Local-field corrected van der Waals potentials in magnetodielectric multilayer systems

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Within the framework of macroscopic quantum electrodynamics in linear, causal media, we study the van der Waals potentials of ground-state atoms in planar magnetodielectric host media. Our investigation extends earlier ones in two aspects: It allows for the atom to be embedded in a medium, thus covers many more realistic systems; and it takes account of the local-field correction. Two- and three-layer configurations are treated in detail both analytically and numerically. It is shown that an interplay of electric and magnetic properties in neighbouring media may give rise to potential wells or walls. Local-field corrections as high as 80% are found. By calculating the full potential including the translationally invariant and variant parts, we propose a way to estimate the (finite) value of the dispersion potential at the surface between two media. Connection with earlier work intended for biological applications is established.

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I. INTRODUCTION

The dispersive interaction between small neutral, unpolarised particles (atoms, molecules etc.) and an uncharged macroscopic object is a manifestation of the quantum nature of the electromagnetic field and related to the zero-point energy [1]. In the first quantum electrodynamical treatment of this van der Waals (vdW) type force [2], and in many other related works, the atom was assumed to be located in free space. In reality, the atom may be submerged in or be a part of a gas, liquid, or even solid — a situation typical in diverse fields such as colloid science [3, 4], surface engineering [5], and biology [6]. As a particular example from biology, one can cite the transfer of a small particle diluted in cell plasma through a cell membrane caused by vdW forces [8]. A question that may arise when the atom is embedded in a medium is how the vdw interaction is to be corrected due to the difference between the local fields acting on the atom and the macroscopic fields averaged over a region which contains a great number of the medium constituents, thus ignoring the gaps between them. In Ref. [9], the vdw interaction between two ground-state atoms embedded in adjacent semi-infinite magnetodielectric media has been considered. Comparison of this result with that deduced from the Casimir force on a thin composite slab in front of a composite semi-infinite medium, both obeying the Clausius-Mossotti relation, suggests a hint on how to account for the local-field correction. This confirmed shortly after in Ref. [10] on the basis on a macroscopic quantum electrodynamics theory and the real-cavity model [11]. A general formula for the vdw potential in an arbitrary geometry has been derived in the form of a sum of a translationally invariant term and and a term containing the uncorrected scattering Green tensor modified by a local-field correction factor [9, 10]. This general formula is applicable for meta-materials [12] and will serve as a starting point for our treatment of the local-field corrected vdw interaction in a stratified magnetodielectric. Note that a generalisation of the formalism has recently been used to study local-field corrected interactions of an excited atom with a ground-state one across an interface between two media [13].

The interaction between a neutral atom and a material surface is customarily split into two parts: a short-range repulsive part, significant when the atomic valence electrons overlap with the surface, and a longer-range dispersive vdw part [14, 15, 16, 17, 18, 19, 20]. Theories that focus on the vdw interaction commonly neglect the first, thus are incapable of correctly predicting the behaviour of the interaction potential at very short distances. They typically yield a power law of $z_A^{-s}$ (z_A, atom–surface distance) for materials with dominant electric properties, and a power law of $z_A^{-4}$ for purely magnetic materials, which lead to divergent values for the vdw potential right on the surface [2, 21, 22]. Due to the importance of phenomena such as physisorption and transport of particles through interfaces and membranes, much effort has been devoted to a better treatment of the atom–surface interaction when the two are at very short distances. With respect to physisorption, this has been done via introducing a reference plane [23]; via characterising the material surface by a more realistic response function which includes spatial dispersion [24], smooth
variation of the dielectric properties at the interface, and
the contribution from d electrons to the screening [23];
and via using an atomic polarisability going beyond the
dipole approximation [17, 22]. These studies typically
produce finite values for the interaction potential at the interface
[22].

In the present paper, the local-field corrected vdW in-
teraction of a ground-state atom embedded in a planar,
dispersing and absorbing magnetoelectric host medium is
studied within the framework of macroscopic quantum
electrodynamics and the real-cavity model. We propose
a procedure that would allow for obtaining an estimate of
the finite vdW energy of an atom right on the interface
even within our predominantly macroscopic framework
treating the atom within electric dipole approximation.
The paper is organised as follows. In Sec. III the main
results concerning the local-field corrected vdW inter-
action of a ground-state atom and an arbitrary absorbing
and dispersing macroscopic body are reviewed, and then
applied to planar multilayer systems. The two-layer case
is considered and a procedure for an estimation of the
vdW potential at the interface is given in Sec. IIII while
the three-layer case is discussed in Sec. IV. Connection
with earlier work which focus on biological systems and
concluding remarks are given in Sec. V.

II. THE MODEL

We set the stage by briefly recalling the results for
the local-field corrected vdW potential of a ground-state
atom within an arbitrary geometry and applying them
to a planar multilayer system.

A. Local-field corrected vdW potentials in
arbitrary geometries

We consider a ground-state guest atom $A$ located at
$r_A$ in an absorbing and dispersing host medium of arbitrary
size and shape characterised by macroscopic $\varepsilon(r, \omega)$
and $\mu(r, \omega)$. To account for the local-field correction we
employ the real-cavity model by assuming the atom to
be surrounded by a small spherical free-space cavity of
radius $R_c$. The radius of the cavity is a measure of the
distance between the guest atom and the surrounding
host atoms [10]. By construction, the macroscopic quan-
ties $\varepsilon(r, \omega)$ and $\mu(r, \omega)$ do not vary appreciably on the
microscopic length scale $R_c$. To apply the real cavity
model one should keep in mind that $\sqrt{\varepsilon(0)\mu(0)}R_c$
should be small compared to the maximum of all characteristic
atomic and medium wavelengths as well as to the separa-
tion from any surface of the host medium. In particular,
the application of model to metals is very problematic.
Using second-order perturbation theory, the vdW poten-
tial for such an atom can be written in the form [10]

$$U(r_A) = U_1(r_A) + U_2(r_A),$$

where $U_1(r_A)$ is constant throughout any homogenous
region and accounts for all scattering processes within the
cavity,

$$U_1(r_A) = -\frac{\hbar \mu_0}{4\pi^2c} \int_0^\infty d\xi \xi^2 \alpha(i\xi)C_A(i\xi),$$

where

$$C_A(\omega) = \frac{h_1^{(1)}(z_0) \left[ z_0 h_1^{(1)}(z) \right]' - \varepsilon_A(\omega) h_1^{(1)}(z) \left[ z_0 h_1^{(1)}(z_0) \right]'}{\varepsilon_A(\omega) h_1^{(1)}(z_0) \left[ z_0 j_1(z_0) \right]' - j_1(\omega) \left[ z_0 h_1^{(1)}(z) \right]'}.$$
\( \omega_{\text{max}} \) represents the maximum of characteristic atomic and medium frequencies (for details, see Ref. 10),

\[
U_1(r_A) = -\frac{h}{4\pi^2\epsilon_0} \int_0^\infty d\xi \alpha \left[ 3 \frac{\varepsilon_A - 1}{\varepsilon_A + 1} \frac{1}{R_c^3} + \frac{9\xi^2}{e^2} \frac{1}{2\varepsilon_A + 1} \frac{3\varepsilon_A + 1}{2\varepsilon_A + 1} \right] (9)
\]

and

\[
U_2(r_A) = \frac{\hbar \mu_0}{2\pi} \int_0^\infty d\xi \xi^2 \alpha \left( \frac{3\varepsilon_A}{2\varepsilon_A + 1} \right)^2 \nabla \text{Tr} \mathbf{G}^{(1)}(r_A, r_A, i\xi). (10)
\]

Here and in the following the dependence of \( \varepsilon, \mu, \) and \( \alpha \) on the \( i\xi \) is suppressed for brevity. Note that in leading order the local-field factor \( \frac{3\varepsilon_A}{(2\varepsilon_A + 1)^2} \) depends on dielectric properties only. The associated (conservative) vdW force is given by

\[
F(r_A) = -\nabla U_2(r_A) = -\frac{\hbar \mu_0}{2\pi} \int_0^\infty d\xi \xi^2 \alpha \left( \frac{3\varepsilon_A}{2\varepsilon_A + 1} \right)^2 \nabla \text{Tr} \mathbf{G}^{(1)}(r_A, r_A, i\xi). (11)
\]

The cavity-induced part of the potential, \( U_1 \) according to Eq. (2) does not lead to a force but to an energy shift whose influence on the overall potential will be studied in Secs. III and IV.

## B. Atom in a magnetoelectric multi-layer system

So far we have not been specific about the geometry of the macroscopic body. Consider a stack of \( n \) layers labeled by \( l (l = 1, \ldots, n) \) of thicknesses \( d_l \) with planar parallel boundary surfaces, where \( \varepsilon(r, \omega) = \varepsilon(\omega) \) and \( \mu(r, \omega) = \mu(\omega) \) in layer \( l \). The coordinate system is chosen so that the layers are perpendicular to the \( z \) axis and extend from \( z = 0 \) to \( z = d_l \) for \( l \neq 1, n \) and from \( z = 0 \) to \( z = -\infty \) (\( \infty \)) for \( l = 1, n \). The scattering part of the Green tensor at imaginary frequencies for \( r \) and \( r' \) in layer \( j \) is given by (see, e.g., Ref. 22)

\[
\mathbf{G}^{(1)}(r, r', i\xi) = \int d^2 q e^{iq \cdot (r-r')} \mathbf{G}^{(1)}(q, z, z', i\xi) (12)
\]

\([q \perp e_z]\) where

\[
\mathbf{G}^{(1)}(q, z, z', i\xi) = -\frac{\mu_j}{8\pi^2 \xi^2} \sum_{s, \rho} \frac{1}{D_j^\sigma} \left[ \begin{array}{c}
\mathbf{e}_s^+ \cdot \mathbf{e}_\sigma \cdot e^{-\beta_j(z-z')} + \mathbf{e}_s^- \cdot \mathbf{e}_\sigma \cdot e^{-\beta_j(z-z')} \\
+ e^{2\beta_j d_j} D_j^\sigma \left[ \mathbf{e}_s^+ \cdot \mathbf{e}_\sigma \cdot e^{-\beta_j(z-z')} + \mathbf{e}_s^- \cdot \mathbf{e}_\sigma \cdot e^{\beta_j(z-z')} \right] \end{array} \right] (13)
\]

\([j > 0, \text{for } j = 0 \text{ set } d_0 = 0] \) with the abbreviation

\[
D_j^\sigma = 1 - r_j^\sigma \cdot r_j^\sigma + e^{-2\beta_j d_j}. (14)
\]

In Eq. (13), \( p(s) \) denotes \( p(s) \) polarisations. The reflection coefficients obey the recursion relations

\[
\begin{align*}
\mathbf{r}_l^\pm &= \mathbf{r}_{l+1}^\pm + e^{-2\beta_l d_l} \mathbf{r}_{l+1}^\pm, \\
\mathbf{r}_{l+1}^\pm &= \frac{\mu_l + \beta_l + \mu_l \beta_l}{\mu_l + \beta_l + \mu_l \beta_l} \mathbf{r}_{l+1}^\pm, \\
\mathbf{r}_{l+1}^- &= \frac{\mu_l + \beta_l + \mu_l \beta_l}{\mu_l + \beta_l + \mu_l \beta_l} \mathbf{r}_{l+1}^+.
\end{align*}
\]

(15)

\([r_{l+1}^- = r_{l+1}^+ = 0] \), where the modulus of wave vector in the \( z \) direction is given by

\[
\beta_l = \sqrt{k_l^2 + q^2} (17)
\]

with \( k_l \), which always appears in the form of \( k_l^2 \) in the Green tensor, Eq. (13), being

\[
k_l^2 = \frac{\xi^2}{c^2} \mu_l \epsilon_l. (18)
\]

The s- and p-polarisation unit vectors are defined as

\[
\mathbf{e}_{s} = e_{q} \times e_{z}, \quad \mathbf{e}_{p} = \frac{1}{i k_j} \left( q e_{z} + i \beta_j e_{q} \right) (19)
\]

\([e_q = q / q, q = |q|]. \) Substitution of Eqs. (12) and (13) into Eq. (10) leads to

\[
U_2(z_A) = \frac{\hbar \mu_0}{8\pi^2} \int_0^\infty d\xi \xi^2 \alpha \mu_j \left[ \frac{3\varepsilon_j}{2\varepsilon_j + 1} \right]^2 \times \int_0^\infty dq \frac{q}{\beta_j} \left\{ e^{-2\beta_j z_A} \left[ \frac{r^+}{D_j^\sigma} - \left( 1 + 2 q^2 e^2 \frac{q}{\xi^2 \varepsilon_j \mu_j} \right) \frac{r^+}{D_j^\sigma} \right] \right. \\
+ e^{-2\beta_j (d_j - z_A)} \left[ \frac{r^+}{D_j^\sigma} - \left( 1 + 2 \frac{q^2 e^2}{\xi^2 \varepsilon_j \mu_j} \right) \frac{r^+}{D_j^\sigma} \right] \right\} + \hbar \mu_0 \int_0^\infty d\xi \xi^2 \alpha \mu_j \left[ \frac{3\varepsilon_j}{2\varepsilon_j + 1} \right]^2 \times \int_0^\infty dq \frac{q}{\beta_j} \sum_{s, \rho} \frac{r^+ r^+ e^{-2\beta_j d_j}}{D_j^\sigma}, (20)
\]

where we have used the relations

\[
\mathbf{e}_{s} \cdot \mathbf{e}_{p} = \mathbf{e}_{s} \cdot \mathbf{e}_{p} = 1, (21)
\]

\[
\mathbf{e}_{s} \cdot \mathbf{e}_{p} = 1, \quad \mathbf{e}_{s} \cdot \mathbf{e}_{p} = -1 - 2 \frac{q^2 e^2}{\xi^2 \varepsilon_j \mu_j} (22)
\]

to calculate the trace. It is worth noting that the term in curly brackets in Eq. (20) describes processes that involve an odd number of reflections at the interfaces while the second term accounts for an even number of reflections, as can be seen from

\[
\begin{align*}
\mathbf{r}_{l+1}^- &= e^{-2\beta_l z_A} \frac{1 - r_j^- r_j^+ e^{-2\beta_j d_j}}{1 - r_j^- r_j^+ e^{-2\beta_j d_j}} = e^{-\beta_j z_A} \mathbf{r}_{l+1}^- e^{-2\beta_j d_j} + e^{-\beta_j z_A} \mathbf{r}_{l+1}^- e^{-\beta_j d_j} + \mathbf{r}_{l+1}^- e^{-\beta_j z_A} + \ldots,
\end{align*}
\]

(23)
\[ r_j^+ e^{-2\beta_j (d_j - z_A)} \left( 1 - r_j^- r_j^+ e^{-2\beta_j d_j} \right) = e^{-\beta_j (d_j - z_A)} r_j^+ e^{-\beta_j (d_j - z_A)} + e^{-\beta_j (d_j - z_A)} r_j^+ e^{-\beta_j d_j} r_j^- e^{-\beta_j (d_j - z_A)} + \ldots \] (24)

and

\[ r_j^- r_j^+ e^{-2\beta_j d_j} \left( 1 - r_j^- r_j^+ e^{-2\beta_j d_j} \right) = e^{-\beta_j z_A} r_j^+ e^{-\beta_j d_j} r_j^- \times e^{-\beta_j (d_j - z_A)} + e^{-\beta_j z_A} r_j^+ e^{-\beta_j d_j} r_j^- e^{-\beta_j d_j} \times r_j^- e^{-\beta_j d_j} r_j^+ e^{-\beta_j (d_j - z_A)} + \ldots \] (25)

Obviously, the expression presented in Eq. (25), which corresponds to even numbers of reflections, is independent of the position of the atom and rapidly decreases with increasing distance between two plates. Hence, it cannot lead to a force but only to a layer-dependent energy shift which is small compared to the other terms. It is completely absent in the two-layer case since only single reflections at the interface occur. It also vanishes for sufficiently dilute media, an expansion for small \( \chi_j = \varepsilon_j - 1 \) and \( \zeta_j = \mu_j - 1 \) showing no contribution to linear order, which reflects the fact that at least three medium-assisted reflection processes are involved. On the contrary, Eqs. (23) and (21) depend on the position of the atom, where waves propagating to the left and to the right of the atom have to be distinguished.

It is worth noting that all formulas in this section are valid for arbitrary (passive) magnetoelectric media, including metamaterials and in particular, left-handed materials with simultaneously negative real parts of \( \varepsilon \) and \( \mu \), due to the fact that \( \sqrt{\varepsilon_j(\omega)\mu_j(\omega)} \) has no branching points in the upper half of the complex frequency plane. However, left-handed material properties being only realized in finite frequency windows, they can not be expected to have a strong influence on ground-state dispersion potentials which depend on the medium response at all frequencies; alternatively, this can be seen from the fact that the potential is expressible in terms of permeittivities and permeabilities taken at imaginary frequencies which are always positive [22, 23]. The situation can change when the atom is in an excited state and the atom-field interaction resonantly depends on the medium response at the atomic transition frequencies [28, 29].

### III. VDW POTENTIAL NEAR AN INTERFACE

Let us first apply the theory to the simplest case of a single interface between two homogeneous semi-infinite magnetoelectric half spaces, where we first concentrate on the position-dependent part of the potential responsible for the vdW force and then interpret the (layer-dependent) constant part.

#### A. Position-dependent part

For a planar magnetoelectric two-layer system with the guest atom placed in, say, layer 2, substitution of \( r_{nn}^+ = 0 \) and \( r_{nn}^- \) in accordance with Eqs. (16) in Eq. (20) leads to the following expression for the position-dependent part of the vdW potential

\[
U_2(z_A) = \frac{\hbar \mu_0}{8\pi^2} \int_0^\infty \xi \xi^2 \alpha \left( \frac{3\varepsilon_2}{2\varepsilon_2 + 1} \right)^2 \times \mu_2 \left[ \frac{\mu_1 \beta_2 - \mu_2 \beta_1}{\mu_1 \beta_2 + \mu_2 \beta_1} \right] \int_0^\infty dq \frac{q}{\beta_2} \left[ \frac{\varepsilon_1 \beta_2 - \varepsilon_2 \beta_1}{\varepsilon_1 \beta_2 + \varepsilon_2 \beta_1} \left( 1 + 2 \frac{q^2 c^2}{\varepsilon_2 \beta_2^2} \right) \right] e^{-2\beta_2 z_A},
\] (26)

which differs from its atom-in-free-space counterpart by the local-field correction factor \( \left( \frac{3\varepsilon_2}{2\varepsilon_2 + 1} \right)^2 \) and by \( \varepsilon_2 \neq 1 \) and \( \mu_2 \neq 1 \) [22].

#### 1. Retarded limit

It is instructive to study the potential in the retarded limit

\[
z_A >> \frac{c}{\omega_A} \text{ and } z_A >> \frac{c}{\omega_M},
\] (27)

where \( \omega_A \) and \( \omega_M \) being the minima of all relevant atomic transition and medium resonance frequencies, respectively. Introducing a new integration variable \( v = c\beta_2 / \xi \) and replacing \( a(i\xi) \approx a(0) \), \( \varepsilon_{1,2}(i\xi) \approx \varepsilon_{1,2}(0) \), and \( \mu_{1,2}(i\xi) \approx \mu_{1,2}(0) \), the integration over \( \xi \) can be performed and we obtain for the potential

\[
U_2(z_A) = \frac{C_4}{z_A^4},
\] (28)

where

\[
C_4 = \frac{3\hbar c}{64\pi^2} \alpha(0) \left( \frac{3\varepsilon_2(0)}{2\varepsilon_2(0) + 1} \right)^2 \mu_2(0) \int_0^\infty dw \frac{\sqrt{\varepsilon_2(0)\mu_2(0)}}{dw} \frac{1}{v^4} \left[ \mu_1(0)v - \mu_2(0)v^2 - \varepsilon_2(0)\mu_2(0) + \varepsilon_1(0)\mu_1(0) \right] \frac{\mu_1(0)v - \mu_2(0)v^2 - \varepsilon_2(0)\mu_2(0) + \varepsilon_1(0)\mu_1(0)}{\mu_1(0)v + \mu_2(0)v^2 - \varepsilon_2(0)\mu_2(0) + \varepsilon_1(0)\mu_1(0)} + \varepsilon_1(0)v - \varepsilon_2(0)v^2 - \varepsilon_2(0)\mu_2(0) + \varepsilon_1(0)\mu_1(0) \right] \times (1 - 2\frac{v^2}{\varepsilon_2(0)\mu_2(0)}). \] (29)

It can be proven that \( \partial C_4 / \partial \varepsilon_1(0) < 0 \), \( \partial C_4 / \partial \mu_1(0) > 0 \), and \( \partial C_4 / \partial \mu_2(0) < 0 \).

To deduce some physics from Eq. (29), we consider some limiting cases. Assuming that the atom is located in free space \( \mu_2(0) = \varepsilon_2(0) = 1 \), it can be shown that, for a purely electric half-space 1,

\[
C_4[\mu_1(0) = 1, \mu_2(0) = 1, \varepsilon_2(0) = 1] < 0
\] (30)
and, for a purely magnetic halfspace 1 with \( \mu_1(0) > 1 \),
\[
C_4[\epsilon_1(0) = 1, \mu_2(0) = 1, \epsilon_2(0) = 1] > 0. \tag{31}
\]
The inequality \( \tag{30} \) means the atom is attracted toward the electric halfspace — the case which is commonly treated in earlier literature. On the other hand, the positivity of \( C_4 \) in Eq. \( \tag{31} \) means the atom is repelled from the magnetic half space. This result generalises the one obtained in Ref. \[22\] to the medium of potential is attractive, whereas when the atom is in a medium of \( \epsilon_2(0)/\mu_2(0) > 23/7 \), a repulsive potential can be realized.

2. Non-retarded limit

The non-retarded limit corresponds to atom–surface distances \( z_A \) small compared with the typical wavelengths of the medium and the atomic system,
\[
z_A \ll \frac{c}{\omega_A [n_1(0) + n_2(0)]} \quad \text{and/or} \quad z_A \ll \frac{c}{\omega_A^+ [n_1(0) + n_2(0)]} \tag{39}
\]
\[
[n_{1,2}(0) = \sqrt{\epsilon_1(2)[\mu_1(2)[\mu_1(2) + 1]}; \quad \omega_A^+ \quad \text{and} \quad \omega_A^-, \quad \text{maxima of the relevant atomic transition and medium resonance frequencies}. \quad \text{The conditions} \tag{39} \] \text{and} \tag{40} \text{imply}
\[
\frac{\xi z_A}{c} \sqrt{[\epsilon_1(2) - \epsilon_2(2)]} \ll 1, \tag{41}
\]
\[
\frac{\xi z_A}{c} \sqrt{[\epsilon_1(2) + \epsilon_2(2)]} \ll 1, \tag{42}
\]
where we have used that the \( \xi \)-integration is practically limited to a region where \( \xi \ll \omega_A^+ \). We substitute
\[
q = \sqrt{\epsilon_2^2(2)[\epsilon_1(2) - \epsilon_2(2)] + \beta_3^2}, \tag{43}
\]
\[
q dq = \beta_3 d \beta_3, \tag{44}
\]
\[
\beta_3 = \sqrt{\epsilon_2^2(2)[\epsilon_1(2) - \epsilon_2(2)] + \beta_3^2}, \tag{45}
\]
in Eq. \( \tag{36} \) and, on recalling Eq. \( \tag{11} \), perform a leading-order Taylor expansion in \( \xi^2(2)[\epsilon_1(2) - \epsilon_2(2)](\epsilon_1(2) + \epsilon_2(2)) \). After carrying out the \( \beta_3 \)-integral, we arrive at
\[
U_2(z_A) = \frac{C_3}{z_A^3} + \frac{C_4}{z_A}. \tag{46}
\]
where
\[
C_3 = \frac{\hbar}{16\pi^2 \epsilon_0} \int_0^\infty d \xi \alpha \left[ \frac{9 \epsilon_2}{(2 \epsilon_2 + 1)^2} \epsilon_1 - \epsilon_2 \right], \tag{47}
\]
\[
C_1 = \frac{\hbar \mu_0}{16\pi^2} \int_0^\infty d \xi \sqrt{\epsilon_2} \mu_2 \left[ \frac{3 \epsilon_2}{2 \epsilon_2 + 1} \right]^2 \left\{ \frac{\mu_1 - \mu_2}{\mu_1 + \mu_2} + \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2} + \frac{2 \epsilon_1 (\epsilon_1 - \epsilon_2 \mu_2)}{\mu_2 (\epsilon_1 + \epsilon_2)^2} \right\}, \tag{48}
\]
and Eq. \( \tag{12} \) has been used to set \( \exp(-2\sqrt{\epsilon_2 \epsilon_2 \xi z_A/c}) \) equal to one. By putting \( \epsilon_2 = \mu_2 = 1 \), Eqs. \( \tag{47} \) and \( \tag{48} \) reduce to those for an atom in free space \( \tag{22} \).

As can be seen from Eqs. \( \tag{46} \)–\( \tag{47} \), one can distinguish two regimes having different power laws. The first regime is where the two contacting media have unequal electric properties. Then the first term in Eq. \( \tag{46} \) dominates and the power law is \( \sim c_A^3 \). The atom is pulled toward (repelled from) the interface if the medium it is located in has stronger (weaker) electric properties than that on the other side of the interface.
In the case of equal electric properties $C_3 = 0$ and $U_2(z_A) = C_1/z_A$ with

$$C_1 = \frac{\mu_0}{16\pi^2} \int_0^\infty d\xi \xi^2 \alpha \left( \frac{3\varepsilon_2}{2\varepsilon_2 + 1} \right) \left( \frac{\mu_2}{\mu_1 + \mu_2} + \frac{1}{2} \right).$$

The atom experiences a force which points away from (toward) the interface if the magnetic properties of the medium the atom is situated in are weaker (stronger) than those of the medium on the other side of the interface.

Note that the dependence of the directions of the forces on the difference in strength of the medium responses is opposite in the two cases of dominantly electric and purely magnetic media. In both cases the strength of the force increases with increasing difference between the electric and magnetic parameters of the contacting media. These results are consistent with earlier ones [8, 30].

A more detailed comparison of our results with those presented in Ref. [3] will be made in the last section. Since the coefficient $C_3$ of the leading-order term depends on electric properties only, the influence of electric properties on the behaviour of the potential tends to dominate that of the magnetic properties, except for the case when the electric properties of the neighboring media are similar. At more moderate distances, competing effects of electric and magnetic properties may create potential walls or wells, as is also evident from the numerical results below.

3. Numerical results

To study the local-field corrected potential at intermediate distances and to elucidate the combined influence of electric and magnetic properties of the media, we calculate the position dependent part $U_2(z_A)$ in accordance with Eq. (20) numerically. A two-level atom of transition frequency $\omega_{ei}$ is assumed and material electric and magnetic properties are described using single-resonance Drude-Lorentz-type permittivities and permeabilities

$$\varepsilon_i(\omega) = 1 + \frac{\omega_{pe}^2}{\omega_{Te}^2 - \omega^2 - i\omega\gamma_{ei}}, \quad \mu_i(\omega) = 1 + \frac{\omega_{p_m}^2}{\omega_{Tm}^2 - \omega^2 - i\omega\gamma_{mi}}, \quad i = 1, 2. \quad (51)$$

Figure 1 (a) illustrates the atom–surface-distance dependence of the $U_2(z_A)$ potential. The interface is at $z_A = 0$, the medium 1 is on the left, while the medium 2 is on the right. The parameters $\varepsilon_1, \mu_1, \mu_2$ are fixed whereas $\varepsilon_2$ takes on three different values of the plasma frequency $\omega_{pe}$. In all three cases $\varepsilon_1$ and $\varepsilon_2$ have same (transverse) resonance frequencies $\omega_{Te}$ and damping constants $\gamma_{ei}$, but different plasma frequencies (i.e., $\varepsilon_1 \neq \varepsilon_2$) and the $z_{A}^{-1}$ term in Eq. (10) is negligibly small. In case (1) $\varepsilon_2 > \varepsilon_1$, it can be seen from the figure that the potential at very short atom–surface distances is repulsive in medium 2 and attractive in medium 1, in consistency with the analytical result (10) and (47). Similarly, in cases (2) and (3) $\varepsilon_2 < \varepsilon_1$, the potential is attractive in medium 2 while repulsive in medium 1. As the atom–surface distance increases, the second term $z_{A}^{-1}$ in the potential (10) gradually comes into play and if the magnetic properties are strong enough, may switch the sign of the potential and create potential walls or wells in the process, as is clearly visible in case (2).

To show how the net effect of the local-field correction depends on the distance and on the properties of the media surrounding the guest atom, we plot the uncorrected potential by dashed lines in Fig. 1 (a), and the
difference between the corrected and uncorrected results in Fig. 1(b). The ratio between the corrected and uncorrected results is not always a good measure of the difference between the two because one of them can vanish. The local-field correction factor \( \frac{3\varepsilon_j / (2\varepsilon_j + 1)}{\varepsilon_j} \) is positive, larger than one, and increases with \( \varepsilon_j \) [\( j \) indicative of the layer containing the guest atom]. It approaches the maximum value of \( 9/4 \) as \( \varepsilon_j \to \infty \). Note that a larger-than-unity local-field correction factor does not necessarily lead to an enhancement of the potential because the uncorrected factor in the integrand can change sign as \( \xi \) varies. The local-field correction has a clear-cut effect of increasing or decreasing the potential only when the uncorrected integrand is purely repulsive or attractive, for which cases (1) and (3) can serve as examples. In the middle case (2), the two curves with and without local-field correction cross, that is, there exists an atom–surface distance at which the effect of the local-field correction is canceled out due to the \( \xi \)-integration. In addition, one can notice that the local-field correction leads a small shift of the position of the peak. Figure 1(b) which shows the difference between the local-field corrected and uncorrected potentials, reveals quite significant corrections of up to 30% of the uncorrected values.

The behaviour of the local-field corrected vdW potential with respect to the static permittivity of the medium the atom is embedded in is shown in Fig. 2 for two different values of the atom–surface distance. Within the scale of the figure, the curves for the larger distance from the interface peak at certain values of \( \varepsilon_2(0) \). The positions of the peaks are different due to the effects of the local field. As \( \omega_{r,\varepsilon_2}/\omega_{10} \) and as a consequence \( \varepsilon_2(0) \) increases, an inspection of the figure reveals that the ratio between the corrected and uncorrected curves tends to the static value of the local-field correction factor \( \frac{3\varepsilon_2(0) / (2\varepsilon_2(0) + 1)}{\varepsilon_2} \) (which lies between 1 and 9/4), in agreement with the analytical analysis given in Sec. III A 1. For the smaller value of the atom–surface distance \( z_{A10}/c = 0.01 \), a crossing point between the corrected and uncorrected curves is observed, where the local-field correction produces no net change.

### B. Layer-dependent constant part

Fig. 3 shows the dependence of the constant part \( U_1 \) of the potential on the real-cavity radius \( R_c \). To gain some insight, we consider the two limiting cases of a purely electric and a purely magnetic material. According to the analytic result \( [9] \), in the first case the leading term is proportional to \( [R_c\omega_{10}/c]^{-3} \), while in the second case the leading term is proportional to \( [R_c\omega_{10}/c]^{-1} \). Thus for small enough \( R_c\omega_{10}/c, [U_1] \) for a pure electric material is generally larger than that for a pure magnetic material - a fact that is confirmed by the figure. It can be seen that \( U_1 < 0 \) in the first case and \( U_1 > 0 \) in the second case, again in agreement with Eq. [9]. The figure also indicates that the magnitude of \( U_1 \), which is entirely due to the local-field correction, decreases with an increasing real-cavity radius, that is, the effects of the local field becomes weaker as the medium becomes more dilute.

For comparison, we also plot the potential \( U_1 \) accord-
ing to the approximate result (dashed curves). It can be seen that for the parameters used in the figure, the approximate result reproduces quite well the exact one, especially in the case of a pure electric material. The agreement in the case of a pure magnetic material is good for very small $R_c\omega_{10}/c$, but worsens as $R_c\omega_{10}/c$ increases.

C. Total vdW potential and its value at the interface

We have separately investigated the position-dependent part $U_2(z_A)$ of the potential, which determines the force acting on the atom, and the constant, layer-dependent part $U_1$, which is related to the local-field correction. For problems such as the transfer of an atom or a small particle through an interface, it is of relevance to evaluate the potential right at the interface. For this purpose, the total value of the potential is needed. In Fig. 4, we have calculated $U_1 + U_2(z_A)$ on both sides of the interface with the medium fixed while the medium 2 varying from vacuum to a more dense medium with balanced electric and magnetic properties. The case represented by dashed line is nothing else rather than case (2) in Fig. 1. Only very short distances $\sqrt{\varepsilon_1\mu_1}z_A\omega_{10}/c \ll 1$ are presented. Since $\varepsilon_1 \neq \varepsilon_2$ in general, the position dependence of the potential at short distances is mostly determined by the $C_{30}$ term which contains $\varepsilon_1 - \varepsilon_2$ in the integrand. Numerical results in the figure are consistent with this and show that the potential is attractive (repulsive) if the atom is located in a medium which is electrically more dilute (dense) than that in the opposite side of the interface. Additional structures in $U_2$ like potential wells or walls are typically overwhelmed by the magnitude of $U_1$. Baring the visual suppression of the potential wells or walls in $U_2$ due to large magnitude of $U_1$, a full potential is more straightforward than $U_2$ alone in predicting the movement of an atom across a surface. Take, for example, case (2) in Fig. 1. An atom located in layer 2 close to the surface will be attracted to it, and if the atom can cross the interface, it will be pushed further away from the surface into layer 1. Fig. 1(dashed line) provides us with some additional information. It shows explicitly that the total potential in layer 2 is higher that in layer 1, by giving the difference between the potentials in the two layers; and it may also help to estimate the amount of energy required for the atom to penetrate into layer 1.

In Fig. 1, we have not displayed the results for distances $|z_A| < R_c\sqrt{|\mu|}$ where the real-cavity model can no longer be applied. This gives rise to a gap between the potentials on the two sides of the interface. To extend our theory so that it can be employed to estimate

![Local-field corrected total vdW potential of a ground-state two-level atom in a magnetodielectric two-layer system as a function of the atom–surface distance.](image)

The potential right at the interface, we suggest that

$$U(z_A = 0) = \frac{1}{2} [U(R_c) + U(-R_c)]$$

$$= -\frac{\hbar}{2\pi^2\varepsilon_0 R_c^2} \int_0^\infty d\xi \alpha \left\{ 12 \left( \frac{\varepsilon_1 - 1}{2\varepsilon_1 + 1} + \frac{\varepsilon_2 - 1}{2\varepsilon_2 + 1} \right) - \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \left[ \frac{1}{\varepsilon_1} \left( \frac{3\varepsilon_1}{2\varepsilon_1 + 1} \right)^2 - \frac{1}{\varepsilon_2} \left( \frac{3\varepsilon_2}{2\varepsilon_2 + 1} \right)^2 \right] \right\}$$

(52)

[recall Eqs. (5), (10), and (17)]. Visually, this means first plotting the potential as a function of the atomic position with respect to surface potential of a molecule of finite size s,

$$U(z_A = 0) = \frac{\hbar}{2\pi^2\varepsilon_0 s^2} \int_0^\infty d\xi \alpha \left\{ \frac{1}{2} \left( \frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} \right) + \frac{1}{3} \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \left( \frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2} \right) \right\}$$

(53)

The second terms in Eqs. (52) and (53), which represent the interface contribution to the potential, agree when setting $s = (\sqrt{16/3}/\pi^{-1/6})R_c \approx 1.4R_c$ and neglecting the local-field correction in Eq. (52) which was not considered in Ref. 31. The first terms, which represent bulk contributions from the two interfacing media, differ in the two approaches, where Eq. (53) still contains self-energy contributions which do not vanish in the vacuum case $\varepsilon_1 = 1$ while Eq. (52) does not. Our result (52)
thus represents an improvement of the previous one in that local-field corrections are taken into account and self-energy contributions have consistently been removed.

IV. THREE-LAYER SYSTEM

A system consisting of an atom in a three-layer planar structure can serve as a prototype for the problem of a small particle near or inside a membrane. The translationally invariant part and position-dependent part of the vdw potential can again be determined in accordance with Eqs. (2) and (20), respectively. If the atom is in one of the two outer layers, Eq. (20) simplifies greatly via either \( r_{j+}^2 = 0 \) or \( r_{j-}^2 = 0 \). If the atom is in the middle layer, the overall form of the potential \( U_2(z_A) \) remains as in Eq. (20) and there exists a term which contains the product \( r_{j-}^2 r_{j+}^2 \) and is position-independent. This position-independent term in \( U_2(z_A) \) is irrelevant when it is the force which is concerned, but has to be kept, together with \( U_1 \), if the potential at the surfaces is of interest. Since the formulas are complicated, we resort to numerical computation.

Figure 5 shows the behaviour of the vdw potential for an atom placed in an asymmetric (left column) and a symmetric (right column) three-layer magnetodielectric structure for different thicknesses of the middle layer. Note that the parameters for layer 1 are the same as those for layer 1 in Fig. 1 and the parameters for layer 3 are vacuum while in the symmetric configuration, layers 2 and 1 have the same characteristics.

Let us first analyse the asymmetric configuration and see how the presence of a third layer on the right, which is vacuum, affects the behaviour of the potential near the 1-2 interface. In case (a) where the middle-layer thickness \( d_2 \omega_{10}/c = 5 \) is the largest among three cases, the behaviour of the potential \( U_2(z_A) \) in the boundary regions is similar to that in the two-layer systems. Near the 1-2 interface, we find a potential well in layer 1 and a potential wall in layer 2, just as in Fig. 1(2). Near the 2-3 interface the potential is repulsive in the more dense medium 2 and attractive in the more dilute medium 3. A new feature appears around the center of the middle layer where a finite potential wall on the left and an attractive one towards the right interface combine to a potential well. Clearly, if an atom at rest is put in the well, it will remain there. When the thickness of the middle layer 2 is reduced, the well becomes more shallow and eventually disappears, as is visible in Figs. 5(b) and (c). For the parameters used in the figure, the potential well in the middle layer occurs when \( d_2 \omega_{10}/c \gg 1 \) and is overwhelmed when \( d_2 \omega_{10}/c \sim 1 \). The curves for the potential can help one to predict the movement of an atom located near or inside a membrane (layer 2). For example, let an atom be initially located in layer 3 (vacuum) of case (a).

First, it will be attracted to the 2-3 interface. If it can be transported through the interface and gather enough momentum going down the slope, it can pass the finite potential wall and is then attracted to the 1-2 interface. After this interface, and maybe some oscillations, it will be suspended in the potential well near the surface.

We now turn to the symmetric configuration (right column of Fig. 5) where the middle layer 2 is sandwiched between two identical layers 1 and 3. The behaviour of the potential on the right is just a mirror image of that on the left with the mirror plane being the one parallel to the surface and passing through the centre of the middle layer. When the thickness of layer 2 is largest \( d_2 \omega_{10}/c = 5 \) [case (d)], we see in layer 2 a combination of two potential walls as found in Fig. 4 with a well in the middle. Thus even as the middle layer is in general less dense than the two surrounding layers in both electric and magnetic aspects, there exists a possibility that an atom initially located in the potential well remains there. With decreasing thickness \( d_2 \), the bottom of the well rises and the two walls eventually merge into one [cases (e) and (f)]. Clearly, in the cases (e) and (f), any atom initially situated in the middle layer will be transported to the
neighboring layers. Numerical computation also shows that the magnitude of the position-independent term in $U_2(z_A)$, i.e., the last term in Eq. (20), is negligible compared to the position-independent terms, due to the small exponential factor.

In Fig. 5, the uncorrected potentials are plotted by dashed lines. In the two outer layers, the effects of the local field almost remain the same as in the two-layer configuration, which can be explained by that the presence of a third layer is screened by the middle layer. For the middle layer, we have found that typically, the local-field correction is most significant around the centre of the layer, as is most manifest in case (f) where a correction $[(U_{2\text{cor}}) - (U_{2\text{uncor}})]/(U_{2\text{uncor}})$ of more than 80% is observed. A variation of the middle layer thickness does not affect much the strength of the local field correction near the surfaces. This can be understood as resulting from the fact that when an atom is located very close to a surface, it will tend to see only the nearest neighboring layer.

If one wish to know the potentials right on the surfaces, one would have to evaluate the full potential $U_1 + U_2(z_A)$ for atom–surface distances large enough such that the macroscopic theory applies, then use it as an input to the procedure proposed in the previous section. Since the position-independent part $U_1$ does not depend on the layer thicknesses, at each surface in a more-than-two-layer system, the results will be closely analogous to those of the two-layer case.

V. DISCUSSION AND SUMMARY

Our results might be of interest in biological applications such as the transfer of a small molecule through a membrane from one cell to another. Earlier theories have been developed to describe the vdW interaction between molecules or small particles and a solvent medium [8]. In particular, such particles were modeled by a small dielectric sphere of radius $R_s$ and (macroscopic) permittivity $\varepsilon_s$. It was found that the nonretarded dispersion potential of such a sphere near the interface of two dielectric media (with the sphere being situated in a medium of permittivity $\varepsilon_2$, and $\varepsilon_1$ denoting the permittivity of the medium on the far side of the interface) is given by

$$U(z_s) = -\frac{h}{16\pi^2 \varepsilon_0^2 z_s^3} \int_0^{\infty} d\xi \frac{\alpha_s \varepsilon_1 - \varepsilon_2}{\varepsilon_2 \varepsilon_1 + \varepsilon_2}. \quad (54)$$

Here, $z_s$ is the distance from the sphere to the surface and

$$\alpha_s(\omega) = 4\pi \varepsilon_0 R_s^3 \varepsilon_2(\omega) \frac{\varepsilon_s(\omega) - \varepsilon_2(\omega)}{\varepsilon_s(\omega) + 2\varepsilon_2(\omega)} \quad (55)$$

is the excess or effective polarisability [32, 33] of the dissolved particle in the medium. This potential already accounts for the fact that the (macroscopic) particle has a finite volume and can hence only move by displacing an equal volume of solvent from its path (with associated pressure forces being present); the excess polarisability and hence also the potential must vanish when a dissolved particle has the same properties as the solvent.

Equation (54) is the macroscopic counterpart of our microscopic equations (10)–(18), where the position-dependent part of our potential for purely dielectric solvent media reads

$$U_2(z_A) = -\frac{h}{16\pi^2 \varepsilon_0^2 z_A^3} \int_0^{\infty} d\xi \frac{\alpha_s}{\varepsilon_2} \left( \frac{3\varepsilon_2}{2\varepsilon_2 + 1} \right)^2 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}. \quad (56)$$

The results from a microscopic description of the particle as a system of bound point charges, leading to our Eq. (54), are thus formally very similar to those from a macroscopic model of the particle as a dielectric sphere, Eq. (55). The main difference is the fact that the microscopic polarisability [8] together with a local-field correction factor appears in Eq. (56), while the macroscopic excess polarisability [35] which effectively accounts for pressure forces enters Eq. (54). Depending on the size of the immersed particle, one of the two models may provide a more realistic description: For very small particles like atoms or small molecules whose size is comparable to the free interspaces between the atoms forming the solvent medium, local-field effects are important while (macroscopic) pressure forces can not even be defined, so that the microscopic result (54) should be used. For larger molecules whose volume covers a region that would otherwise be occupied by a large number of solvent atoms, local-field effects can be neglected while pressure forces become relevant, so Eq. (54) should be given preference.

As an additional difference, note that our microscopic calculation has also given layer-dependent constant contributions to the potential, which are absent in Eq. (54).

Similar considerations apply in the retarded limit, where the macroscopic potential of the small sphere was found to be [8]

$$U(z_s) = -\frac{23hc}{320\pi^2 \varepsilon_0^2 z_s^2} \frac{\alpha_s(0)}{\varepsilon_2^2} \frac{\varepsilon_s(0) - \varepsilon_2(0)}{(\varepsilon_1(0) + \varepsilon_2(0))}. \quad (57)$$

whereas our microscopic result as given by Eqs. (28) and (29) reads

$$U_2(z_A) = \frac{3hc}{64\pi^2 \varepsilon_0^2 z_A^2} \frac{\alpha(0)}{\varepsilon_2^2} \left[ \frac{3\varepsilon_2(0)}{2\varepsilon_2(0) + 1} \right]^2$$

$$\times \int_1^{\infty} dy \left[ \frac{1}{y^2 - 1 + a} \frac{ay - \sqrt{y^2 - 1 + a}}{ay + \sqrt{y^2 - 1 + a}} + \frac{1}{y^2 - 1 + a} \frac{1}{y^2 + \sqrt{y^2 - 1 + a}} \right] \quad (58)$$

$[a = \varepsilon_1(0)/\varepsilon_2(0)]$. In addition to the observations made for the nonretarded limit, the interface-dependent proportionality constants [i.e., the last factors in Eqs. (57) and (58)] are now also different in general, note that they
do agree in the limit of small dielectric contrast between the media, $\chi(0) = \varepsilon_1(0) - \varepsilon_2(0) \ll \varepsilon_2(0)$.

To conclude, we have the local-field corrected vdW potential of a ground state atom embedded in a planar magnetodielectric multilayer system by analytical and numerical means. The theory allows us to extend earlier studies of the same system in two important aspects: first, one can allow for the atom to be embedded in a medium thus making the theory applicable to a larger range of realistic situations; second, the effects of the local-field correction is elucidated.

The formulas for the interaction potential have been derived for an arbitrary number of layers where the case of two- and three-layer systems have been studied in detail. We have shown that the potential can be decomposed into two parts: A layer-dependent constant part which depends on the real cavity radius, i.e., the density of the medium the atom is placed in; and a position-dependent part which contains the local-field correction as a factor in the integral over frequency. For the latter, we have presented retarded and non-retarded limits and the considered case of neighboring media of similar properties. Distance laws have been reestablished with effects of the local field included where the local-field correction has been found to be as high as 80% in certain cases. Further, numerical calculations show that an interplay between electric and magnetic properties of the neighboring media may lead to the appearance of potential wells or walls near the surface. These structures are potentially helpful as a trapping mechanism. Although these structures are much less intense in magnitude than those occurring for an excited atom [28, 29], they are more permanent because an atom in the ground state has an infinitely long lifetime.

The constant part of the potential, which originates from local-field effects, does not contribute to the vdW forces, but it can facilitate our understanding of the movement of an atom near an interface, and is instrumental in our proposed estimate of the on-surface value of the potential: After calculating the total potential in both sides of an interface up to distances equal to the radius of the (real) cavity, beyond which a macroscopic model no longer applies, the average of the two potential values taken at these distances can be regarded as the potential at the interface. Our procedure improves previous similar estimates by including local-field effects and consistently removing self-interactions.

In the case of the three-layer system, emphasis was given to the influence of the thickness of the middle layer. While new features may arise for a very thin middle layer, the behaviour of the potential is simply those at the interfaces combined if the middle layer is thick enough.

Our results, which have been obtained on the basis of an exact, microscopic model of the atom–field coupling, are complementary to previous more macroscopic dispersion potentials of particles modelled as small spheres. The model of preference depends on the size of the particle in the specific situations considered. In the future, efforts should be taken to find a dispersion potential which holds for all possible ranges of particle sizes and includes both the microscopic and macroscopic potentials as limiting cases. Our considerations may easily be extended to other geometries, such as spherically or cylindrically layered host media.

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