Inverse dielectric response function of a dielectric sphere

Ami C. Sharma*

Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge, CB3 0HE, United Kingdom (Received 16 September 1986; revised manuscript received 16 January 1987)

We present a model inverse random-phase-approximation dielectric response function $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$ of a dielectric sphere of radius d. $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$ is applied to the calculation of the image potentials when the dielectric sphere is in the field of a point charge and in a uniform electric field.

I. INTRODUCTION

In our previous papers^{1,2} we studied one of the most basic properties (image formation) of a planar surface by performing a model calculation of the real-space inversion of the dielectric response function (DRF), $\epsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega)$, of a dielectric slab and that of a semi-infinite dielectric media. One is always interested in a spherical surface after studying a planar surface. In this paper we extend our calculation of $\epsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega)$ to a dielectric sphere. We present a compact form of $\epsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega)$ for a dielectric sphere taking into consideration the long-range dipoledipole interaction. The DRF, thus obtained, has been applied to calculations of the image potentials (a) when the dielectric sphere is kept in the field of a point charge, and (b) when it is in a uniform electric field.

Spherical particles have been the subject of extensive investigations in a recent past.³⁻²¹ The distinct characteristic of a spherical particle is the size dependence of its various properties such as image potentials, surface excitations, and optical and transport properties. The theoretical treatments of a spherical particle have followed two routes. The first is to modify the usual bulk properties by introducing the necessary boundary conditions. The second rate is to treat the particle as a microscopic quantum-mechanical system and to evaluate its properties from first principles. During the recent past the second route has been followed for a metallic particle by a number of researchers, who model it as a free-electron system.⁸⁻¹⁹ Comparatively less work has been done on nonmetallic particles because of the complexities involved.^{5,6,20,21} In this paper we study the dielectric sphere, modeling it as a system composed of polarizable atoms which interact with each other via a multipolemultipole interaction on the application of an external field. Using the extreme-tight-binding (ETB) model, we first calculate the random-phase-approximation $\epsilon^{-1}(\mathbf{r},\mathbf{r},\omega)$ of a dielectric sphere, with which we than calculate the

image potentials when the dielectric sphere is in the field of a point charge, and when it is in a uniform electric field.

II. INVERSION OF DIELECTRIC RESPONSE FUNCTION

In order to obtain $\epsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega)$ we evaluate the matrix $(Q_{\mathbf{R}\mathbf{R}'}^{\nu\nu'})^{-1}$ which includes the multipole-multipole interactions [see Eqs. (1) to (5) of Ref. 1]. The matrix $(Q_{\mathbf{R}\mathbf{R}'}^{\nu\nu'})^{-1}$ can be expressed as a series given below.^{1,2}

$$\underline{Q}^{-1} = 1 + N_0 \underline{C} + N_0^2 \underline{C} \underline{C} + N_0^3 \underline{C} \underline{C} \underline{C} + \cdots , \qquad (1)$$

where

$$N_{0} = -4E_{g}/(E_{g}^{2} - \hbar^{2}\omega^{2}) , \qquad (2)$$

$$\underline{C} = \int \int d^{3}\lambda d^{3}\rho A_{\nu}(\lambda - \mathbf{R})v(\lambda - \rho)A_{\nu}^{*}(\rho - \mathbf{R}) . \qquad (3)$$

 E_g , v, **R**, and $v(\lambda - \rho)$ denote he energy gap, the orientation index, the location of an atomic site, and the Coulomb interaction, respectively. $A_v(\lambda - \mathbf{R})$ is the product of valence- and conduction-band orbitals at an atomic site **R**. Since $A_v(\lambda - \mathbf{R})$ and $A_v^*(\rho - \mathbf{R})$ are localized, matrix <u>C</u> can be expressed as

$$\underline{C} = e^{2} \int \int d^{3}r \, d^{3}r' A_{\nu}(\mathbf{r}) \\ \times \sum_{n=0}^{\infty} (\mathbf{r} \cdot \nabla)^{n} \sum_{m=0}^{\infty} (\mathbf{r}' \cdot \nabla')^{m} \phi(\mathbf{R} - \mathbf{R}') A_{\nu'}^{*}(\mathbf{r}') ,$$
(4)

where $\phi(\mathbf{R} - \mathbf{R}') = 1 / |\mathbf{R} - \mathbf{R}'|$, ∇ and ∇' are gradient operators of **R** and **R**'. Separating the long-range interactions from the short-range interactions, we write

$$\underline{C} = \underline{C}_{l} + \underline{C}_{s} , \qquad (5)$$

where

$$\underline{C}_{l} = \mathbf{d}_{v} \cdot \nabla [\mathbf{d}_{v'} \cdot \nabla' \phi(\mathbf{R} - \mathbf{R}')],$$

$$\underline{C}_{s} = \sum_{n=2}^{\infty} \int d^{3}r \ A_{v}(\mathbf{r})(\mathbf{r} \cdot \nabla)^{n} \left[\mathbf{d}_{v'} \cdot \nabla' \phi(\mathbf{R} - \mathbf{R}') + \frac{1}{2} \sum_{m=2}^{\infty} \int d^{3}r' \ A_{v'}^{*}(\mathbf{r}')(\mathbf{r}' \cdot \nabla')^{m} \phi(\mathbf{R} - \mathbf{R}') \right] .$$

$$+ \left[\mathbf{d}_{v} \cdot \nabla + \frac{1}{2} \sum_{n=2}^{\infty} \int d^{3}r \ A_{v}(r)(\mathbf{r} \cdot \nabla)^{n} \right] \sum_{m=2}^{\infty} \int d^{3}r' \ A_{v'}^{*}(\mathbf{r}')(\mathbf{r}' \cdot \nabla')^{m} \phi(\mathbf{R} - \mathbf{R}') ,$$
(6)

36 4413

AMI C. SHARMA

36

(18)

where \mathbf{d}_{v} is the dipole momentum. In order to calculate various matrix products of Eq. (1), we evaluate $\underline{C} \underline{C}$. The matrix product $\underline{C} \underline{C}$ cannot be calculated analytically unless we truncate Eq. (4). \underline{C}_{s} is significant only at atomic scale. In order to calculate $\underline{C} \underline{C}$, we sum on **R** over the sphere. $\underline{C}_{l} \underline{C}_{l}$, therefore, makes a large contribution to $\underline{C} \underline{C}$ unless the sphere is very small. We therefore can safely write $\underline{C} \underline{C} = \underline{C}_{l} \underline{C}_{l}$ for a reasonably big sphere in order to obtain $\epsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega)$ for practical use. We can write [see Eq. (12) of Ref. 1]

$$\underline{C} \underline{C} = d^2 n_0 \mathbf{d}_v \cdot \nabla \left[\int d\mathbf{s} \cdot \nabla'' \phi(\mathbf{R} - \mathbf{R}'') \mathbf{d}_{v'} \cdot \nabla' \phi(\mathbf{R}'' - \mathbf{R}') - \int d^3 R'' (\nabla'')^2 \phi(\mathbf{R} - \mathbf{R}'') \mathbf{d}_{v'} \cdot \nabla' \phi(\mathbf{R}'' - \mathbf{R}') \right],$$
(8)

where n_0 is the atomic density, d^2 is the average squared dipole moment, and ds is the unit area along the outward normal to the surface. On the right-hand side of Eq. (8) finite-geometry effects appear in the first term while the second term contains the pure bulk effects. The calculation of the second term is straightforward. We calculate the first term by performing the surface integration over a sphere of radius d. Choosing the origin at the center of the sphere, **R**' along the z direction, **R** along the direction (α,β) , and **R**'' along the direction (θ,ϕ) , we obtain

$$\underline{C} \, \underline{C} = A \left(\underline{C} - \underline{D}_{1} \right) \,, \tag{9}$$

where

$$A = 4\pi n_0 d^2 , \qquad (10)$$

$$\underline{D}_1 = \sum_{n=0}^{\infty} \left[\frac{n+1}{2n+1} \right] \frac{\mathbf{d}_{v} \cdot \nabla}{d^{2n+1}} \{ R^n \mathbf{d}_{v'} \cdot \nabla' [R'^n P_n(\cos\alpha)] \} , \qquad (11)$$

 $P_n(\cos \alpha)$ being the Legendre function. It may be noted that <u>C</u> is the dipole-dipole interaction matrix between the real dipoles, while <u>D</u>₁ is the dipole-dipole interaction matrix between the real dipoles and the first-order image dipoles.

In order to evaluate $\underline{C} \underline{C} \underline{C}$, we calculate the matrix product $\underline{C}D_1$. Proceeding as in the calculation of $\underline{C} \underline{C}$, we get

$$\underline{C}\,\underline{D}_{1} = A\underline{D}_{2} , \qquad (12)$$

Similarly,

$$\underline{C}\,\underline{D}_2 = A\underline{D}_3 \,. \tag{13}$$

In general, we have

$$\underline{C}\,\underline{D}_{m-1} = AD_m \quad , \tag{14}$$

where

$$\underline{D}_{m} = A \sum_{n=0}^{\infty} \frac{n^{m-1}(n+1)}{(2n+1)^{m}} \frac{1}{d^{2n+1}} \mathbf{d}_{v} \cdot \nabla \times [R^{n} \mathbf{d}_{v'} \cdot \nabla' \{R'^{n} P_{n}(\cos \alpha)\}].$$
(15)

Substituting the various matrix products in Eq. (1), and then summing up various series, we obtain

$$(Q_{\mathbf{R}\mathbf{R}'}^{\nu\nu'})^{-1} = B_{\mathbf{R}\mathbf{R}'}^{\nu\nu'} + D_{\mathbf{R}\mathbf{R}'}^{\nu\nu'} , \qquad (16)$$

where

$$B_{\mathbf{R}\mathbf{R}'}^{\nu\nu'} = \delta_{\mathbf{R}\mathbf{R}'}^{\nu\nu'} + \frac{N_0(\omega)}{1 - AN_0(\omega)} C_{\mathbf{R}\mathbf{R}'}^{\nu\nu'} , \qquad (17)$$

and

$$D_{\mathbf{R}\mathbf{R}'}^{\nu\nu'} = -\frac{AN_0^2(\omega)}{1 - AN_0(\omega)} \sum_{n=0}^{\infty} \frac{(n+1)}{[2n+1 - AN_0(\omega)]} \times \frac{\mathbf{d}\nu \cdot \nabla}{\mathbf{d}^{2n+1}} \{ \mathbf{R}^n \mathbf{d}_{\nu'} \cdot \nabla' \times [\mathbf{R}'^n \mathbf{P}_n(\cos\alpha)] \}$$

The matrix $B_{RR'}^{\nu\nu'}$ involves the pure bulk effects. It contains the on-site dipole-dipole interaction and the screened dipole-dipole interaction between the real dipoles. On the other hand, the matrix $D_{RR'}^{\nu\nu'}$ is the screened dipole-dipole interaction between the real dipoles and the image dipoles of different orders. $D_{RR'}^{\nu\nu'}$, a distinct characteristic of a dielectric sphere, is added to the bulk terms to obtain $(Q_{RR'}^{\nu\nu'})^{-1}$ for a sphere. $D_{RR'}^{\nu\nu'}$ provides all the information about the spherical surface and the finite radius. As $d \to \infty$, $D_{RR'}^{\nu\nu'}$ is vanishingly small and, consequently $(Q_{RR'}^{\nu\nu'})^{-1}$ reduces to the matrix $B_{RR'}^{\nu\nu'}$, as it should. On the other hand, for small values of d, $D_{RR'}^{\nu\nu'}$ dominates over $B_{RR'}^{\nu\nu'}$. This shows that surface effects are more important than bulk effects in the case of a small sphere. The response function $\epsilon^{-1}(\mathbf{r},\mathbf{r'},\omega)$ of a dielectric sphere can be now given by^{2,22}

$$\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}') + N_0(\omega) \sum_{\nu,\mathbf{R}} \int d^3 r'' \nu (\mathbf{r}-\mathbf{r}') A_{\nu}(\mathbf{r}''-\mathbf{R}) (B_{\mathbf{R}\mathbf{R}'}^{\nu\nu'} + D_{\mathbf{R}\mathbf{R}'}^{\nu\nu'}) A_{\nu'}^{*}(\mathbf{r}'-\mathbf{R}') .$$
(19)

Although we have neglected the short-range interactions in obtaining \underline{Q}^{-1} , Eq. (19) still contains a great deal of information about the short-range interactions.

INVERSE DIELECTRIC RESPONSE FUNCTION OF A ...

III. IMAGE POTENTIALS

In order to demonstrate the physical correctness of Eq. (19), we calculate the image potentials when the dielectric sphere is kept in the field of a point charge, and when it is a uniform electric field. The field of the point charge, q_0 , at location **a** and the uniform electric field, E_0 , are

$$v_{\text{ext}}(\mathbf{r}) = q_0 / |\mathbf{r} - \mathbf{a}| \equiv q_0 \phi(\mathbf{r} - \mathbf{a}) , \qquad (20)$$

and

$$v_{\text{ext}}(\mathbf{r}) = E_0 z = E_0 r \cos\theta . \tag{21}$$

The image potential can be calculated as

$$v_{\text{tot}}(\mathbf{r}) = \int d^3 \mathbf{r}' \, \boldsymbol{\epsilon}^{-1}(\mathbf{r}, \mathbf{r}', \omega) v_{\text{ext}}(\mathbf{r}') \,. \tag{22}$$

Substituting Eqs. (20) and (19) into Eq. (22) we can write

$$v_{\text{tot}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + v_1(\mathbf{r}) + v_2(\mathbf{r}) + v_3(\mathbf{r}) , \qquad (23)$$

where $v_1(\mathbf{r})$ and $v_2(\mathbf{r})$ correspond to the second and third terms, while $v_3(\mathbf{r})$ corresponds to the fourth term on the righthand side of Eq. (19). We can define $v_1(\mathbf{r})$ as the on-site potential, and $v_2(\mathbf{r})$ and $v_3(\mathbf{r})$ as the interaction potentials. Keeping in mind the localized nature of $A_v(\mathbf{r}-\mathbf{R})$, $v_1(\mathbf{r})$ can be expressed as

$$v_{1}(\mathbf{r}) = \sum_{\nu,\mathbf{R}} \left[\sum_{n=0}^{\infty} \int d^{2}r^{\prime\prime} A_{\nu}(\mathbf{r}^{\prime\prime})(\mathbf{r}^{\prime\prime}\cdot\nabla)^{n} v(\mathbf{r}-\mathbf{R}) \right] \left[\sum_{m=0}^{\infty} \int d^{3}r^{\prime} A_{\nu}^{*}(\mathbf{r}^{\prime})(\mathbf{r}^{\prime}\cdot\nabla)^{m} v(\mathbf{r}^{\prime}-\mathbf{a}) \right].$$
(24)

Separating the long-range interaction potential from the short-range interaction potential, we can write

$$v_1(\mathbf{r}) = v_{1l}(\mathbf{r}) + v_{1s}(\mathbf{r})$$
, (25)

with

$$v_{1l}(\mathbf{r}) = \sum_{v,\mathbf{R}} \left[\mathbf{d}_{v} \cdot \nabla \phi(\mathbf{r} - \mathbf{R}) \right] \left[\mathbf{d}_{v} \cdot \nabla \phi(\mathbf{R} - \mathbf{a}) \right],$$
(26)

and

$$V_{1s}(\mathbf{r}) = \sum_{\nu, \mathbf{R}} \left[\mathbf{d}_{\nu} \cdot \nabla \phi(\mathbf{r} - \mathbf{R}) \sum_{m=2}^{\infty} \int d^{3}r' A_{\nu}^{*}(\mathbf{r}') (\mathbf{r}' \cdot \nabla')^{m} \phi(\mathbf{R} - \mathbf{a}) \right. \\ \left. + \mathbf{d}_{\nu} \cdot \nabla \phi(\mathbf{R} - \mathbf{a}) \sum_{n=2}^{\infty} \int d^{3}r'' A_{\nu}(\mathbf{r}'') (\mathbf{r}'' \cdot \nabla'')^{m} v(\mathbf{r} - \mathbf{R}) \right].$$

$$(27)$$

 $v_{1l}(\mathbf{r})$ can be calculated analytically while $v_{1s}(\mathbf{r})$ cannot. However, we can numerically calculate $v_{1s}(\mathbf{r})$ by substituting the appropriate value of $A_{y}(\mathbf{r})$ as has been done for a bulk semiconductor in Sec. III of Ref. 22. We here notice that depending on the position of field point (r) and the source point (a), $v_1(\mathbf{r})$ has the following four possible values which correspond to the cases: (i) r < d and a < d, (ii) r < d and a > d, (iii) r > d and a < d, and (iv) r > d and a > d. We see from Eq. (27) that $v_{1s}(\mathbf{r})$ has a substantial contribution to $v_1(\mathbf{r})$ only when either r or a, or both r and a are in the vicinity of the spherical surface. On the other hand, when both r and a are away from the surface, the contribution of $v_{1s}(\mathbf{r})$ to $v_1(\mathbf{r})$ is insignificant and $v_1(\mathbf{r}) \simeq v_{1l}(\mathbf{r})$. The main object of this paper is to obtain a model $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$ of a sphere and to demonstrate the correctness of our model $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$. We therefore neglect the short-range potentials and calculate only $v_{1l}(\mathbf{r})$ in order to obtain analytic results. We similarly calculate only long-range interaction parts of potentials $v_2(\mathbf{r})$ and $v_3(\mathbf{r})$. Our results are given, for case (i) r < d and a < d, as

$$v_1(\mathbf{r}) = AN_0(\omega) \left[v_{\text{ext}}(\mathbf{r}) - q_0 \sum_{n=0}^{\infty} \lambda_n \right], \qquad (28)$$

$$v_{2}(\mathbf{r}) = \frac{A^{2}N_{0}^{2}(\omega)}{1 - AN_{0}(\omega)} \left[v_{\text{ext}}(\mathbf{r}) - q_{0} \sum_{n=0}^{\infty} \left[1 + \frac{n}{n+1} \right] \lambda_{n} \right],$$
(29)

$$v_{3}(\mathbf{r}) = -\frac{A^{3}N_{0}^{3}(\omega)}{1 - AN_{0}(\omega)}q_{0}$$

$$\times \sum_{n=0}^{\infty} \left[\frac{n^{2}}{2n+1}\right] \frac{\lambda_{n}}{\left[2n+1 - AN_{0}(\omega)\right]}, \quad (30)$$

where

$$\lambda_n = \left[\frac{n+1}{2n+1}\right] \frac{r^n a^n}{d^{2n+1}} P_n \cos(\theta') ,$$

with

$$\mathbf{r} \cdot \mathbf{a} = ra \cos \theta'$$
.

Similarly, neglecting the short-range interactions $v_1(\mathbf{r})$, $v_2(\mathbf{r})$, and $v_3(\mathbf{r})$ for cases (ii)–(iv) are given by

$$v_1(\mathbf{r}) = AN_0(\omega)q_0 \sum_{n=0}^{\infty} \phi_n$$
, (31)

$$v_{2}(\mathbf{r}) = \frac{A^{2}N_{0}^{2}(\omega)q_{0}}{1 - AN_{0}(\omega)} \sum_{n=0}^{\infty} \left[\frac{n}{n+1}\right] \phi_{n} , \qquad (32)$$

and

$$v_{3}(\mathbf{r}) = -\frac{A^{3}N_{0}^{3}(\omega)}{1 - AN_{0}(\omega)}q_{0}\sum_{n=0}^{\infty} \left[\frac{n}{2n+1}\right] \times \frac{\phi_{n}}{[2n+1 - AN_{0}(\omega)]}, \quad (33)$$

where for cases (ii)–(iv) ϕ_n is given by

$$\phi_n = \left[\frac{n}{2n+1}\right] \frac{r^n}{a^{2n+1}} P_n(\cos\theta') ,$$

$$\phi_n = \left[\frac{n}{2n+1}\right] \frac{a^n}{r^{2n+1}} P_n(\cos\theta') ,$$

$$\phi_n = \left[\frac{n}{2n+1}\right] \frac{d^{2n+1}}{r^{n+1}a^{n+1}} P_n(\cos\theta') ,$$

respectively. On substituting Eqs. (28)-(30) into Eq. (23), we get for case (i)

$$v_{\text{tot}}(\mathbf{r}) = \frac{v_{\text{ext}}(\mathbf{r})}{\epsilon(\omega)} - v_{\text{ind}}(\mathbf{r}) , \qquad (34)$$

where

$$v_{\text{ind}}(\mathbf{r}) = \frac{\epsilon(\omega) - 1}{\epsilon(\omega)} q_0 \sum_{n=0}^{\infty} \frac{(n+1)}{[n\epsilon(\omega) + n + 1]} \frac{r^n a^n}{d^{2n+1}} P_n(\cos\theta') .$$
(35)

Here $\epsilon(\omega)$ is the "long-wavelength" dielectric function. For cases (ii)-(iv) we substitute Eqs. (31)-(33) into Eq. (23). We obtain

$$v_{\text{tot}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) - v_{\text{ind}}(\mathbf{r})$$
, (36)

where

$$v_{\text{ind}}(\mathbf{r}) = [\epsilon(\omega) - 1] q_0 \sum_{n=0}^{\infty} \frac{(2n+1)}{[n\epsilon(\omega) + n + 1]} \phi_n .$$
(37)

For the case of a uniform electric field, $v_1(\mathbf{r})$, $v_2(\mathbf{r})$, and $v_3(\mathbf{r})$ have two values according to cases (a) r < d and (b) r > d. Neglecting the short-range interaction part, $v_1(\mathbf{r})$, $v_2(\mathbf{r})$, and $v_3(\mathbf{r})$ are given for case (a) as

$$v_1(\mathbf{r}) = \frac{A}{3} N_0(\omega) E_0 r \cos\theta , \qquad (38)$$

$$v_2(\mathbf{r}) = \frac{A^2 N_0^2(\omega)}{g \left[1 - A N_0(\omega)\right]} E_0 r \cos\theta , \qquad (39)$$

and

$$v_{3}(\mathbf{r}) = -\frac{2}{9} \frac{A^{3} N_{0}^{3}(\omega)}{[1 - A N_{0}(\omega)][3 - A N_{0}(\omega)]} E_{0} \mathbf{r} \cos\theta .$$
(40)

For case (b)

$$v_1(\mathbf{r}) = \frac{A}{3} N_0(\omega) \frac{d^3}{r^2} E_0 \cos\theta , \qquad (41)$$

$$v_{2}(\mathbf{r}) = \frac{A^{2}N_{0}^{2}(\omega)}{g\left[1 - AN_{0}(\omega)\right]} \frac{d^{3}}{r^{2}} E_{0}\cos\theta , \qquad (42)$$

and

$$v_{3}(\mathbf{r}) = -\frac{2}{9} \frac{A^{3}N_{0}^{3}(\omega)}{[1 - AN_{0}(\omega)][3 - AN_{0}(\omega)]} \frac{d^{3}}{r^{2}} E_{0}\cos\theta .$$
(43)

Here we again neglected the short-range potentials, in order to avoid numerical computation. The short-range potentials substantially contribute to $v_{tot}(\mathbf{r})$ when r is in vicinity of surface. The $v_{tot}(\mathbf{r})$ can be given by

$$v_{\text{tot}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) - v_{\text{ind}}(\mathbf{r}) .$$
(44)

Here for case (a) r < d

$$v_{\rm ind}(\mathbf{r}) = \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 2} E_0 r \cos\theta .$$
(45)

For case (b) r > d

$$v_{\rm ind}(\mathbf{r}) = \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 2} \frac{d^3}{r^2} E_0 \cos\theta . \qquad (46)$$

IV. DISCUSSION AND CONCLUSIONS

Our results for the image potentials, given is Eqs. (35), (37), (45), and (46), are exactly the same as those obtained using classical electrodynamics,²³ as they should be because we have considered only long-range interaction effects. This demonstrates the physical correctness of our model $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$. Our results for the image potential are obtained using a quantum-mechanical approach which is based on the dielectric response function of the sphere, and which does not involve any matching conditions. Thus our calculation of image potentials provides a quantum-mechanical proof of old classical results. We note here that the evaluation of Eq. (23) with the use of appropriate bond orbitals gives short-range fluctuating terms in the image potentials. This information about short-range fluctuations in the image potentials can be obtained by performing a numerical computation of Eq. (27). We have, however, confined ourselves to only the analytically obtainable results in this paper.

To conclude, we have reported a simple analytic expres-

4416

sion for a model $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$, which incorporates the basic and most distinct features of a dielectric sphere. Equation (19) yields a good model RPA $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$ unless the radius of the sphere is very small. The imaginary part of ETB model $\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega)$ contains a δ function, and therefore, it does not give a physically correct answer for optical properties. Our calculation should be extended beyond the ETB model in order to study the optical properties of a dielectric sphere.^{5,6} A further modification of our calculation is the inclusion of the quantum size effects.

ACKNOWLEDGMENTS

I thank Dr. T. Takemori for many useful discussions on the subject of this paper at Cavendish Laboratory. I am thankful to Professor S. S. Mathur and Professor K. P. Jain for their generous help in various ways, at the Indian Institute of Technology (IIT), Delhi. I acknowledge with thanks the financial assistance of Science and Engineering Research Council (U.K.) at Cavendish Laboratory, and of Scientific and Industrial Research Council (India) at IIT, Delhi.

- *Present address: Laser Technology Research Program, Department of Physics, Indian Institute of Technology, Delhi, Hauz Khas, New Delhi-110016, India.
- ¹A. C. Sharma, Phys. Rev. B 34, 1165 (1986).
- ²J. C. Inkson and A. C. Sharma, J. Phys. C 18, 5435 (1985).
- ³G. Mie, Ann. Phys. 25, 377 (1980).
- ⁴A. Liebsch and P. V. Gonzalez, Phys. Rev. B **29**, 6907 (1984). ⁵M. Inoue and K. Ohtaka, Phys. Rev. B **26**, 3487 (1982); M.
- Inoue, K. Ohtaka, and S. Yanagawa, *ibid*. **25**, 689 (1982). ⁶K. Ohtaka and M. Inoue, J. Phys. C **15**, 6463 (1982); M. Inoue
- and K. Ohtaka, J. Phys. Soc. Jpn. 52, 554 (1982), M. Hidde
- ⁷J. A. A. J. Parenboom, P. Wyder, and F. Meier, Phys. Rep. 78, 173 (1981).
- ⁸J. Crowell and R. H. Ritchie, Phys. Rev. 172, 436 (1968).
- ⁹A. Kawabata and R. Kuba, J. Phys. Soc. Jpn. 21, 1765 (1966);
 J. D. Ganiere, R. Rechsteiner, and M.-A. Smithard, Solid State Commun. 16, 113 (1975).
- ¹⁰A. A. Lushnikov and A. J. Simonov, Z. Phys. 270, 17 (1974).
- ¹¹R. Ruppin, Phys. Rev. B 11, 2871 (1975).
- ¹²D. R. Penn and R. W. Rendell, Phys. Rev. Lett. 47, 1067

- (1981); D. R. Penn and R. W. Rendell, Phys. Rev. B 26, 3047 (1982).
- ¹³D. M. Wood and N. W. Aschroft, Phys. Rev. B 25, 6255 (1982).
- ¹⁴W. Ekardt, Phys. Rev. B **29**, 1558 (1984); W. Ekardt, Phys. Rev. Lett. **52**, 1925 (1984); G. Berstsch and W. Ekardt, Phys. Rev. B **32**, 7659 (1985).
- ¹⁵A. Schmitt-Ott, P. Schurtenberger, and H. C. Siegmann, Phys. Rev. Lett. 45, 1284 (1980).
- ¹⁶D. R. Sinder and R. S. Sorbello, Phys. Rev. B 28, 5702 (1983).
- ¹⁷M. J. Rice, W. R. Schneider, and S. Strassler, Phys. Rev. B 8, 474 (1975).
- ¹⁸K. Hilpert, Phys. Chem. 88, 132 (1984).
- ¹⁹M. Inoue and K. Ohtaka, J. Phys. Soc. Jpn. **52**, 3853 (1983); K. Ohtaka and M. Inoue, Phys. Rev. B **25**, 677 (1982).
- ²⁰B. B. Dasgupta and R. Fuchs, Phys. Rev. B 24, 554 (1981).
- ²¹J. I. Gersten and A. Nitzan, Phys. Rev. B 29, 3852 (1984).
- ²²M. P. Ortuno and J. C. Inkson, J. Phys. C 12, 1065 (1979).
- ²³C. J. F. Bottcher, Theory of Electric Polarization (Elsevier, Amsterdam, 1973).