclusion of nondiagonal density-response matrix elements $-A_{Qqq'}$, along with the diagonal ones, $D_{Qq}\delta_{qq'}/\eta_q$ [Eq. (15)].

If we introduce the diagonal approximation and neglect $-A_{Qqq'}$, it is well known that in the semi-infinite limit [recall that we are previously committed to neglecting terms of order $O(1/d)$]

$$\widetilde{E}_{Qqq'}\to 4\pi\Delta_{Qq}\delta_{qq'}\to(Q^2+q^2+4\pi D_{Qq})\delta_{qq'}$$
$$\to(Q^2+q^2)\epsilon_\infty^{3D}(\mathbf{q},\omega)\delta_{qq'}\ , \tag{26}$$

where $\epsilon_\infty^{3D}(\mathbf{q},\omega)$ (3D denotes three dimensional) is the bulk dielectric function of the thick-slab material, and

$$\widetilde{E}^{-1}_{Qqq'}=[(Q^2+q^2)\epsilon_\infty^{3D}(\mathbf{q},\omega)]^{-1}\delta_{qq'}\ , \tag{27}$$

whence

$$\sum_{q'(A,S)}\widetilde{E}^{-1}_{Qqq'}=[(Q^2+q^2)\epsilon_\infty^{3D}(\mathbf{q},\omega)]^{-1} \tag{27'}$$

[same for (A) and (S)]. Moreover, the same results for (A) and (S) are derived from

$$\sum_{q(A,S)}\to\frac{d}{2\pi}\int_0^\infty dq$$

for the semi-infinite thick-slab limit, and thus $\sum_{A+S}\to 2$. In the diagonal approximation, we thus obtain

$$(\epsilon_Q^{(A,S)})^{-1}=\epsilon_Q^{-1}=\frac{2Q}{\pi}\int_0^\infty dq[(Q^2+q^2)\epsilon_\infty^{3D}(\mathbf{q},\omega)]^{-1}\ , \tag{28}$$

$$V_Q^{(A,S)}(0,\omega)=V_Q(0,\omega)$$
$$=(1+\epsilon_Q)^{-1}[\delta(z')-2\epsilon_Q K_\infty^{3D}(\bar{Q},z';\omega)\eta_+(z')]\ , \tag{29}$$

where we have defined

$$K_\infty^{3D}(\bar{Q},z';\omega)=\pi^{-1}\int_0^\infty dq\cos(qz')/\epsilon_\infty^{3D}(\mathbf{q},\omega)$$

and will also introduce

$$v_\infty^{3D}(\bar{Q},z';\omega)=2\pi^{-1}\int_0^\infty dq\cos(qz')/[(q^2+Q^2)\epsilon_\infty^{3D}(\mathbf{q},\omega)]\ .$$

The "diagonal" result for $\kappa(\bar{Q},z,z';\omega)$ is finally given for the thick-slab semi-infinite limit [neglecting terms of order $O(1/d)$] as follows:

$$\kappa(\bar{Q},z,z';\omega)=\eta_+(-z)\left[\delta(z-z')-\frac{\epsilon_Q}{1+\epsilon_Q}e^{Qz}\delta(z')+\frac{2\epsilon_Q}{1+\epsilon_Q}K_\infty^{3D}(\bar{Q},z';\omega)e^{Qz}\eta_+(z')\right]$$
$$+\eta_+(z)\left[v_\infty^{3D}(\bar{Q},z;\omega)\left[\frac{Q\epsilon_Q}{1+\epsilon_Q}\delta(z')-\frac{2Q\epsilon_Q}{1+\epsilon_Q}K_\infty^{3D}(\bar{Q},z';\omega)\eta_+(z')\right]+[K_\infty^{3D}(\bar{Q},z+z';\omega)+K_\infty^{3D}(\bar{Q},z-z';\omega)]\eta_+(z')\right]\ . \tag{30}$$

For the local limit we have

$$\epsilon_Q=\epsilon_\infty^{3D}(\omega)\to\epsilon(\omega),\quad \eta_+(0)\to\tfrac{1}{2},\quad K_\infty^{3D}(\bar{Q},z';\omega)=\delta(z')/\epsilon(\omega),\quad v_\infty^{3D}(\bar{Q},z';\omega)=e^{-Q|z'|}/Q\epsilon(\omega)\ ,$$
$$\kappa(\bar{Q},z,z';\omega)=\eta_+(-z)\left[\delta(z-z')+\delta(z')e^{Qz}\left[\frac{1-\epsilon(\omega)}{1+\epsilon(\omega)}\right]\right]+\eta_+(z)\left[\frac{\delta(z-z')}{\epsilon(\omega)}+\delta(z')e^{-Qz}\frac{1}{\epsilon(\omega)}\left[\frac{\epsilon(\omega)-1}{\epsilon(\omega)+1}\right]\right]\ . \tag{31}$$

It should be noted that these results are consistent with Bechstedt's dynamically screened Coulomb potential in that we have verified that our Eq. (31) follows from applying the Laplacian to Bechstedt's Eq. (26) in the local limit, but these results disagree with Bechstedt's Eq. (28). It should be further noted that the correct dynamically screened image potential generated by a Coulombic impurity follows from our Eqs. (3) and (30) by using Eq. (7)

above, as one can readily verify.

Our results for the infinite-barrier model, Eqs. (25), (30), and (31), are explicitly revealing in regard to the manner in which image fields are embodied in the structure of the inverse dielectric function $\kappa(\bar{Q},z,z';\omega)$ through boundary terms localized in the vicinity of the surface by $\delta(z')$ factors. This stands in contrast to the elegant but rather formal results for $\kappa(\bar{Q},z,z';\omega)$ presented by Hertel,[4] which are not illustrative in this manner. However, on the other hand, Hertel's results have a broader generality and can be applied to boundary conditions other than the specular reflection infinite-barrier model to which we are committed. It should be noted that such problems have also been addressed by Eguiluz[5] and others from rather different points of view. Moreover, our results should provide useful insight into problems of interaction and correlation at surfaces (as well as of screening and normal modes) as even greater complexity is introduced into infinite-barrier problems, such as the inclusion of a magnetic field.[6]

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