Dispersion potentials of paramagnetic atoms in the presence of magnetoelectric media

(Dispersionspotentiale paramagnetischer Atome bei Anwesenheit magnetoelektrischer Medien)

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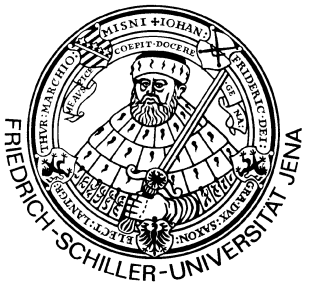

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Chapter 1

Introduction

In free space, in the absence of any electric charge and current, the classical electrodynamics formalism results in traveling waves, which represent the transport of energy from one point to another with the energy density being proportional to the squared of the field amplitude. In particular, in "vacuum", i.e., vanishing electromagnetic field amplitude, this formalism leads to vanishing energy as a trivial consequence. Whereas the quantum electrodynamics (QED), according to the Heisenberg uncertainty principle, predicts a fluctuating zero-point or vacuum field even in the absence of any source, although the field vanishes on average. In other words there is no vacuum in the ordinary sense of nothingness. Vacuum fluctuations of the electromagnetic field is known to be responsible for various phenomena, for example, spontaneous decay, Lamb shift, and dispersion forces, as pure quantum effects. The dispersion interactions are known as the interactions between neutral and unpolarized (but polarizable) objects among atoms[1] and macroscopic bodies. These interactions may be classified into three categories as, the interaction between an atom and a macroscopic body, the interaction between atoms, and the interaction between macroscopic bodies. In this work we are going to focus on the first two categories, briefly referred to as single-atom vdW interaction and two-atom vdW interaction, respectively.

Dispersion interactions play an important role in the understanding of many phenomena, mostly in the field of surface science, such as surface tension [1, 2], adhesion [3], capillarity [4, 5], adsorption of inert gas atoms to a solid surface [6, 7, 8], wetting properties of liquids on such surfaces [8, 9, 10], but also in chemical physics, such as colloidal interactions [1, 11] and stability [12]. The dispersion interactions also play roles in astrophysics, e.g., the dust aggregation leading to form a planet around a star is known to be initiated by these interactions [13]. In biology, the interaction of molecules with cell membranes and cell-membranes interactions leading to cell adhesion are attributed to dispersion forces [14, 15]. Recently, the ability of a gecko to climb on sheer surfaces has been attributed to dispersion forces [16].

To present the motivation for fulfilling the present work, let us first give a brief review on previous theoretical or experimantal studies on the dispersion interactions. Since bringing

[1] Atoms and molecules are briefly referred to as atoms throughout.

the complete list of the studies recorded is very cumbersome and unnecessary, we have selected the ones which we have found to be in close relation to this work.

The vdW interaction potential of two electric[2] atoms in free space was first studied by London in the nonretarded limit, i.e., the atom-atom distances being small compared to the wave length of the relevant fluctuating field, using second-order perturbation theory [17]. In this limit, the interaction may be regarded as being the mutual interaction of the fluctuating electric dipole moments of the atoms. The result is an attractive potential proportional to l^{-6} with l being the interatomic distance. Later, the force on a ground-state electric atom in the presence of a conducting wall was studied by Lennard–Jones [18] treating the atom-wall interaction as the one between the atomic dipole moment and its image in the conducting wall. The result is a z^{-3}-dependent attractive potential with z being the atom-wall separation.

The London formula was extended to arbitrary distances by Casimir and Polder within the framework of full QED using the normal-mode expansion method and calculating the vdW potential as the position-dependent shift of the ground-state energy of the system by fourth-order perturbative calculations [19]. When the interatomic distance exceeds the nonretarded limit, the retardation effects due to the finite speed of light become pronounced and the interaction is due to the ground-state fluctuations of both the atomic dipole moments and the electromagnetic far field. In particular, they found an attractive potential proportional to l^{-7} for large separations (retarded limit). Recently, a closely related Casimir interaction between two magnetoelectric spheres has been studied by means of a scattering method [20], where the inclusion of higher-order multipoles have been shown to lead to corrections of the Casimir–Polder result. Casimir and Polder also considered the potential of an electric atom in the presence of a perfectly conducting wall [19, 21]. Their result is an attractive potential showing a z^{-3}-dependence in the nonretarded limit, in agreement with that of Lennard–Jones, and is proportional to z^{-4} in the retarded limit.

The theory was generalized in many respects, and various factors affecting the interactions were taken into account. It was extended to magnetic atoms by Feinberg and Sucher [22] who studied the retarded interaction of two electromagnetic atoms based on a calculation of photon scattering amplitudes. Their results were later reproduced in Ref. [23] using a zero-point energy technique; It is found that in this limit, the vdW interaction of two magnetic atoms is again an attractive potential proportional to l^{-7}, while for two

[2]Here and henceforth, we refer to the "electrically polarizable" (atoms or media) as "electric". The same with "(para)magnetically polarizable" for which we use the term "magnetic".

atoms of opposed type — one electric and one magnetic — the vdW potential obeys the same power-law, but repulsive. Later on, Feinberg and Sucher extended their formula to arbitrary distances [24]. In particular, in the nonretarded limit the interaction potential of two opposed-type atoms is found to be repulsive and proportional to l^{-4}. The retarded Feinberg–Sucher potential was extended to atoms possessing crossed electric-magnetic polarizabilities on the basis of a duality argument [25]. For the single-atom case, the atom-wall vdW potential — calculated by Casimir and Polder — in the retarded limit was generalized to atoms with both electric and magnetic polarizabilities [23], showing that a magnetic atom is repelled by the conducting wall due to a potential proportional to z^{-4}, in contrast to the attractive potential with the same power-law for electric atoms.

Although in some situations the effect of material environment on the dispersion interactions can be disregarded or approximately equated to the effect of conducting walls (e.g., metal surfaces), when recalculating the nonretarded atom-wall potential in Ref. [26] it was pointed out that a metal surface can be treated as a perfect conductor only when slowly moving charges are dealt with, but in the case of sufficiently fast rotating dipoles a metal behaves like a dielectric body rather than an ideally polarizable structure. Further, to develop the theory to more realistic cases the effect of arbitrarily shaped media on the vacuum fluctuations must be taken into account. To this aim, the normal-mode QED (on which the early studies were based), which requires specifying the geometry of the system at the very beginning of the calculation, is not a suitable method since it is not applicable in the presence of absorption and it has not been fully developed for bodies owning magnetic properties. Moreover, extending the normal-mode QED to various geometries is extremely difficult, even for simple geometries. The single-atom vdW potential of an electric atom in the presence of an electric half-space was first given in Ref. [27] in the nonretarded limit, based on the S-matrix approach. A geometry-independent formula expressing the single- and two-atom vdW potentials of electric atoms in the presence of electric media was first obtained in Ref. [28, 29] based on linear-response theory, in terms of the (classical) Green tensor of the macroscopic Maxwell equations and the polarizabilities of the atoms. Later, the medium-assisted vdW interaction potential between two electric atoms was given by treating the effect of the bodies semiclassically in Refs. [30, 31, 32], and was applied to the case of two atoms placed between two planar perfectly conducting plates [31]. The nonretarded single- and two-atom potentials in the presence of an electric half-space were later derived using the method of image charges [33] and by linear-response formalism [34]. Other

scenarios such as two atoms embedded in bulk magnetoelectric [35] or non-local electric material [36] or placed in front of a metallic [37, 38, 39] or within a planar, electric, three-layer geometry [40], or two anisotropic atoms in front of an electric half-space or within a planar electric cavity [34] have also been studied.

The efforts in extending the theory was not confined to ground-state atoms and zero temperature. The single-atom vdW force on an electric atom in an arbitrary energy-eigenstate in the presence of an electric media was calculated making use of linear-response formalism [41]. Within the framework of macroscopic QED, the dynamics of the single-atom vdW in the presence of magnetoelectric media, abandoning the potential approach, was studied in Ref. [42] via calculating the Lorentz force on an electric atom in an arbitrary energy-eigenstate. The case where an excited atom is in a strong coupling with the electromagnetic field, which may be realized when an excited atom is placed within a cavity or another resonator-like geometry and results in a periodic exchange of excitation between the atom and the field (Rabi oscillations), is studied in Ref. [43]. In studying the effect of finite temperatures, thermal photons have been shown to result in the same power-law as in the zero temperature for the single-atom vdW potential in the presence of a perfectly conducting wall [44], whereas regarding to the two-atom vdW potential, it has been shown that the temperature effects mask the retardation effects as soon as the interatomic separation exceeds the wavelength of the dominant photons, and lead to a change of the free-space result from a l^{-7}- to a l^{-6}-dependence [44, 45, 46, 47, 48]. The situation of two electric atoms between two perfectly conducting plates was later reconsidered taking into account finite temperature effects [49]. The single-atom vdW potential of an excited magnetic atom placed inside a planar cavity for all distance regimes has been studied invoking a full QED treatment [50]. Further studies on the two-atom vdW interaction have included the cases of one [51] or both atoms [52, 53] being excited, leading to potentials that vary as r^{-6} and r^{-2} in the nonretarded and retarded limits, respectively. Modifications of the two-atom interaction due to external fields have been shown to lead to a potential varying as r^{-3} in the nonretarded limit when the applied field is unidirectional [54].

In the three-atom case, a non-additive term prevents the potential from just being the sum of three pairwise contributions, as the presence of each atom modifies the atomic dipole fluctuations in the others; the three-atom dispersion potential in free space was first calculated in the nonretarded limit by pursuing the perturbation calculation to the third order [55, 56, 57] and then extended to arbitrary interatomic distances by using sixth-order

perturbation calculation [58], where the potentials were seen to depend on the relative positions of the atoms in a rather complicated way. A general formula for the non-additive N-atom vdW potential in free space was derived by summing up the response of each atom to the quantized field caused by the other atoms [59] and by calculating the difference in the zero-point energy of the electromagnetic field of a large cavity with and without the atoms [60]. Later on, the nonretarded three-atom vdW potential was derived for the case with one atom being excited [61].

For atoms that are embedded in an optically dense host body or medium, the local electromagnetic field experienced by the atoms differs from the macroscopic one. Hence, the theory of dispersion interactions must be modified by taking local-field corrections into account. One approach to this problem is the real-cavity model, where one assumes that each guest atom is surrounded by a small, empty, spherical cavity [62]. It has been used to study the local-field corrections to the spontaneous decay rate of an atom embedded in an arrangement of magnetoelectric bodies and/or media [63], and was recently applied to obtain local-field corrected formulas for single- and two-atom vdW potentials of electric atoms within such geometries [64]. Local-field corrections to the vdW potentials have also been addressed in Ref. [65].

On the experimental side, the single-atom vdW interaction was traced first time by experiments on the deflexion of a beam of ground-state atoms passing near a dielectric or metal surface [66]. It was found that the attraction vdW force is proportional to z^{-4} for sufficiently small atom-body separations, in agreement with the theoretical results [18, 19, 21]. Similar experiments on an atomic beam passing through two conducting walls showed a strong enhancement of the vdW potential for excited atoms [67], and later it was found that for large atom-plate separations the vdW force on ground-state atoms become proportional to z^{-5} [68] in agreement with the findings of Casimir and Polder [19, 21]. Later, by experiments on selective reflection spectroscopy of optically active atoms near a dielectric surface, the influence of the surface to atomic spectra recorded was attributed to the vdW interaction [69]. The interaction between a single atom and a body has also been explored by means of detecting the intensity of an atomic beam transmitted through a parallel-plate cavity [70], direct force measurement using atomic-mirror techniques [71, 72], measuring the intensity of a diffracted atomic beam from a transmission-grating [73], making use of quantum reflection from a solid surface at nonretarded [74] and retarded [75, 76] atom–surface separations, or determining their effect on the collective oscillation frequency of the

magnetically trapped atoms [77]. Observations of interatomic vdW interactions based on a determination of the scattering cross sections in the atomic collisions between two ground-state atomic beams [78], between an atomic beam and the atoms of a stationary target gas [79, 80], and between a beam of ground-state atoms and a beam of excited atoms [81] have been reported.

As mentioned earlier, in obtaining general results for dispersion interactions, the methods based on linear-response theory overcame the problems which normal-mode QED encounters with, e.g., being applicable for various geometries. On the other hand, since the linear-response approach is not based on an explicit quantization scheme it is less rigorous than the normal-mode QED. This work aims to generalize the medium-assisted single-atom [28, 29, 42, 82] and two-atom vdW potentials found for electric atoms via linear-response theory [28, 29] or semiclassical treatments [30], within the framework of macroscopic QED to the cases where the atoms possess both electric and magnetic polarizabilities.

In chapter 2 we present the quantization scheme for a system consisting of macroscopic magnetoelectric media, electromagnetic field, and charged particles, starting with macroscopic Maxwell equations. By grouping the charged particles into neutral atoms and rewriting the Hamiltonian in the multipolar coupling form, we facilitate expressing the atom-field interaction Hamiltonian in terms of electric and magnetic dipole moments of the atoms using the long-wavelength approximation. In order to describe the paramagnetic properties of the atoms correctly, the spin of the charged particles are included in the formalism [HS5].

In chapter 3 the formula of the vdW potential of a single ground-state atom in the presence of an arbitrary arrangement of magnetoelectric media — previously found for electric atoms — is generalized to atoms with both electric and magnetic polarizabilities, using leading (second) order perturbation theory. The local-field corrections to the formula given in Refs. [64, 65] is also generalized to the case of magnetic atoms [HS5]. The formula is applied to obtain the vdW potential of an atom in the presence of a planar magnetoelectric multilayer system or in the presence of a homogeneous magnetoelectric sphere.

The generalization of the formula of interatomic vdW potential between two ground-state atoms, to atoms having both electric and magnetic polarizabilities is performed using fourth-order perturbation theory in chapter 4 [HS1, HS5], where the local-field corrected formulae for the cases where one or both atoms are embedded in host media are also generalized to paramagnetic atoms [HS5]. The formula is applied to obtain the vdW interaction between two atoms embedded in a bulk magnetoelectric media [HS1, HS5], two atoms in

the presence of a planar magnetoelectric multilayer [HS1], and two atoms in the presence of a homogeneous magnetoelectric sphere [HS4, HS5]. In the multilayer example, particular cases of a perfectly reflecting plate and a thick magnetoelectric plate have been explored with special emphasis on the limiting cases of retarded and nonretarded and specified arrangements of the atoms with respect to the body. To illustrate the effect of the media on the interatomic potentials, numerical results are presented. The body-induced reduction or enhancement in the nonretarded vdW interaction potential (shown by numerical results) is, qualitatively, explained by the method of image charges [HS1, HS3, HS4].

Summary of the main results of this work is given in chapter 5 together with some unaddressed questions as possible subjects of further studies. Long calculations are shifted to separate appendices for the sake of transparency.

Chapter 2

Macroscopic QED in linear media

In studying the dynamics of a system consisting of matter and the electromagnetic field, due to the vast number of the atoms forming the bodies, it is impossible to find the analtytical dynamic properties of each individual atom in such a complex system. However, in cases where the dynamics of the constituents of (continuum) bodies are not of interest, it is useful to devide the matter into a background part and an active part whose dynamics need to be treated more explicitly, e.g., discrete atoms (if present). By means of an averaging procedure, the problem can thus be reduced to the study of the dynamics of each continuum body, the electromagnetic field, and the atoms. A suitable averaging leads to the well-known Maxwell's macroscopic equations where the media enter into account via their constitutive relations.

2.1 Basic formalism

In the frame of macroscopic electrodynamics, the electromagnetic phenomena are governed by the Maxwell equations

$$\boldsymbol{\nabla} \cdot \mathbf{D}(\mathbf{r}) = \rho(\mathbf{r}), \tag{2.1}$$

$$\boldsymbol{\nabla} \times \mathbf{E}(\mathbf{r}) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r}), \tag{2.2}$$

$$\boldsymbol{\nabla} \cdot \mathbf{B}(\mathbf{r}) = 0, \tag{2.3}$$

$$\boldsymbol{\nabla} \times \mathbf{H}(\mathbf{r}) = \mathbf{j}(\mathbf{r}) + \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r}) \tag{2.4}$$

where ρ and $\mathbf{j}$ are free[1] electric-charge and current densities, respectively, $\mathbf{D}$ and $\mathbf{B}$ are displacement and (magnetic) induction fields related to the electric field $\mathbf{E}$ and magnetic field $\mathbf{H}$ as follows

$$\mathbf{D}(\mathbf{r}) = \varepsilon_0 \mathbf{E}(\mathbf{r}) + \mathbf{P}(\mathbf{r}), \tag{2.5}$$

$$\mathbf{B}(\mathbf{r}) = \mu_0[\mathbf{H}(\mathbf{r}) + \mathbf{M}(\mathbf{r})], \tag{2.6}$$

with $\mathbf{P}$ and $\mathbf{M}$ being, respectively, the electric and magnetic polarization of the medium.

[1] In the study of the dispersion interactions, which is the focus of this work, the atoms among the discrete ones and the ones forming the macroscopic bodies have no net charges, so that the free electric-charge density refers to macroscopic excess charges.

Assuming that the response of the media to the electromagnetic field is linear, local, and isotropic, the general relations between the polarizations and the electromagnetic field being in agreement with the causality and fluctuation-dissipation theorem [83] are

$$\mathbf{P}(\mathbf{r},t) = \varepsilon_0 \int_0^\infty \mathrm{d}\tau\, \chi_e(\mathbf{r},\tau)\mathbf{E}(\mathbf{r},t-\tau) + \mathbf{P}_N(\mathbf{r},t), \tag{2.7}$$

$$\mathbf{M}(\mathbf{r},t) = \frac{1}{\mu_0} \int_0^\infty \mathrm{d}\tau\, \chi_m(\mathbf{r},\tau)\mathbf{B}(\mathbf{r},t-\tau) + \mathbf{M}_N(\mathbf{r},t), \tag{2.8}$$

where χ_e and χ_m are given as

$$\chi_e(\mathbf{r},t) = \int_{-\infty}^\infty \mathrm{d}\omega [\varepsilon(\mathbf{r},\omega) - 1] e^{-i\omega t}\,, \tag{2.9}$$

$$\chi_m(\mathbf{r},t) = \int_{-\infty}^\infty \mathrm{d}\omega \left[1 - \frac{1}{\mu(\mathbf{r},\omega)}\right] e^{-i\omega t} \tag{2.10}$$

with $\varepsilon(\mathbf{r},\omega)$ and $\mu(\mathbf{r},\omega)$ being, respectively, the position-dependent complex-valued (relative) electric permittivity and magnetic permeability of the media, with real and imaginary parts — responsible for dispersion and absorption [$\mathrm{Im}\,\varepsilon(\mathbf{r},\omega) > 0$, $\mathrm{Im}\,\mu(\mathbf{r},\omega) > 0$; $\forall\,\mathbf{r}$] — satisfying the Kramers-Kronig relations in accordance with causality [84]. In the cases where empty-space regions are involved, the limits $\mathrm{Im}\,\varepsilon(\mathbf{r},\omega) \to 0$ and $\mathrm{Im}\,\mu(\mathbf{r},\omega) \to 0$ may be performed after taking the expectation values and having the valume integrals performed (if any). This way we allow the electromagnetic filed quantization scheme to be valid for arbitrary arrangemnt of linear, causal magnetoelectric bodies with $\mathrm{Im}\,\varepsilon(\mathbf{r},\omega) \geqslant 0$ and $\mathrm{Im}\,\mu(\mathbf{r},\omega) \geqslant 0$. In Eqs. (2.7) and (2.8), $\mathbf{P}_N$ and $\mathbf{M}_N$ are, respectively, the noise polarization and noise magnetization associated with the absorption. Substituting Eqs. (2.7) and (2.8) into Eqs. (2.5) and (2.6) together with Fourier transformation, leads to the constitutive relations

$$\underline{\mathbf{D}}(\mathbf{r},\omega) = \varepsilon_0 \varepsilon(\mathbf{r},\omega)\underline{\mathbf{E}}(\mathbf{r},\omega) + \underline{\mathbf{P}}_N(\mathbf{r},\omega), \tag{2.11}$$

$$\underline{\mathbf{B}}(\mathbf{r},\omega) = \mu_0 \mu(\mathbf{r},\omega)[\underline{\mathbf{H}}(\mathbf{r},\omega) + \underline{\mathbf{M}}_N(\mathbf{r},\omega)], \tag{2.12}$$

where $\underline{\mathcal{O}}(\,\mathbf{r},\omega)$ denotes the field components of $\mathcal{O}(\mathbf{r})$ in the frequency domain

$$\mathcal{O}(\mathbf{r}) = \int_0^\infty \mathrm{d}\omega\, \underline{\mathcal{O}}(\mathbf{r},\omega) + c.c.\,. \tag{2.13}$$

Using Eqs. (2.11) and (2.12), the Maxwell equations in the case of vanishing free electric charge and current densities are found to be

$$\varepsilon_0 \boldsymbol{\nabla} \cdot \varepsilon(\mathbf{r},\omega)\underline{\mathbf{E}}(\mathbf{r},\omega) = \underline{\rho}_N(\mathbf{r},\omega), \tag{2.14}$$

$$\boldsymbol{\nabla} \times \underline{\mathbf{E}}(\mathbf{r},\omega) = i\omega\mu_0 \mu(\mathbf{r},\omega)[\underline{\mathbf{H}}(\mathbf{r},\omega) + \underline{\mathbf{M}}_N(\mathbf{r},\omega)], \tag{2.15}$$

$$\boldsymbol{\nabla} \cdot \underline{\mathbf{B}}(\mathbf{r}, \omega) = 0, \tag{2.16}$$

$$\boldsymbol{\nabla} \times \underline{\mathbf{H}}(\mathbf{r}, \omega) = -i\omega[\varepsilon_0 \varepsilon(\mathbf{r}, \omega) \underline{\mathbf{E}}(\mathbf{r}, \omega) + \underline{\mathbf{P}}_N(\mathbf{r}, \omega)], \tag{2.17}$$

where the noise charge density ρ_N is defined by

$$\underline{\rho}_N(\mathbf{r}, \omega) = -\boldsymbol{\nabla} \cdot \underline{\mathbf{P}}_N(\mathbf{r}, \omega). \tag{2.18}$$

By combining Eqs. (2.15) and (2.17) it is seen that $\underline{\mathbf{E}}(\,\mathbf{r}, \omega)$ obeys the differential equation

$$\boldsymbol{\nabla} \times \kappa(\mathbf{r}, \omega) \boldsymbol{\nabla} \times \underline{\mathbf{E}}(\mathbf{r}, \omega) - \frac{\omega^2}{c^2} \varepsilon(\mathbf{r}, \omega) \underline{\mathbf{E}}(\mathbf{r}, \omega) = i\omega\mu_0 \underline{\mathbf{j}}_N(\mathbf{r}, \omega), \tag{2.19}$$

[$\kappa(\mathbf{r}, \omega) = 1/\mu(\mathbf{r}, \omega)$] with $\mathbf{j}_N$ being the noise current density introduced as

$$\underline{\mathbf{j}}_N(\mathbf{r}, \omega) = -i\omega \underline{\mathbf{P}}_N(\mathbf{r}, \omega) + \boldsymbol{\nabla} \times \underline{\mathbf{M}}_N(\mathbf{r}, \omega), \tag{2.20}$$

satisfying the continuity equation

$$\boldsymbol{\nabla} \cdot \underline{\mathbf{j}}_N(\mathbf{r}, \omega) - i\omega \underline{\rho}_N(\mathbf{r}, \omega) = 0. \tag{2.21}$$

Representing the solution of Eq. (2.19) in the form suggested by the method of Green function

$$\underline{\mathbf{E}}(\mathbf{r}, \omega) = i\omega\mu_0 \int \mathrm{d}^3\mathbf{r}\, \boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) \cdot \underline{\mathbf{j}}_N(\mathbf{r}', \omega), \tag{2.22}$$

it is seen that the Green tensor $\boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega)$ has to obey the differential equation

$$\boldsymbol{\nabla} \times \kappa(\mathbf{r}, \omega) \boldsymbol{\nabla} \times \boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) - \frac{\omega^2}{c^2} \varepsilon(\mathbf{r}, \omega) \boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) = \boldsymbol{I}\delta(\mathbf{r} - \mathbf{r}') \tag{2.23}$$

[$\boldsymbol{I}$ is unit tensor] together with the boundary condition at infinity

$$\boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) \to \mathbf{0} \quad \text{for} \quad |\mathbf{r} - \mathbf{r}'| \to \infty. \tag{2.24}$$

Note that the electromagnetic and geometric properties of the medium are fully incorporated in the Green tensor via the space- and frequency-dependent permittivity and permeability. In addition, the Green tensor is uniquely defined by Eq. (2.23), analytic in the upper half of the complex-frequency plane, and has the following properties [85]

$$\boldsymbol{G}^*(\mathbf{r}, \mathbf{r}', \omega) = \boldsymbol{G}(\mathbf{r}, \mathbf{r}', -\omega^*), \tag{2.25}$$

$$\boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) = \boldsymbol{G}^{\mathsf{T}}(\mathbf{r}', \mathbf{r}, \omega), \tag{2.26}$$

$$\int \mathrm{d}^3 s \left\{ \mathrm{Im}\kappa(\mathbf{s}, \omega) \left[\boldsymbol{G}(\mathbf{r}, \mathbf{s}, \omega) \times \overleftarrow{\boldsymbol{\nabla}}_s \right] \cdot \left[\boldsymbol{\nabla}_s \times \boldsymbol{G}^*(\mathbf{s}, \mathbf{r}', \omega) \right] + \frac{\omega^2}{c^2} \mathrm{Im}\varepsilon(\mathbf{s}, \omega)\, \boldsymbol{G}(\mathbf{r}, \mathbf{s}, \omega) \cdot \boldsymbol{G}^*(\mathbf{s}, \mathbf{r}', \omega) \right\} = \mathrm{Im}\, \boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega), \tag{2.27}$$

Where the superscript T denotes transposition and $\overleftarrow{\boldsymbol{\nabla}}$ introduces differentiation to the left.

2.2 Electromagnetic field Hamiltonian

So far, the electromagnetic field is expressed in terms of the continuous sets of complex-valued noise polarization $\underline{\mathbf{P}}_N(\mathbf{r},\omega)$ and noise magnetization $\underline{\mathbf{M}}_N(\mathbf{r},\omega)$, which can therefore be considered as playing the role of dynamical variables of the overall system consisting of the electromagnetic field and the medium including the dissipative system. For later uses, it is convenient to split off some factors from the noise fields to define the fundamental dynamical variables $\mathbf{f}_\lambda(\mathbf{r},\omega)$ ($\lambda\in\{e,m\}$) according to

$$\underline{\mathbf{P}}_N(\mathbf{r},\omega)=i\sqrt{\frac{\hbar\varepsilon_0}{\pi}\mathrm{Im}\varepsilon(\mathbf{r},\omega)}\mathbf{f}_e(\mathbf{r},\omega), \tag{2.28}$$

$$\underline{\mathbf{M}}_N(\mathbf{r},\omega)=\sqrt{-\frac{\hbar}{\pi\mu_0}\mathrm{Im}\kappa(\mathbf{r},\omega)}\mathbf{f}_m(\mathbf{r},\omega). \tag{2.29}$$

Now, the transition from classical to quantum theory can be performed by the replacement of the classical fields $\mathbf{f}_\lambda(\mathbf{r},\omega)$ and $\mathbf{f}^*_\lambda(\mathbf{r},\omega)$ by the operator-valued bosonic fields $\hat{\mathbf{f}}_\lambda(\mathbf{r},\omega)$ and $\hat{\mathbf{f}}^\dagger_\lambda(\mathbf{r},\omega)$ which are associated with the excitations of the composed system of the electromagnetic field and the magnetoelectric media and have the following commutation relations

$$\Big[\hat{f}_{\lambda i}(\mathbf{r},\omega),\hat{f}^\dagger_{\lambda' i'}(\mathbf{r}',\omega')\Big]=\delta_{\lambda\lambda'}\delta_{ii'}\delta(\mathbf{r}-\mathbf{r}')\delta(\omega-\omega'), \tag{2.30}$$

$$\Big[\hat{f}_{\lambda i}(\mathbf{r},\omega),\hat{f}_{\lambda' i'}(\mathbf{r}',\omega')\Big]=0 \tag{2.31}$$

(for a similar treatment in quantization scheme see also [86]). The medium-assisted electric field expressed in terms of the bosonic field operators can be obtained by substituting Eq. (2.20) together with Eqs. (2.28) and (2.29) into Eq. (2.22),

$$\hat{\mathbf{E}}(\mathbf{r})=\sum_{\lambda=e,m}\int\mathrm{d}^3r'\int_0^\infty\mathrm{d}\omega\boldsymbol{G}_\lambda(\mathbf{r},\mathbf{r}',\omega)\cdot\hat{\mathbf{f}}_\lambda(\mathbf{r}',\omega)+H.c., \tag{2.32}$$

where

$$\boldsymbol{G}_e(\mathbf{r},\mathbf{r}',\omega)=i\frac{\omega^2}{c^2}\sqrt{\frac{\hbar}{\pi\varepsilon_0}\mathrm{Im}\varepsilon(\mathbf{r}',\omega)}\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega), \tag{2.33}$$

$$\boldsymbol{G}_m(\mathbf{r},\mathbf{r}',\omega)=-i\frac{\omega}{c}\sqrt{-\frac{\hbar}{\pi\varepsilon_0}\mathrm{Im}\kappa(\mathbf{r}',\omega)}\big[\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega)\times\overleftarrow{\boldsymbol{\nabla}}'\big]. \tag{2.34}$$

Note that the integral relation (2.27) can be rewritten as

$$\sum_{\lambda=e,m}\int\mathrm{d}^3s\,\boldsymbol{G}_\lambda(\mathbf{r},\mathbf{s},\omega)\cdot\boldsymbol{G}^{*\mathsf{T}}_\lambda(\mathbf{r}',\mathbf{s},\omega)=\frac{\hbar\mu_0}{\pi}\omega^2\mathrm{Im}\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega). \tag{2.35}$$

To express all other relevant fields in terms of the dynamical variables, one can make use of the Maxwell equations (2.14)–(2.17) and the constitutive relations (2.11) and (2.12)

which leads, for example, for the induction field to

$$\hat{\mathbf{B}}(\mathbf{r}) = \sum_{\lambda=e,m} \int \mathrm{d}^3 r' \int_0^\infty \frac{\mathrm{d}\omega}{i\omega} \boldsymbol{\nabla} \times \boldsymbol{G}_\lambda(\mathbf{r}, \mathbf{r}', \omega) \cdot \hat{\mathbf{f}}_\lambda(\mathbf{r}', \omega) + H.c.\,. \tag{2.36}$$

The correct time dependence of the electromagnetic field, fulfilling the Maxwell equations (2.2) and (2.4) with vanishing current density can be generated from the Heisenberg equation of motion

$$\dot{\hat{\mathcal{O}}} = \frac{1}{i\hbar}[\hat{\mathcal{O}}, \hat{H}], \tag{2.37}$$

by introducing the Hamiltonian of the medium-assisted electromagnetic field as

$$\hat{H}_F = \sum_{\lambda=e,m} \int \mathrm{d}^3 r \int_0^\infty \mathrm{d}\omega\, \hbar\omega\, \hat{\mathbf{f}}_\lambda^\dagger(\mathbf{r}, \omega) \cdot \hat{\mathbf{f}}_\lambda(\mathbf{r}, \omega). \tag{2.38}$$

It should be noted that the formalism presented here is based on the assumption of locally responding media that has been taken into account, in frequency domain, via the constitutive relations (2.11) and (2.12). A more general formalism is given in Ref. [87] with taking into account the spatial dispersion of the media response to the electromagnetic field, from which, our formalism may be recovered for locally responding media. However we restrict our considerations to the local media throughout.

Comparing (2.38) to the Hamiltonian of a set of harmonic oscillators, it turns out that the ground state of the medium-assisted electromagnetic field (vacuum state $|\{0\}\rangle$) can be defined by

$$\hat{\mathbf{f}}_\lambda(\mathbf{r}, \omega)|\{0\}\rangle = \mathbf{0}, \quad \forall\, \lambda, \mathbf{r}, \omega \tag{2.39}$$

and the Hilbert space can be spanned by the Fock states obtained by repeated application of the creation operator $\hat{\mathbf{f}}_\lambda^\dagger(\mathbf{r}, \omega)$ to this vacuum state. In particular, the single quantum excitation and two quanta excitation of the medium-assisted electromagnetic field that will be involved in the calculation of the vdW potentials are given by

$$|\mathbf{1}_\lambda(\mathbf{r}, \omega)\rangle = \hat{\mathbf{f}}_\lambda^\dagger(\mathbf{r}, \omega)|\{0\}\rangle, \tag{2.40}$$

$$|\mathbf{1}_\lambda(\mathbf{r}, \omega), \mathbf{1}_{\lambda'}(\mathbf{r}', \omega')\rangle = \frac{1}{\sqrt{2}} \hat{\mathbf{f}}_\lambda^\dagger(\mathbf{r}, \omega) \hat{\mathbf{f}}_{\lambda'}^\dagger(\mathbf{r}', \omega')|\{0\}\rangle. \tag{2.41}$$

It is worth mentioninig that the introduction of noise variables in Eqs. (2.7) and (2.8) which is due to the lack of precise knowledge of the field sources, differ from the inclusion of the noice operators in QED formalism, where fluctuations are always present due to the Heisenberg uncertainty principle. In particular, classical electromagnetic vacuum does not fluctuate and results in a vanishing field, while in quantum vacuum state, which is an eigenstate of

the Hamiltonian (although not the electric or magnetic field operators), the electric field does not achieve a definite value and is found to have nonzero dispersion, determined by the imaginary part of the Green tensor

$$\begin{aligned}\langle\{0\}|\big[\Delta\hat{\mathbf{E}}(\mathbf{r})\big]^2|\{0\}\rangle &= \langle\{0\}|\hat{\mathbf{E}}^2(\mathbf{r})|\{0\}\rangle - \langle\{0\}|\hat{\mathbf{E}}(\mathbf{r})|\{0\}\rangle \\ &= \frac{\hbar\mu_0}{\pi}\int_0^\infty \mathrm{d}\omega\,\omega^2\mathrm{Tr}[\mathrm{Im}\boldsymbol{G}(\mathbf{r},\mathbf{r},\omega)],\end{aligned} \tag{2.42}$$

and fluctuates around its vanishing mean value

$$\langle\{0\}|\hat{\mathbf{E}}(\mathbf{r})|\{0\}\rangle = 0. \tag{2.43}$$

In order to study the interaction between the electromagnetic field and charged particles it is useful to introduce the scalar potential $\hat{\varphi}$ and vector potential $\hat{\mathbf{A}}$ related to the electric and induction fields as

$$\hat{\mathbf{E}}(\mathbf{r}) = -\boldsymbol{\nabla}\hat{\varphi}(\mathbf{r}) - \dot{\hat{\mathbf{A}}}(\mathbf{r}), \tag{2.44}$$

$$\hat{\mathbf{B}}(\mathbf{r}) = \boldsymbol{\nabla}\times\hat{\mathbf{A}}(\mathbf{r}). \tag{2.45}$$

Obviously, the potentials are not unique and can be chosen in different ways. In Coulomb gauge which is introduced upon suggesting a solenoidal vector potential, $\boldsymbol{\nabla}\cdot\hat{\mathbf{A}}(\mathbf{r}) = 0$, the first and second terms on the right-hand side of Eq. (2.44) correspond to the longitudinal ($||$) and transverse ($\perp$) parts of the electric field where

$$\mathbf{v}^{||(\perp)}(\mathbf{r}) = \int \mathrm{d}^3r'\boldsymbol{\delta}^{||(\perp)}(\mathbf{r}-\mathbf{r}')\cdot\mathbf{v}(\mathbf{r}) \tag{2.46}$$

with

$$\boldsymbol{\delta}^{||}(\mathbf{r}) = -\boldsymbol{\nabla}\boldsymbol{\nabla}\Big(\frac{1}{4\pi r}\Big), \quad \boldsymbol{\delta}^{\perp}(\mathbf{r}) = \delta(\mathbf{r})\boldsymbol{I} - \boldsymbol{\delta}^{||}(\mathbf{r}) \tag{2.47}$$

for an arbitrary vector field $\mathbf{v}(\mathbf{r})$. Therefore, from Eq. (2.44), $\boldsymbol{\nabla}\hat{\varphi}$ and $\hat{\mathbf{A}}$ may be expressed in terms of bosonic variables $\hat{\mathbf{f}}_\lambda$ and $\hat{\mathbf{f}}_\lambda^\dagger$

$$\boldsymbol{\nabla}\hat{\varphi}(\mathbf{r}) = -\sum_{\lambda=e,m}\int \mathrm{d}^3r'\int_0^\infty \mathrm{d}\omega\ {}^{||}\boldsymbol{G}_\lambda(\mathbf{r},\mathbf{r}'\omega).\hat{\mathbf{f}}_\lambda(\mathbf{r}',\omega) + H.c., \tag{2.48}$$

$$\hat{\mathbf{A}}(\mathbf{r}) = \sum_{\lambda=e,m}\int \mathrm{d}^3r'\int_0^\infty \frac{\mathrm{d}\omega}{i\omega}\,{}^{\perp}\boldsymbol{G}_\lambda(\mathbf{r},\mathbf{r}'\omega).\hat{\mathbf{f}}_\lambda(\mathbf{r}',\omega) + H.c., \tag{2.49}$$

where

$${}^{||(\perp)}\boldsymbol{T}(\mathbf{r},\mathbf{r}') = \int \mathrm{d}^3s\ \boldsymbol{\delta}^{||(\perp)}(\mathbf{r}-\mathbf{s})\cdot\boldsymbol{T}(\mathbf{s},\mathbf{r}') \tag{2.50}$$

for an arbitrary tensor field $\boldsymbol{T}(\mathbf{r},\mathbf{r}')$.

2.3 Atomic Hamiltonian

The dynamics of a system consisted of charged particles in the absence of external electromagnetic field, is governed by the Hamiltonian

$$\hat{H}_p = \sum_\alpha \frac{\hat{\mathbf{p}}_\alpha^2}{2m_\alpha} + \frac{1}{8\pi\varepsilon_0}\sum_\alpha\sum_{\beta\neq\alpha}\frac{q_\alpha q_\beta}{|\hat{\mathbf{r}}_\alpha - \hat{\mathbf{r}}_\beta|}\,, \tag{2.51}$$

where q_α and m_α are the electric charge and mass of the particle α, and $\hat{\mathbf{r}}_\alpha$ and $\hat{\mathbf{p}}_\alpha$ are its (operator-valued) position and canonical momentum having following commutation relations

$$\begin{aligned}[\hat{r}_{\alpha i}, \hat{r}_{\beta j}] &= [\hat{p}_{\alpha i}, \hat{p}_{\beta j}] = 0,\\ [\hat{r}_{\alpha i}, \hat{p}_{\beta j}] &= i\hbar\delta_{ij}\delta_{\alpha\beta}\,.\end{aligned} \tag{2.52}$$

In Eq. (2.51) the first term on the right-hand side is the kinetic energy of the system. Although in the present case, the canonical momentum $\hat{\mathbf{p}}_\alpha$ is identical to the kinetic momentum $m_\alpha\dot{\hat{\mathbf{r}}}_\alpha$, this identity does not apply in general. The second term on the right-hand side is the electrostatic potential energy of the system and can be written in terms of the charge density and the Coulomb potential of the system. In particular, in the case where the particles may be grouped into atoms it is useful to introduce center-of-mass and relative coordinates

$$\hat{\mathbf{r}}_A = \sum_{\alpha\in A}\frac{m_\alpha}{m_A}\hat{\mathbf{r}}_\alpha, \quad \hat{\tilde{\mathbf{r}}}_\alpha = \hat{\mathbf{r}}_\alpha - \hat{\mathbf{r}}_A \tag{2.53}$$

for an arbitrary atom A ($m_A = \sum_{\alpha\in A} m_\alpha$) and associated canonical momentums

$$\hat{\mathbf{p}}_A = \sum_{\alpha\in A}\hat{\mathbf{p}}_\alpha, \quad \hat{\tilde{\mathbf{p}}}_\alpha = \hat{\mathbf{p}}_\alpha - \frac{m_\alpha}{m_A}\hat{\mathbf{p}}_A\,. \tag{2.54}$$

This provides rewriting Eq. (2.51) in the form

$$\hat{H}_p = \sum_A \hat{H}_A + \frac{1}{2}\sum_A\sum_{B\neq A}\hat{H}_{AB}, \tag{2.55}$$

where $\hat{H}_A$ and $\hat{H}_{AB}$ are, respectively, the atomic and interatomic Hamiltonians given as

$$\hat{H}_A = \frac{\hat{\mathbf{p}}_A^2}{2m_A} + \sum_{\alpha\in A}\frac{\hat{\tilde{\mathbf{p}}}_\alpha^2}{2m_\alpha} + \frac{1}{2}\int \mathrm{d}^3r\hat{\rho}_A(\mathbf{r})\hat{\varphi}_A(\mathbf{r}) = \frac{\hat{\mathbf{p}}_A^2}{2m_A} + \sum_k E_k^A|k_A\rangle\langle k_A| \tag{2.56}$$

with E_n^A and $|n_A\rangle$ denoting the eigenenergies and energy eigenstates of atomic internal Hamiltonian, $\hat{\rho}_A$ and $\hat{\varphi}_A$ being, respectively, the charge density and the Coulomb potential of atom A

$$\hat{\rho}_A(\mathbf{r}) = \sum_{\alpha\in A} q_\alpha\delta(\mathbf{r} - \hat{\mathbf{r}}_\alpha), \tag{2.57}$$

$$\hat{\varphi}_A(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\int \mathrm{d}^3r' \frac{\hat{\rho}_A(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{4\pi\varepsilon_0}\sum_{\alpha\in A}\frac{q_\alpha}{|\mathbf{r}-\hat{\mathbf{r}}_\alpha|}, \tag{2.58}$$

and

$$\hat{H}_{AB} = \int \mathrm{d}^3r \hat{\rho}_A(\mathbf{r})\hat{\varphi}_B(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\sum_{\alpha\in A}\sum_{\beta\in B}\frac{q_\alpha q_\beta}{|\hat{\mathbf{r}}_\alpha-\hat{\mathbf{r}}_\beta|}. \tag{2.59}$$

It can be inferred easily that the Coulomb potential and the charge density obey the Poisson equation

$$\nabla^2\hat{\varphi}_A(\mathbf{r}) = -\frac{\hat{\rho}_A(\mathbf{r})}{\varepsilon_0}, \tag{2.60}$$

and the continuity relation

$$\dot{\hat{\rho}}_A(\mathbf{r}) + \boldsymbol{\nabla}\cdot\hat{\mathbf{j}}_A(\mathbf{r}) = 0, \tag{2.61}$$

where $\hat{\mathbf{j}}_A$ denotes the atomic current density given by

$$\hat{\mathbf{j}}_A(\mathbf{r}) = \sum_{\alpha\in A}\frac{q_\alpha}{2}\left[\dot{\hat{\mathbf{r}}}_\alpha\delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha) + \delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha)\dot{\hat{\mathbf{r}}}_\alpha\right]. \tag{2.62}$$

Further atomic quantities of interest are the atomic polarization and magnetization

$$\hat{\mathbf{P}}_A(\mathbf{r}) = \sum_{\alpha\in A} q_\alpha\hat{\bar{\mathbf{r}}}_\alpha\int_0^1 \mathrm{d}\sigma\delta(\mathbf{r}-\hat{\mathbf{r}}_A-\sigma\hat{\bar{\mathbf{r}}}_\alpha), \tag{2.63}$$

$$\hat{\mathbf{M}}_A(\mathbf{r}) = \sum_{\alpha\in A}\frac{q_\alpha}{2}\int_0^1 \mathrm{d}\sigma\,\sigma\left[\delta(\mathbf{r}-\hat{\mathbf{r}}_A-\sigma\hat{\bar{\mathbf{r}}}_\alpha)\hat{\bar{\mathbf{r}}}_\alpha\times\dot{\hat{\bar{\mathbf{r}}}}_\alpha - \dot{\hat{\bar{\mathbf{r}}}}_\alpha\times\hat{\bar{\mathbf{r}}}_\alpha\delta(\mathbf{r}-\hat{\mathbf{r}}_A-\sigma\hat{\bar{\mathbf{r}}}_\alpha)\right]. \tag{2.64}$$

As a consequence of these definitions, the atomic charge and current densities can be expressed in terms of the atomic polarization and magnetization as follows:

$$\hat{\rho}_A(\mathbf{r}) = -\boldsymbol{\nabla}\cdot\hat{\mathbf{P}}_A(\mathbf{r}), \tag{2.65}$$

$$\hat{\mathbf{j}}_A(\mathbf{r}) = \dot{\hat{\mathbf{P}}}_A(\mathbf{r}) + \boldsymbol{\nabla}\times\hat{\mathbf{M}}_A(\mathbf{r}) + \frac{1}{2}\boldsymbol{\nabla}\times\left[\hat{\mathbf{P}}_A(\mathbf{r})\times\dot{\hat{\mathbf{r}}}_A - \dot{\hat{\mathbf{r}}}_A\times\hat{\mathbf{P}}_A(\mathbf{r})\right], \tag{2.66}$$

where the third term in Eq. (2.66) is the Röntgen current density [88, 89] due to the center-of-mass motion of the atom.

2.4 Atom-field interaction Hamiltonian

For a system consisting of atoms and a medium-assisted electromagnetic field the Hamiltonian can be obtained by summing H_F and H_p and taking into account the atom-field interaction Hamiltonian. As it is discussed extensively in Refs. [85, 42, 90] this can be done by adding the Coulomb interaction between atomic charges and the medium-assisted elctromagnetic field and replacing $\hat{\mathbf{p}}_\alpha$ with $\hat{\mathbf{p}}_\alpha - q_\alpha\hat{\mathbf{A}}(\hat{\mathbf{r}}_\alpha)$ (in Coulomb gauge) according to the

principle of minimal atom-field coupling. In order to describe correctly the paramagnetic properties of the atoms, it is crucial to take into consideration the spins of their constituents. Therefore, for each particle α, in addition to mass m_α and charge q_α, we denote its spin by $\hat{\mathbf{s}}_\alpha$ that gives rise to a magnetic dipole moment $\gamma_\alpha \hat{\mathbf{s}}_\alpha$ with γ_α being the gyromagnetic ratio of the particle [$\gamma_e = -eg_e/(2m_e)$ for electrons with $-e$: electron charge; $g_e \simeq 2$, electric g-factor; m_e: electron mass]. Hence, for the abovementioned system the Hamiltonian has to include a Pauli term describing the interaction between the spins and the induction field [HS5], viz.,

$$\begin{aligned}\hat{H} = &\sum_{\lambda=e,m} \int \mathrm{d}^3 r \int_0^\infty \mathrm{d}\omega\, \hbar\omega\, \hat{\mathbf{f}}_\lambda^\dagger(\mathbf{r},\omega)\cdot\hat{\mathbf{f}}_\lambda(\mathbf{r},\omega) + \sum_A \sum_{\alpha\in A} \frac{1}{2m_\alpha}\left[\hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}(\hat{\mathbf{r}}_\alpha)\right]^2 \\ &+ \sum_A \int \mathrm{d}^3 r \hat{\rho}_A(\mathbf{r})\hat{\varphi}(\mathbf{r}) + \frac{1}{2}\sum_A \sum_B \int \mathrm{d}^3 r \hat{\rho}_A(\mathbf{r})\hat{\varphi}_B(\mathbf{r}) - \sum_A \sum_{\alpha\in A} \gamma_\alpha\, \hat{\mathbf{s}}_\alpha \cdot \hat{\mathbf{B}}(\mathbf{r}_\alpha).\end{aligned} \tag{2.67}$$

With $\hat{H}_F$, $\hat{H}_A$, and $\hat{H}_{AB}$ given by Eqs. (2.38), (2.56), and (2.59), respectively, Eq. (2.67) can be written as

$$\hat{H} = \hat{H}_F + \sum_A \hat{H}_A + \frac{1}{2}\sum_A \sum_{B\neq A} \hat{H}_{AB} + \sum_A \hat{H}_{AF}\,, \tag{2.68}$$

where

$$\hat{H}_{AF} = \int \mathrm{d}^3 r \hat{\rho}_A(\mathbf{r})\hat{\varphi}(\mathbf{r}) - \sum_{\alpha\in A} \frac{q_\alpha}{m_\alpha}\hat{\mathbf{p}}_\alpha \cdot \hat{\mathbf{A}}(\hat{\mathbf{r}}_\alpha) + \sum_{\alpha\in A} \frac{q_\alpha^2}{2m_\alpha}\hat{\mathbf{A}}^2(\hat{\mathbf{r}}_\alpha) - \sum_{\alpha\in A} \gamma_\alpha\, \hat{\mathbf{s}}_\alpha \cdot \hat{\mathbf{B}}(\hat{\mathbf{r}}_\alpha) \tag{2.69}$$

is the atom-field interaction Hamiltonian. The last term on the right-hand side of (2.69) is the newly introduced Pauli interaction [HS5].

The electric and displacement fields are not affected by the spin of the particles but by their charges, so that the total fields are given by

$$\hat{\boldsymbol{\mathcal{E}}}(\mathbf{r}) = \hat{\mathbf{E}}(\mathbf{r}) - \sum_A \boldsymbol{\nabla}\hat{\varphi}_A(\mathbf{r}), \tag{2.70}$$

$$\hat{\boldsymbol{\mathcal{D}}}(\mathbf{r}) = \hat{\mathbf{D}}(\mathbf{r}) - \varepsilon_0 \sum_A \boldsymbol{\nabla}\hat{\varphi}_A(\mathbf{r}), \tag{2.71}$$

while the total induction and magnetic fields remain equal to the medium-assisted ones

$$\hat{\boldsymbol{\mathcal{B}}}(\mathbf{r}) = \hat{\mathbf{B}}(\mathbf{r}), \quad \hat{\boldsymbol{\mathcal{H}}}(\mathbf{r}) = \hat{\mathbf{H}}(\mathbf{r}). \tag{2.72}$$

Further, the atomic current density given by Eq. (2.62) for spinless particles, in the presence of spin has to be generalized to

$$\hat{\mathbf{j}}_A(\mathbf{r}) = \sum_{\alpha\in A} \frac{q_\alpha}{2}\left[\dot{\hat{\mathbf{r}}}_\alpha \delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha) + \delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha)\dot{\hat{\mathbf{r}}}_\alpha\right] - \sum_{\alpha\in A} \gamma_\alpha \hat{\mathbf{s}}_\alpha \times \boldsymbol{\nabla}\delta(\mathbf{r}-\hat{\mathbf{r}}_\alpha). \tag{2.73}$$

Note that

$$m_\alpha \dot{\hat{\mathbf{r}}}_\alpha = \hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}(\hat{\mathbf{r}}_\alpha), \tag{2.74}$$

as it can be verified easily by using the Heisenberg equation of motion for $\hat{\mathbf{r}}_\alpha$. Since the current density associated with the spin is transverse, the continuity relation (2.61) remains valid. Moreover, the atomic charge and current densities are still related to the atomic polarization and magnetization via Eqs. (2.65) and (2.66) with the atomic magnetization being modified as

$$\begin{aligned}\hat{\mathbf{M}}_A(\mathbf{r}) =& \sum_{\alpha\in A} \frac{q_\alpha}{2} \int_0^1 \mathrm{d}\sigma\, \sigma \left[\delta(\mathbf{r} - \hat{\mathbf{r}}_A - \sigma\hat{\tilde{\mathbf{r}}}_\alpha)\hat{\tilde{\mathbf{r}}}_\alpha \times \dot{\hat{\tilde{\mathbf{r}}}}_\alpha - \dot{\hat{\tilde{\mathbf{r}}}}_\alpha \times \hat{\tilde{\mathbf{r}}}_\alpha \delta(\mathbf{r} - \hat{\mathbf{r}}_A - \sigma\hat{\tilde{\mathbf{r}}}_\alpha)\right] \\ &+ \sum_{\alpha\in A} \gamma_\alpha \hat{\mathbf{s}}_\alpha \delta(\mathbf{r} - \hat{\mathbf{r}}_\alpha).\end{aligned} \tag{2.75}$$

The consistency of the Hamiltonian (2.67) can be verified by showing that it leads to correct time-dependence for the electromagnetic field

$$\boldsymbol{\nabla} \times \hat{\boldsymbol{\mathcal{E}}}(\mathbf{r}) = -\frac{\partial}{\partial t}\hat{\boldsymbol{\mathcal{B}}}(\mathbf{r}), \tag{2.76}$$

$$\boldsymbol{\nabla} \times \hat{\boldsymbol{\mathcal{H}}}(\mathbf{r}) = \sum_A \hat{\mathbf{j}}_A(\mathbf{r}) + \frac{\partial}{\partial t}\hat{\boldsymbol{\mathcal{D}}}(\mathbf{r}) \tag{2.77}$$

and the Newton equations of motion for the particles

$$m_\alpha \ddot{\hat{\mathbf{r}}}_\alpha = q_\alpha \hat{\boldsymbol{\mathcal{E}}}(\hat{\mathbf{r}}_\alpha) + \frac{q_\alpha}{2}\left[\dot{\hat{\mathbf{r}}}_\alpha \times \hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\alpha) - \hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\alpha) \times \dot{\hat{\mathbf{r}}}_\alpha\right] + \gamma_\alpha \boldsymbol{\nabla}_\alpha \left[\hat{\mathbf{s}}_\alpha \cdot \hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\alpha)\right] \tag{2.78}$$

(Appendix A). In Eq. (2.78) the first two term on the right-hand side represent the Lorentz force on the charged particles and the third term is the Zeeman force resulting from the action of the induction field on the particle spins.

In most cases of interest the atoms can be assumed to be small compared to the wave length of the relevant electromagnetic field and hence it is useful to employ center-of-mass and relative coordinates (2.53) and apply the long wave-length approximation. This can be done by performing a Taylor expansion for the atom-field interaction Hamiltonian (2.69) in the center-of-mass of the atoms and keeping the leading-order terms. For neutral atoms ($\sum_{\alpha\in A} q_\alpha = 0$) this leads to [42, HS5]

$$\hat{H}_{AF} = -\hat{\mathbf{d}}_A \cdot \hat{\mathbf{E}}^{||}(\hat{\mathbf{r}}_A) - \sum_{\alpha\in A} \frac{q_\alpha}{m_\alpha} \hat{\mathbf{p}}_\alpha \cdot \hat{\mathbf{A}}(\hat{\mathbf{r}}_A) + \sum_{\alpha\in A} \frac{q_\alpha^2}{2m_\alpha} \hat{\mathbf{A}}^2(\hat{\mathbf{r}}_A) - \sum_{\alpha\in A} \gamma_\alpha\, \hat{\mathbf{s}}_\alpha \cdot \hat{\mathbf{B}}(\hat{\mathbf{r}}_A), \tag{2.79}$$

where

$$\hat{\mathbf{d}}_A = \sum_{\alpha\in A} q_\alpha \hat{\mathbf{r}}_\alpha = \sum_{\alpha\in A} q_\alpha \hat{\tilde{\mathbf{r}}}_\alpha \tag{2.80}$$

is the electric dipole moment of the atom which emerges from the atomic polarization (2.63) in this approximation. In analogy to Eq. (2.80), one can introduce the magnetic dipole moment of the atom arising from Eq. (2.64) as

$$\hat{\mathbf{m}}_A = \sum_{\alpha\in A}\left[\frac{q_\alpha}{2}\hat{\mathbf{r}}_\alpha \times \dot{\hat{\mathbf{r}}}_\alpha + \gamma_\alpha \hat{\mathbf{s}}_\alpha\right] = \sum_{\alpha\in A}\left[\frac{q_\alpha}{2}\hat{\tilde{\mathbf{r}}}_\alpha \times \dot{\hat{\tilde{\mathbf{r}}}}_\alpha + \gamma_\alpha \hat{\mathbf{s}}_\alpha\right]. \tag{2.81}$$

Due to the large number of atom-field and atom-atom interaction terms, the Hamiltonian (2.67) is not very practical for calculations. It can be represented in a proper form, known as multipolar-coupling Hamiltonian, by applying the Power–Zienau–Woolley transformation [91, 92] on the variables, which is defined according to

$$\hat{\mathcal{O}}' = \hat{U}\hat{\mathcal{O}}\hat{U}^\dagger \tag{2.82}$$

with $\hat{U}$ being the unitary operator defined as

$$\hat{U} = \exp\left[\frac{i}{\hbar}\sum_A \int \mathrm{d}^3 r \hat{\mathbf{P}}_A(\mathbf{r})\cdot\hat{\mathbf{A}}(\mathbf{r})\right]. \tag{2.83}$$

In Eqs. (2.32), (2.36), (2.48), and (2.49) the fields are given as linear expressions in terms of the fundamental variables $\hat{\mathbf{f}}_\lambda$ and $\hat{\mathbf{f}}_\lambda^\dagger$ and hence the transformed fields will have the same form but in terms of the transformed variables $\hat{\mathbf{f}}'_\lambda$ and $\hat{\mathbf{f}}'^\dagger_\lambda$. Using (2.82) together with (2.83) and exploiting the Baker-Hausdorff lemma

$$\mathrm{e}^{\hat{S}}\hat{O}\mathrm{e}^{-\hat{S}} = \hat{O} + [\hat{S},\hat{O}] + \frac{1}{2!}[\hat{S},[\hat{S},\hat{O}]] + \dots, \tag{2.84}$$

it will be found that

$$\hat{\mathbf{f}}'_\lambda(\mathbf{r},\omega) = \hat{\mathbf{f}}_\lambda(\mathbf{r},\omega) + \frac{1}{\hbar\omega}\sum_A \int \mathrm{d}^3 r' \hat{\mathbf{P}}_A^\perp(\mathbf{r}')\cdot \boldsymbol{G}^*_\lambda(\mathbf{r}',\mathbf{r},\omega). \tag{2.85}$$

The multipolar Hamiltonian can be obtained by rewriting the Hamiltonian (2.67) in terms of the transformed variables. In particular, for neutral atoms it is found to be (cf. Ref. [42])

$$\begin{aligned}\hat{H} = {} & \sum_{\lambda=e,m}\int \mathrm{d}^3 r \int_0^\infty \mathrm{d}\omega\, \hbar\omega\, \hat{\mathbf{f}}'^\dagger_\lambda(\mathbf{r},\omega)\cdot\hat{\mathbf{f}}'_\lambda(\mathbf{r},\omega) + \sum_A\sum_{\alpha\in A}\frac{1}{2m_\alpha}\left[\hat{\mathbf{p}}'_\alpha + \int \mathrm{d}^3 r \hat{\boldsymbol{\Xi}}'_\alpha \times \hat{\mathbf{B}}'(\mathbf{r})\right]^2 \\ & - \sum_A \int \mathrm{d}^3 r \hat{\mathbf{P}}'_A(\mathbf{r})\cdot\hat{\mathbf{E}}'(\mathbf{r}) + \frac{1}{2\varepsilon_0}\sum_A\sum_B\int \mathrm{d}^3 r \hat{\mathbf{P}}'_A(\mathbf{r})\cdot\hat{\mathbf{P}}'_B(\mathbf{r}) - \sum_A\sum_{\alpha\in A}\gamma_\alpha\,\hat{\mathbf{s}}'_\alpha\cdot\hat{\mathbf{B}}'(\mathbf{r}_\alpha),\end{aligned} \tag{2.86}$$

where

$$\hat{\boldsymbol{\Xi}}'_\alpha(\mathbf{r}) = q_\alpha\hat{\tilde{\mathbf{r}}}'_\alpha\int_0^1 \mathrm{d}\sigma\,\sigma\delta(\mathbf{r}-\hat{\mathbf{r}}'_A-\sigma\hat{\tilde{\mathbf{r}}}'_\alpha) - \frac{m_\alpha}{m_A}\sum_{\beta\in A} q_\beta\hat{\tilde{\mathbf{r}}}'_\beta\int_0^1 \mathrm{d}\sigma\,\sigma\delta(\mathbf{r}-\hat{\mathbf{r}}'_A-\sigma\hat{\tilde{\mathbf{r}}}'_\alpha) + \frac{m_\alpha}{m_A}\hat{\mathbf{P}}'_A(\mathbf{r}) \tag{2.87}$$

and the transformed electric field is found to have the physical meaning of a displacement field with respect to the atomic polarizations

$$\hat{\mathbf{E}}'(\mathbf{r}) = \hat{\mathbf{E}}(\mathbf{r}) + \sum_A \frac{\hat{\mathbf{P}}_A^{\perp}(\mathbf{r})}{\varepsilon_0}\,. \tag{2.88}$$

Note that since the quantities $\hat{\tilde{\mathbf{r}}}_\alpha$, $\hat{\mathbf{s}}_\alpha$, $\hat{\mathbf{P}}_A$ and $\hat{\mathbf{A}}$ commute with both $\hat{\mathbf{P}}_A$ and $\hat{\mathbf{A}}$, they remain unchanged under the transformation (2.82)

$$\hat{\tilde{\mathbf{r}}}'_\alpha = \hat{\tilde{\mathbf{r}}}_\alpha, \quad \hat{\mathbf{r}}'_A = \hat{\mathbf{r}}_A, \quad \hat{\mathbf{s}}'_\alpha = \hat{\mathbf{s}}_\alpha, \quad \hat{\mathbf{P}}'_A(\mathbf{r}) = \hat{\mathbf{P}}_A(\mathbf{r}), \quad \hat{\mathbf{B}}'(\mathbf{r}) = \hat{\mathbf{B}}(\mathbf{r}). \tag{2.89}$$

On the right-hand side of Eq. (2.86), the term in the squared brackets is equal to the mechanical momentum $\hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}(\hat{\mathbf{r}}_\alpha)$ and the fourth term is comprised of the terms associated with the internal Hamiltonian of the atoms ($A = B$) and the terms associated with the interatomic Hamiltonians ($A \neq B$). The latter can be ignored in the cases where the atoms are well separated from each other, i.e.,

$$\int \mathrm{d}^3 r\, \hat{\mathbf{P}}'_A(\mathbf{r}) \cdot \hat{\mathbf{P}}'_B(\mathbf{r}) = \delta_{AB} \int \mathrm{d}^3 r\, \hat{\mathbf{P}}'^2_A(\mathbf{r}), \tag{2.90}$$

thus, as one of the advantages of multipolar formalism, the interaction between the atoms contributes to the Hamiltonian (only) via the electromagnetic field implicitly, and hence the Hamiltonian (2.86) may be written as

$$\hat{H} = \hat{H}'_F + \sum_A \hat{H}'_A + \sum_A \hat{H}'_{AF}, \tag{2.91}$$

where

$$\hat{H}'_F = \sum_{\lambda=e,m} \int \mathrm{d}^3 r \int_0^\infty \mathrm{d}\omega\, \hbar\omega\, \hat{\mathbf{f}}^{\dagger\prime}_\lambda(\mathbf{r},\omega) \cdot \hat{\mathbf{f}}'_\lambda(\mathbf{r},\omega), \tag{2.92}$$

$$\hat{H}'_A = \sum_{\alpha\in A} \frac{\hat{\mathbf{p}}'^2_\alpha}{2m_\alpha} + \frac{1}{2\varepsilon_0} \int \mathrm{d}^3 r\, \hat{\mathbf{P}}'^2_A(\mathbf{r}) = \frac{\hat{\mathbf{p}}'^2_A}{2m_A} + \sum_k E_k^{A'} |k'_A\rangle\langle k'_A|, \tag{2.93}$$

$$\begin{aligned}\hat{H}'_{AF} = &- \int \mathrm{d}^3 r\, \hat{\mathbf{P}}'_A(\mathbf{r}) \cdot \hat{\mathbf{E}}'(\mathbf{r}) - \int \mathrm{d}^3 r\, \hat{\mathbf{M}}'_A(\mathbf{r}) \cdot \hat{\mathbf{B}}'(\mathbf{r}) + \sum_{\alpha\in A} \frac{1}{2m_\alpha} \left[\int \mathrm{d}^3 r\, \hat{\boldsymbol{\Xi}}'_\alpha \times \hat{\mathbf{B}}'(\mathbf{r})\right]^2 \\ &+ \frac{1}{m_A} \int \mathrm{d}^3 r\; \hat{\mathbf{p}}'_\alpha \cdot \hat{\mathbf{P}}'_A(\mathbf{r}) \times \hat{\mathbf{B}}'(\mathbf{r}),\end{aligned} \tag{2.94}$$

with $\hat{\mathbf{M}}'_A$ being the (transformed) magnetization of the atom

$$\begin{aligned}\hat{\mathbf{M}}'_A(\mathbf{r}) = &\sum_{\alpha\in A} \frac{q_\alpha}{2m_\alpha} \int_0^1 \mathrm{d}\sigma\, \sigma \left[\delta(\mathbf{r} - \hat{\mathbf{r}}'_A - \sigma\hat{\tilde{\mathbf{r}}}'_\alpha)\hat{\tilde{\mathbf{r}}}'_\alpha \times \hat{\tilde{\mathbf{p}}}'_\alpha - \hat{\tilde{\mathbf{p}}}'_\alpha \times \hat{\tilde{\mathbf{r}}}'_\alpha \delta(\mathbf{r} - \hat{\mathbf{r}}'_A - \sigma\hat{\tilde{\mathbf{r}}}'_\alpha)\right] \\ &+ \sum_{\alpha\in A} \gamma_\alpha \hat{\mathbf{s}}'_\alpha \delta(\mathbf{r} - \hat{\mathbf{r}}'_\alpha).\end{aligned} \tag{2.95}$$

Needless to say that since the multipolar- and minimal-coupling Hamiltonians are the same, the eigenenergies of the total system remain the same in both formalism as well as the equation of motion of the physical variables. However the decomposition of the Hamiltonian into parts as field, atomic, atom-atom interactions, and atom-field interactions is different in the two formalism, hence the eigenstates of the medium-assisted field in the multipolar scheme, differ from the eigenstates of $\hat{H}_F$. In particular, the ground state of the medium-assisted field in multipolar formalism is defined by [cf. Eq. (2.39)]

$$\hat{\mathbf{f}}'_\lambda(\mathbf{r},\omega)|\{0'\}\rangle = \mathbf{0}, \quad \forall\,\lambda,\mathbf{r},\omega\,. \tag{2.96}$$

Similarly the eigenstates $|k'_A\rangle$ of $\hat{H}'_A$ are different from the eigenstates $|k_A\rangle$ of $\hat{H}_A$.

Again, in the long wave-length approximation, retaining the leading-order terms in the relative coordinates, Eq. (2.94) can be presented as

$$\begin{aligned}\hat{H}'_{AF} =& -\hat{\mathbf{d}}'_A\cdot\hat{\mathbf{E}}'(\hat{\mathbf{r}}'_A) - \hat{\mathbf{m}}'_A\cdot\hat{\mathbf{B}}'(\hat{\mathbf{r}}'_A) + \sum_{\alpha\in A}\frac{q_\alpha^2}{8m_\alpha}\left[\hat{\tilde{\mathbf{r}}}'_\alpha\times\hat{\mathbf{B}}'(\hat{\mathbf{r}}'_A)\right]^2 + \frac{3}{8m_A}\left[\hat{\mathbf{d}}'_A\times\hat{\mathbf{B}}'(\hat{\mathbf{r}}'_A)\right]^2\\ &+\frac{1}{m_A}\hat{\mathbf{p}}'_A\cdot\hat{\mathbf{d}}'_A\times\hat{\mathbf{B}}'(\hat{\mathbf{r}}'_A),\end{aligned} \tag{2.97}$$

where

$$\hat{\mathbf{d}}'_A = \sum_{\alpha\in A} q_\alpha\hat{\tilde{\mathbf{r}}}'_\alpha = \hat{\mathbf{d}}_A, \quad \hat{\mathbf{m}}'_A = \sum_{\alpha\in A}\left[\frac{q_\alpha}{2m_\alpha}\hat{\tilde{\mathbf{r}}}'_\alpha\times\hat{\tilde{\mathbf{p}}}'_\alpha + \gamma_\alpha\hat{\mathbf{s}}'_\alpha\right]. \tag{2.98}$$

Equation (2.97) exhibits one other advantage of using the multipolar formalism as it facilitates expansion of the atom-field interaction Hamiltonian in terms of atomic dipole moments. The first two terms in Eq. (2.97) are the electric and magnetic dipole interactions, respectively, the next two terms represent the diamagnetic interaction and the last term is the Röntgen interaction due to the translational motion of center-of-mass, which becomes important when studying dissipative forces such as quantum friction [93] and can be omitted for nonrelativistic motion. Hence, ignoring the diamagnetic properties of the atoms, the atom-field interaction Hamiltonian in multipolar formalism reduces to

$$\hat{H}'_{AF} = -\hat{\mathbf{d}}'_A\cdot\hat{\mathbf{E}}'(\hat{\mathbf{r}}'_A) - \hat{\mathbf{m}}'_A\cdot\hat{\mathbf{B}}'(\hat{\mathbf{r}}'_A). \tag{2.99}$$

Chapter 3

van der Waals potential of a single atom

It is well known that a neutral atom in the presence of macroscopic bodies is subject to a force, known as the van der Waals (vdW) force, even if both atom and medium-assisted electromagnetic field are in their ground states. According to the well-known concept of Casimir and Polder [19, 21], the vdW force on an atom A at a given position $\mathbf{r}_A$ can be derived from the associated vdW potential $U(\mathbf{r}_A)$ according to

$$\mathbf{F}(\mathbf{r}_A) = -\boldsymbol{\nabla}_A U(\mathbf{r}_A). \tag{3.1}$$

3.1 General expression

The Hamiltonian for a system consisting of an atom with nonrelativistic center-of-mass motion and the medium-assisted electromagnetic field, in electric dipole approximation, as shown in chapter 2, can be presented in the form

$$\hat{H} = \hat{H}_F + \hat{H}_A + \hat{H}_{AF}, \tag{3.2}$$

with $\hat{H}_F$, $\hat{H}_A$, and $\hat{H}_{AF}$ being given by Eqs. (2.92), (2.93), and (2.99) (note that here and in the following, we drop all the primes indicating Power–Zienau–Woolley transformation). We apply the Born-Oppenheimer approximation that follows from the inertia of electrons to be negligible in comparison to the atom to which they are bound; the fast electronic motion can thus be assumed to be uncoupled to the slow center-of-mass motion of the atom. By this approximation the operator-valued center-of-mass posintion $\hat{\mathbf{r}}_A$ may be replaced by real-valued $\mathbf{r}_A$, and the atomic Hamiltonian $\hat{H}_A$ can thus, effectively, be thought of as being the internal Hamiltonian of the atom

$$\hat{H}_A = \sum_k E_k^A |k_A\rangle\langle k_A|. \tag{3.3}$$

Let us assume that both the atom and the electromagnetic field are prepared in their unperturbed ground states and consider $\hat{H}_A + \hat{H}_F$ as the unperturbed Hamiltonian such that the unperturbed state of the combined system is given as $|0\rangle = |0_A\rangle|\{0\}\rangle$. Due to the atom-field coupling, the ground-state energy of the combined system is expected to have a shift that can be deduced from a perturbative calculation for sufficiently weak atom-field

coupling[1], by treating $\hat{H}_{AF}$ as the perturbation. The vdW potential will be the position-dependent part of this energy shift

$$\Delta E = \langle 0|\hat{H}_{AF}|0\rangle - \sum_{I\neq 0} \frac{\langle 0|\hat{H}_{AF}|I\rangle\langle I|\hat{H}_{AF}|0\rangle}{E_I - E_0} + \dots \tag{3.4}$$

with the summation on the right-hand side including position and frequency integrals. Recalling the interaction Hamiltonian (2.99), since the electric and magnetic dipole moments have no diagonal matrix element in the basis of atomic eigenstates, and each of electric and magnetic fields may be given as linear combinations of $\hat{\mathbf{f}}_\lambda(\mathbf{r},\omega)$ and $\hat{\mathbf{f}}^\dagger_\lambda(\mathbf{r},\omega)$ [Eqs. (2.32) and (2.36)], it can be seen that the first term on the right-hand side of Eq. (3.4) (first-order energy shift) vanishes and the vdW potential follows from the second-order energy shift. Further, it can be seen that only intermediate states in which the atom is in an excited state and a single quantum of the fundamental field is excited contribute to the sum. In other words the matrix element $\langle 0|\hat{H}_{AF}|I\rangle$ may be thought of as being related to virtual processes consisted of one photon exchange between the atom and the electromagnetic field together with a transition (from the ground state to an excited state or vice versa) in the atom. Hence Eq. (3.4) may be specified to

$$\Delta E = -\frac{1}{\hbar}\sum_{k\neq 0}\sum_{\lambda=e,m}\int \mathrm{d}^3 r \int_0^\infty \frac{\mathrm{d}\omega}{\omega+\omega_A^k}\left|\langle 0_A|\langle\{0\}|\hat{H}_{AF}|\mathbf{1}_\lambda(\mathbf{r},\omega)\rangle|k_A\rangle\right|^2, \tag{3.5}$$

where $\omega_A^k = (E_k^A - E_0^A)/\hbar$ is the atomic transition frequency. With $\hat{H}_{AF}$ being given by Eq. (2.99) together with the expansions (2.32) and (2.36), the matrix elements of the interaction Hamiltonian (3.5) are found to be

$$\langle 0_A|\langle\{0\}|\hat{H}_{AF}|\mathbf{1}_\lambda(\mathbf{r},\omega)\rangle|k_A\rangle = -\mathbf{d}_A^{0k}\cdot\boldsymbol{G}_\lambda(\mathbf{r}_A,\mathbf{r},\omega) - \frac{\mathbf{m}_A^{0k}\cdot\boldsymbol{\nabla}_A\times\boldsymbol{G}_\lambda(\mathbf{r}_A,\mathbf{r},\omega)}{i\omega} \tag{3.6}$$

[$\mathbf{d}_A^{0k} = \langle 0_A|\hat{\mathbf{d}}_A|k_A\rangle$, $\mathbf{m}_A^{0k} = \langle 0_A|\hat{\mathbf{m}}_A|k_A\rangle$], where the commutation relations (2.30) and (2.31) and Eq. (2.39) have been used. Since ΔE, Eq.(3.5), is quadratic in the matrix elements, there are three classes of contributions to the energy shift. The contribution involving two electric-dipole transitions is known to lead to the electric part of the signle-atom vdW potential. It can be found by replacing the matrix elecment in Eq. (3.5) by the first term on the right-hand side of Eq. (3.6) that results in [28, 29, 41, 82, 42]

$$U_e(\mathbf{r}_A) = \frac{\hbar\mu_0}{2\pi}\int_0^\infty \mathrm{d}u\, u^2 \mathrm{Tr}\big[\boldsymbol{\alpha}_A(iu)\cdot\boldsymbol{G}^{(1)}(\mathbf{r}_A,\mathbf{r}_A,iu)\big], \tag{3.7}$$

[1] A treatment on strong atom-field coupling, which is the case when the atom is in a resonator-like geometry, is given in Ref. [43]

where $\boldsymbol{\alpha}_A(\omega)$ is the lowest-order electric polarizability of the atom [94]

$$\boldsymbol{\alpha}_A(\omega) = \lim_{\epsilon\to 0^+} \frac{2}{\hbar}\sum_k \frac{\omega_A^k \mathbf{d}_A^{0k}\mathbf{d}_A^{k0}}{(\omega_A^k)^2 - \omega^2 - i\omega\epsilon}\,, \tag{3.8}$$

and $\boldsymbol{G}^{(1)}$ is the scattering part of the Green tensor defined by

$$\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega) = \boldsymbol{G}^{(0)}(\mathbf{r},\mathbf{r}',\omega) + \boldsymbol{G}^{(1)}(\mathbf{r},\mathbf{r}',\omega) \tag{3.9}$$

with $\boldsymbol{G}^{(0)}(\mathbf{r},\mathbf{r}',\omega)$ being the free-space part. In particular for an isotropic atom, where

$$\boldsymbol{\alpha}_A(\omega) = \lim_{\epsilon\to 0^+} \frac{2}{3\hbar}\sum_k \frac{\omega_A^k |\mathbf{d}_A^{0k}|^2}{(\omega_A^k)^2 - \omega^2 - i\omega\epsilon}\,\boldsymbol{I} \equiv \alpha_A(\omega)\boldsymbol{I}, \tag{3.10}$$

Eq. (3.7) simplifies to

$$U_e(\mathbf{r}_A) = \frac{\hbar\mu_0}{2\pi}\int_0^\infty \mathrm{d}u\, u^2 \alpha_A(iu)\mathrm{Tr}\boldsymbol{G}^{(1)}(\mathbf{r}_A,\mathbf{r}_A,iu). \tag{3.11}$$

The $\mathbf{r}_A$-independent term associated with the bulk part of the Green tensor gives rise to the well-known Lamb shift and is not of interest here. Let us point out that the decomposition (3.9) is applicable when the positions referred to as $\mathbf{r}$ and $\mathbf{r}'$ can be connected without crossing boundaries (discontinuity surfaces with respect to permittivity and permeability functions) in the media; the scattering part thus account for the presence of media interfaces. In the calculation of the single-atoms potential the Green tensor always refers two equal positions $\mathbf{r}=\mathbf{r}'=\mathbf{r}_A$ and there is no doubt in the mentioned decomposition, but this is not the case in the calculation of two-atom interaction potential as it will be shown in chapter 4. However in all the examples presented through this work Eq. (3.9) is applicable.

The contribution ΔE^m to ΔE which involves two magnetic-dipole transitions can be calculated by substituting the second term on the right-hand side of Eq. (3.6) into Eq. (3.5), resulting in

$$\Delta E^m = \frac{1}{\hbar}\sum_k \sum_{\lambda=e,m}\int \mathrm{d}^3 r_1 \int_0^\infty \frac{\mathrm{d}\omega}{\omega^2(\omega+\omega_A^k)} \times \left[\mathbf{m}_A^{0k}\cdot\boldsymbol{\nabla}\times\boldsymbol{G}_\lambda(\mathbf{r},\mathbf{r}_1,\omega)\cdot\boldsymbol{G}_\lambda^{*\mathsf{T}}(\mathbf{r}',\mathbf{r}_1,\omega)\times\overleftarrow{\boldsymbol{\nabla}}'\cdot\mathbf{m}_A^{0k}\right]_{\mathbf{r}=\mathbf{r}'=\mathbf{r}_A} \tag{3.12}$$

[HS5], where the identities $\mathbf{a}\cdot\boldsymbol{T}=\boldsymbol{T}^{\mathsf{T}}\cdot\mathbf{a}$ and $(\boldsymbol{\nabla}\times\boldsymbol{T})^{\mathsf{T}} = -\boldsymbol{T}^{\mathsf{T}}\times\overleftarrow{\boldsymbol{\nabla}}$ are used ($\mathbf{a}$ and $\boldsymbol{T}$ are, respectively, arbitrary vector and tensor fields). The volume integral in Eq. (3.12) can be performed using the integral relation (2.35) leading to

$$\Delta E^m = \frac{\mu_0}{\pi}\sum_k \int_0^\infty \frac{\mathrm{d}\omega}{\omega+\omega_A^k}\left[\mathbf{m}_A^{0k}\cdot\boldsymbol{\nabla}\times\mathrm{Im}\;\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega)\times\overleftarrow{\boldsymbol{\nabla}}'\cdot\mathbf{m}_A^{k0}\right]_{\mathbf{r}=\mathbf{r}'=\mathbf{r}_A}. \tag{3.13}$$

To perform the frequency integral, we first use the identity $\mathrm{Im}\,\boldsymbol{G} = (\boldsymbol{G} - \boldsymbol{G}^*)/(2i)$, and the relation (2.25), to write

$$\int_0^\infty \frac{\mathrm{d}\omega}{\omega + \omega_A^k} \mathrm{Im}\,\boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{2i}\left[\int_0^\infty \frac{\mathrm{d}\omega}{\omega + \omega_A^k}\,\boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) + \int_{-\infty}^0 \frac{\mathrm{d}\omega}{\omega - \omega_A^k}\boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega)\right]. \quad (3.14)$$

The integrands on the right-hand side of Eq. (3.14) are analytic in the upper half of the complex frequency plane including the real axis apart from a possible pole at the origin. We may therefore apply Cauchy's theorem and replace the first(second) integral by a contour integral along the positive imaginary half-axis introducing the purely imaginary frequency $\omega = iu$, along an infinitely large quarter-circle in the first(second) quadrant of the complex frequency plane, and around an infinitely small quarter-circle around the origin in the first(second) quadrant. The integrals along the infinitely large quarter-circles vanish, the ones around the infinitely small quarter-circles cancel each other, and summing the remaining contributions from the two integrals in Eq. (3.14) leads to

$$\Delta E^m = \frac{\mu_0}{\pi} \sum_k \int_0^\infty \mathrm{d}u \frac{\omega_A^k}{\omega_A^k + u^2} \left[\mathbf{m}_A^{0k} \cdot \boldsymbol{L}(\mathbf{r}, \mathbf{r}', iu) \cdot \mathbf{m}_A^{k0}\right]_{\mathbf{r}=\mathbf{r}'=\mathbf{r}_A}, \quad (3.15)$$

where

$$\boldsymbol{L}(\mathbf{r}, \mathbf{r}', \omega) = \boldsymbol{\nabla} \times \boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega) \times \overleftarrow{\boldsymbol{\nabla}}'. \quad (3.16)$$

The relevant, position-dependent part of ΔE^m can be obtained by replacing the Green tensor with its scattering part. We may thus represent the vdW potential of a (para)magnetic atom as

$$U_A^m(\mathbf{r}_A) = \frac{\hbar\mu_0}{2\pi} \int_0^\infty \mathrm{d}u\, \mathrm{Tr}\left[\boldsymbol{\beta}_A(iu) \cdot \boldsymbol{L}^{(1)}(\mathbf{r}_A, \mathbf{r}_A, iu)\right] = \frac{\hbar\mu_0}{2\pi} \int_0^\infty \mathrm{d}u\, \beta_A(iu) \mathrm{Tr}\boldsymbol{L}^{(1)}(\mathbf{r}_A, \mathbf{r}_A, iu), \quad (3.17)$$

where $\boldsymbol{\beta}_A(\omega)$ is the lowest-order ground-state magnetizability defined as

$$\boldsymbol{\beta}_A(\omega) = \lim_{\epsilon \to 0^+} \frac{2}{\hbar} \sum_k \frac{\omega_A^k \mathbf{m}_A^{0k} \mathbf{m}_A^{k0}}{(\omega_A^k)^2 - \omega^2 - i\omega\epsilon} = \lim_{\epsilon \to 0^+} \frac{2}{3\hbar} \sum_k \frac{\omega_A^k |\mathbf{m}_A^{0k}|^2}{(\omega_A^k)^2 - \omega^2 - i\omega\epsilon}\, \boldsymbol{I} \equiv \beta_A(\omega)\boldsymbol{I} \quad (3.18)$$

Note that $\boldsymbol{L}^{(1)}$ is given by the right-hand side of (3.16) with $\boldsymbol{G}^{(1)}$ instead of $\boldsymbol{G}$, and the second equality in Eq. (3.17) and (3.18) is valid for isotropic atoms.

We restrict our considerations to atoms with centers of inversion (non-chiral atoms), whose energy eigenstates can be chosen to be eigenstates of the parity operator. Contributions to the energy shift that contain one electric-dipole transition and one magnetic-dipole transition can then be excluded, since $\hat{\mathbf{d}}_A$ is odd and $\hat{\mathbf{m}}_A$ is even under spatial reflection that leads to a vanishing crossed electric-magnetic polarizability, defined as

$$\boldsymbol{X}_A(\omega) = \lim_{\epsilon \to 0^+} \frac{2}{\hbar} \sum_k \frac{\omega_A^k \mathbf{d}_A^{0k} \mathbf{m}_A^{k0}}{(\omega_A^k)^2 - \omega^2 - i\omega\epsilon}. \quad (3.19)$$

Hence, the general formula for the total vdW potential of a single ground-state atom that is both polarizable and (para)magnetizable, and is placed within an arbitrary environment of magnetoelectric bodies reads [HS5]

$$U_A(\mathbf{r}_A) = U_e(\mathbf{r}_A) + U_A^m(\mathbf{r}_A), \tag{3.20}$$

with U_e and U_A^m being given by Eqs. (3.7) and (3.17), respectively.

3.2 Local-field corrections

Equations (3.7) and (3.17) refer to an atom that is not embedded in medium, i.e., $\varepsilon(\mathbf{r}_A,\omega) = \mu(\mathbf{r}_A,\omega) = 1$. In the case where the atom under consideration is located in a host medium one needs to include local-field corrections in the calculations to account for the difference between the macroscopic electromagnetic field and the local field experienced by the atom. A possible way to treat local-field effects is offered by the real-cavity model [62], where a small spherical empty cavity of radius R_c surrounding the atom is introduced. As shown in Ref. [64], the needed local-field corrected form of the Green tensor reads, in linear order of $\omega R_\mathrm{c}/c$,

$$\begin{aligned}\boldsymbol{G}^{(1)}_{\mathrm{loc}}(\mathbf{r}_A,\mathbf{r}_A,\omega) = \frac{\omega}{2\pi c}\Bigg\{&\frac{\varepsilon_A-1}{2\varepsilon_A+1}\,\frac{c^3}{\omega^3 R_c^3} + \frac{3}{5}\,\frac{\varepsilon_A^2(5\mu_A-1)-3\varepsilon_A-1}{(2\varepsilon_A+1)^2}\,\frac{c}{\omega R_c}\\ &+ i\left[\frac{3\varepsilon_A n_A^3}{(2\varepsilon_A+1)^2} - \frac{1}{3}\right]\Bigg\}\boldsymbol{I} + \left(\frac{3\varepsilon_A}{2\varepsilon_A+1}\right)^2 \boldsymbol{G}^{(1)}(\mathbf{r}_A,\mathbf{r}_A,\omega),\end{aligned} \tag{3.21}$$

where $\varepsilon_A = \varepsilon_A(\omega) = \varepsilon(\mathbf{r}_A,\omega)$ and $\mu_A = \mu_A(\omega) = \mu(\mathbf{r}_A,\omega)$ are, respectively, the permittivity and permeability of the unperturbed host medium at the position of the guest atom, $n_A = \sqrt{\varepsilon_A\mu_A}$, and $\boldsymbol{G}^{(1)}$ is the scattering part of the uncorrected Green tensor. Inserting the corrected Green tensor into Eqs. (3.7), one obtains the local-field corrected electric contribution to the vdW potential [64],

$$U_e(\mathbf{r}_A) = \frac{\hbar\mu_0}{2\pi}\int_0^\infty \mathrm{d}u\, u^2 \left[\frac{3\varepsilon_A(iu)}{2\varepsilon_A(iu)+1}\right]^2 \mathrm{Tr}\left[\boldsymbol{\alpha}_A(iu)\cdot\boldsymbol{G}^{(1)}(\mathbf{r}_A,\mathbf{r}_A,iu)\right], \tag{3.22}$$

where the position-independent first term on the right-hand side of Eq. (3.21) is discarded.

For (para)magnetic atoms the vdW potential depends on spatial derivatives of the Green tensor. The respective local-field corrected tensor cannot be derived directly from Eq. (3.21), because the correction procedure does not commute with these derivatives. The local field corrected version of the tensor $\boldsymbol{L}$ defined by Eq. (3.16) can be derived in a complete analogy to the derivation of Eq. (3.21), which is given in Refs. [63, 64]. For this purpose we recall

that the first term in Eq. (3.21), i.e., the position-independent part of $\boldsymbol{G}^{(1)}_{\rm loc}(\mathbf{r}_A,\mathbf{r}_A,\omega)$, stems from the scattering Green tensor $\boldsymbol{G}^{(1)}_c(\mathbf{r}_A,\mathbf{r}_A,\omega)$ with position $\mathbf{r}_A$ at the center of a small spherical cavity of radius R_c which is embedded in an infinitely extended bulk material of permittivity ε_A and permeability μ_A. The respective tensor $\boldsymbol{L}^{(1)}_c(\mathbf{r}_A,\mathbf{r}_A,\omega)$ reads [100]

$$\boldsymbol{L}^{(1)}_c(\mathbf{r}_A,\mathbf{r}_A,\omega) = -\frac{i\omega^3}{6\pi c^3}\,C(\omega)\boldsymbol{I}, \tag{3.23}$$

where

$$C(\omega) = -\frac{\mu_A h_1^{(1)}(y)\left[y_0 h_1^{(1)}(y_0)\right]' - h_1^{(1)}(y_0)\left[y h_1^{(1)}(y)\right]'}{\mu_A h_1^{(1)}(y)\left[y_0 j_1(y_0)\right]' - j_1(y_0)\left[y h_1^{(1)}(y)\right]'} \tag{3.24}$$

[$y_0 = \omega R_c/c,\ y = n_A y_0$]. The local-field correction factor multiplying $\boldsymbol{G}^{(1)}$ in Eq. (3.21) is determined by comparing the Green tensor $\boldsymbol{G}_c(\mathbf{r},\mathbf{r}_A,\omega)$ (with $\mathbf{r}_A$ at the center of the cavity and $\mathbf{r}$ at an arbitrary position outside the cavity) with the bulk Green tensor $\boldsymbol{G}_{\rm bulk}(\mathbf{r},\mathbf{r}_A,\omega)$ of an infinite homogeneous medium without the cavity [86],

$$\boldsymbol{G}_{\rm bulk}(\mathbf{r},\mathbf{r}_A,\omega) = -\frac{c^2 \mathrm{e}^{ik\rho}}{4\pi\varepsilon_A\omega^2\rho^3}\,\left\{f(-ik\rho)\boldsymbol{I} - g(-ik\rho)\mathbf{e}_\rho\mathbf{e}_\rho\right\} \tag{3.25}$$

with

$$f(x) = 1 + x + x^2, \quad g(x) = 3 + 3x + x^2 \tag{3.26}$$

[$k = n_A\omega/c$, $\rho = |\mathbf{r} - \mathbf{r}_A|$, $\mathbf{e}_\rho = (\mathbf{r} - \mathbf{r}_A)/\rho$]. In the present case, the required tensor $\boldsymbol{L}_c(\mathbf{r},\mathbf{r}_A,\omega)$ reads [100]

$$\boldsymbol{L}_c(\mathbf{r},\mathbf{r}_A,\omega) = \frac{\mathrm{e}^{ik\rho}}{4\pi n_A^2\rho^3}\,D(\omega)\left\{f(-ik\rho)\boldsymbol{I} - g(-ik\rho)\mathbf{e}_\rho\mathbf{e}_\rho\right\}, \tag{3.27}$$

where

$$D(\omega) = \mu_A\frac{h_1^{(1)}(y_0)\left[y_0 j_1(y_0)\right]' - j_1(y_0)\left[y_0 h_1^{(1)}(y_0)\right]'}{\mu_A h_1^{(1)}(y)\left[y_0 j_1(y_0)\right]' - j_1(y_0)\left[y h_1^{(1)}(y)\right]'}, \tag{3.28}$$

and from Eqs. (3.16) and (3.25), $\boldsymbol{L}_{\rm bulk}(\mathbf{r},\mathbf{r}_A,\omega)$ can be found as

$$\boldsymbol{L}_{\rm bulk}(\mathbf{r},\mathbf{r}_A,\omega) = \frac{\mu_A \mathrm{e}^{ik\rho}}{4\pi\rho^3}\,\left\{f(-ik\rho)\boldsymbol{I} - g(-ik\rho)\mathbf{e}_\rho\mathbf{e}_\rho\right\}. \tag{3.29}$$

Comparing Eqs. (3.29) and (3.27), and using similar arguments as in Refs. [63, 64], we can conclude that the magnetic local-field correction factor is given by $D/(\mu_A n_A^2)$. Combining this with Eq. (3.28) and following the line of reasoning of Refs. [63, 64], we expand all the terms within leading order in $R_c\omega/c$ to obtain the local-field corrected tensor $\boldsymbol{L}^{(1)}_{\rm loc}$ to be

$$\begin{aligned}\boldsymbol{L}^{(1)}_{\rm loc}(\mathbf{r}_A,\mathbf{r}_A,\omega) = -\frac{\omega^3}{2\pi c^3}\Bigg\{&\frac{\mu_A-1}{2\mu_A+1}\,\frac{c^3}{\omega^3 R_c^3} + \frac{3}{5}\,\frac{\mu_A^2(5\varepsilon_A-1)-3\mu_A-1}{(2\mu_A+1)^2}\,\frac{c}{\omega R_c}\\ &+ i\left[\frac{3\mu_A n_A^3}{(2\mu_A+1)^2} - \frac{1}{3}\right]\Bigg\}\boldsymbol{I} + \left(\frac{3}{2\mu_A+1}\right)^2\boldsymbol{L}^{(1)}(\mathbf{r}_A,\mathbf{r}_A,\omega).\end{aligned} \tag{3.30}$$

Replacing in Eq. (3.17) $\boldsymbol{L}^{(1)}$ with $\boldsymbol{L}^{(1)}_{\rm loc}$ from Eq. (3.30), we obtain the local-field corrected magnetic single-atom potential [HS5]

$$U_A^m(\mathbf{r}_A) = \frac{\hbar\mu_0}{2\pi}\int_0^\infty \mathrm{d}u\,\left[\frac{3}{2\mu_A(iu)+1}\right]^2 \mathrm{Tr}\left[\boldsymbol{\beta}_A(iu)\cdot\boldsymbol{L}^{(1)}(\mathbf{r}_A,\mathbf{r}_A,iu)\right], \tag{3.31}$$

where a position-independent term has been discarded, as in the electric case. Needless to say that Eqs. (3.22) and (3.31) reduce to Eqs. (3.7) and (3.17), respectively, when the atom is situated in free space so that $\varepsilon_A = \mu_A = 1$.

3.3 Applications

In order to illustrate, more explicitly, the dependence of the vdW potential on the electromagnetic and geometric properties of the media, as well as its position-dependence, it is required to specify the material environment, which may be done by substituting the appropriate Green tensors into the formula. We now apply the theory to some examples and compare the result with the familiar results for nonmagnetic atoms, with special emphsis on whether the total potential for electromagnetic atom is invariant under a global duality transformation $\varepsilon \leftrightarrow \mu$, $c^2\alpha_A \leftrightarrow \beta_A$ [95, HS6].

3.3.1 Planar multilayer media

Let us consider an isotropic atom A, possessing both electric and magnetic polarizabilities, in front of a planar magnetoelectric multilayer system consisting of N adjoined layers labeled by j ($j = 0, 1, 2, \ldots, N-1$) with thicknesses d_j ($d_0 \to \infty$), permittivities $\varepsilon_j(\omega)$, and permeabilities $\mu_j(\omega)$, as sketched in Fig. 3.1. We choose the coordinate system such as the z axis is perpendicular to the layers, with the origin being on the interface between layer $j = N-1$ and the free-space region, which can be regarded as layer $j = N$ [$d_N \to \infty$, $\varepsilon_N(\omega) \equiv 1$, $\mu_N(\omega) \equiv 1$].

Let us first evaluate the electric part of the potential, which can be calculated using Eq. (3.22). The scattering part of the Green tensor for a planar multilayer system can be given in the form [96]

$$\boldsymbol{G}^{(1)}(\mathbf{r},\mathbf{r}',\omega) = \frac{1}{8\pi^2}\int \frac{\mathrm{d}^2q}{b_N}\, e^{i(\mathbf{w}\cdot\mathbf{r}-\mathbf{w}^*\cdot\mathbf{r}')}(r_N^s \mathbf{e}_s^+\mathbf{e}_s^- + r_N^p \mathbf{e}_p^+\mathbf{e}_p^-), \tag{3.32}$$

($z, z' > 0$, $\mathbf{q} \perp \mathbf{e}_z$, $\mathbf{w} = \mathbf{q} + i\, b_N\, \mathbf{e}_z$), where $b_N = \sqrt{-\omega^2/c^2 + q^2}$ is derived from the definition

$$b_j = b_j(q,\omega) = \sqrt{-\frac{\omega^2}{c^2}\varepsilon_j(\omega)\mu_j(\omega) + q^2}, \tag{3.33}$$

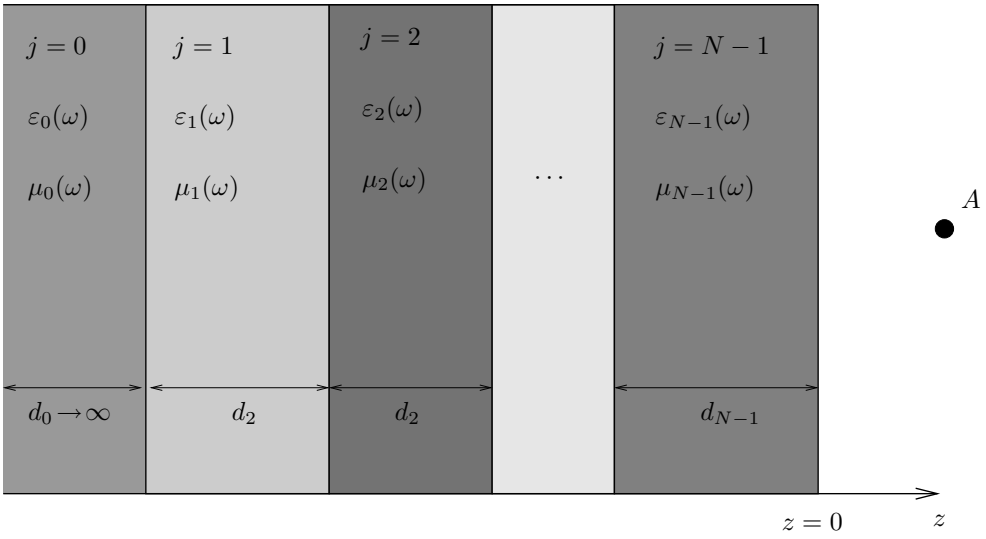

Figure 3.1: Sketch of the planar multilayer medium.

and the unit vectors $\mathbf{e}_s^{\pm}$ and $\mathbf{e}_p^{\pm}$ are, respectively, the polarization vectors for $s-$ and $p-$ polarized waves, propagating in the positive/negative z direction:

$$\mathbf{e}_s^{\pm} = \mathbf{e}_q \times \mathbf{e}_z \equiv \mathbf{e}_s, \quad \mathbf{e}_p^{\pm} = \frac{c}{\omega}\left(q\,\mathbf{e}_z \mp i b_N \mathbf{e}_q\right). \tag{3.34}$$

Further, the (generalized) reflection coefficients r_j^{σ} with respect to the left boundary of the jth layer ($j=1,2,3,\ldots,N$) can be obtained from the recurrence relations

$$r_j^s = r_j^s(q,u) = \frac{\left(\frac{\mu_{j-1}}{b_{j-1}} - \frac{\mu_j}{b_j}\right) + \left(\frac{\mu_{j-1}}{b_{j-1}} + \frac{\mu_j}{b_j}\right) e^{-2b_{j-1}d_{j-1}}\, r_{j-1}^{\sigma}}{\left(\frac{\mu_{j-1}}{b_{j-1}} + \frac{\mu_j}{b_j}\right) + \left(\frac{\mu_{j-1}}{b_{j-1}} - \frac{\mu_j}{b_j}\right) e^{-2b_{j-1}d_{j-1}}\, r_{j-1}^{\sigma}} \tag{3.35}$$

and

$$r_j^p = r_j^p(q,u) = \frac{\left(\frac{\varepsilon_{j-1}}{b_{j-1}} - \frac{\varepsilon_j}{b_j}\right) + \left(\frac{\varepsilon_{j-1}}{b_{j-1}} + \frac{\varepsilon_j}{b_j}\right) e^{-2b_{j-1}d_{j-1}}\, r_{j-1}^{\sigma}}{\left(\frac{\varepsilon_{j-1}}{b_{j-1}} + \frac{\varepsilon_j}{b_j}\right) + \left(\frac{\varepsilon_{j-1}}{b_{j-1}} - \frac{\varepsilon_j}{b_j}\right) e^{-2b_{j-1}d_{j-1}}\, r_{j-1}^{\sigma}} \tag{3.36}$$

with $r_0^{\sigma}=0$ ($\sigma=s,p$). In the Cartesian coordinate system mentioned above, the scattering Green tensor (3.32) referring to equal positions can be written as

$$\boldsymbol{G}^{(1)}(\mathbf{r},\mathbf{r},\omega) = \frac{1}{8\pi}\int_0^{\infty} \frac{q\,\mathrm{d}q}{b_N}\,\mathrm{e}^{-2b_N z}\left[\left(r_N^s + \frac{c^2 b_N^2}{\omega^2} r_N^p\right)(\mathbf{e}_x\mathbf{e}_x + \mathbf{e}_y\mathbf{e}_y) + 2\frac{c^2 q^2}{\omega^2} r_N^p \mathbf{e}_z\mathbf{e}_z\right]. \tag{3.37}$$

The electric part U_e of the single-atom vdW potential, as shown in Ref. [97], will be obtained by substituting $\boldsymbol{G}^{(1)}$ from Eq. (3.37) into Eq. (3.11) as

$$U_e(\mathbf{r}_A) = \frac{\hbar\mu_0}{8\pi^2}\int_0^{\infty}\mathrm{d}u\,u^2\alpha_A(iu)\int_0^{\infty}\mathrm{d}q\frac{q}{b_N}\,\mathrm{e}^{-2b_N z_A}\left[r_N^s - \left(1+2\frac{q^2c^2}{u^2}\right) r_N^p\right]. \tag{3.38}$$

Equation (3.38) agrees with the results derived in Refs. [98] based on a linear-response approach. A detailed analysis of Eq. (3.38) requires numerical computation, which needs

to determine magnetoelectric properties of each individual layer [i.e., $\varepsilon_j(\omega)$, $\mu_j(\omega)$] and to specify the atom [via specifying $\alpha_A(\omega)$].

Let us, as a simpler example, consider a sufficiently thick plate so that the model of a (semi-infinite) half-space applies ($N=1$). The electric part of the vdW potential is given by Eq. (3.38) with the reflection coefficients given by Eqs. (3.35) and (3.36) being reduced to

$$r_s \equiv r_1^s = \frac{\varepsilon(iu)b - b_0}{\varepsilon(iu)b + b_0}\,, \qquad r_p \equiv r_1^p = \frac{\mu(iu)b - b_0}{\mu(iu)b + b_0}\,, \tag{3.39}$$

where

$$b \equiv b_1 = \sqrt{u^2/c^2 + q^2}, \qquad b_0 = \sqrt{\varepsilon(iu)\mu(iu)u^2/c^2 + q^2}. \tag{3.40}$$

Further analytical processing of the potential is possible in two limiting cases of retarded (i.e., long-distance) and nonretarded (i.e., short-distance) limits. In the retarded limit, where $z_A \gg c/\omega_{\min}$ with $\omega_{\min}$ being the minimum of the characteristic atomic and medium frequencies, it turns out that the vdW force can be derived from an attractive potential proportional to z_A^{-4} [97, 99]

$$U_e(z_A) = \frac{3\hbar c\alpha_A(0)}{64\pi^2\varepsilon_0 z_A^4}\int_1^\infty \mathrm{d}v\left[\frac{1}{v^4}r_s(v) - \left(\frac{2}{v^2} - \frac{1}{v^4}\right)r_p(v)\right], \tag{3.41}$$

where, according to Eq. (3.39), the static reflection coefficients $r_s(v)$ and $r_p(v)$ read

$$r_s(v) = \frac{\mu(0)v - \sqrt{n^2(0) - 1 + v^2}}{\mu(0)v + \sqrt{n^2(0) - 1 + v^2}}\,, \quad r_p(v) = \frac{\varepsilon(0)v - \sqrt{n^2(0) - 1 + v^2}}{\varepsilon(0)v + \sqrt{n^2(0) - 1 + v^2}} \tag{3.42}$$

[$n(\omega) = \sqrt{\varepsilon(\omega)\mu(\omega)}$]. In the opposite limit of nonretarded, where $z_A \ll c/[n(0)\omega_{\max}]$ with $\omega_{\max}$ being the maximum of the characteristic atomic and medium frequencies, the vdW potential obeys different power laws in z_A, depending on the strength of the permittivity and permeability of the half-space. Unless the permittivity is very weak, the vdW potential is found to be attractive and proportional to z_A^{-3} [97]

$$U_e(z_A) = -\frac{\hbar}{16\pi^2\varepsilon_0 z_A^3}\int_0^\infty \mathrm{d}u\,\alpha_A(iu)\,\frac{\varepsilon(iu) - 1}{\varepsilon(iu) + 1}\,, \tag{3.43}$$

otherwise it is a repulsive potential proportional to z^{-1} [97]

$$U_e(z_A) = \frac{\hbar\mu_0}{32\pi^2 z_A}\int_0^\infty \mathrm{d}u\,u^2\alpha_A(iu)\frac{[\mu(iu) + 3][\mu(iu) - 1]}{\mu(iu) + 1}\,. \tag{3.44}$$

Equation. (3.43) was also derived in Ref. [33] using method of image-charges.

Let us now evaluate the magnetic part of the vdW potential of the atom in front of the multilayer system [HS5]. To this purpose we need to determine the tensor $\boldsymbol{L}^{(1)}$ that can be done by combining Eq. (3.32) with (3.16) that leads to

$$\boldsymbol{L}^{(1)}(\mathbf{r}, \mathbf{r}', \omega) = \frac{-\omega^2}{8\pi^2 c^2}\int \frac{\mathrm{d}^2 q}{b_N}\, e^{i(\mathbf{w}\cdot\mathbf{r} - \mathbf{w}^*\cdot\mathbf{r}')}(r_N^p \mathbf{e}_s^+\mathbf{e}_s^- + r_N^s \mathbf{e}_p^+\mathbf{e}_p^-). \tag{3.45}$$

Comparing Eqs. (3.17) [together with Eq. (3.45)] and (3.11) [together with Eq. (3.32)], it is seen that the magnetic part U_A^m can be found from the electric part U_e given by Eq. (3.38) by replacing α_A with β_A/c^2 and interchanging of r_N^s and r_N^p on the right-hand side [or equivalently, interchanging of ε and μ; recall Eqs. (3.35) and (3.36)], in agreement with the electromagnetic duality principle [95, HS6]. Needless to say that this symmetry between the electric and magnetic parts of the vdW potential, holds for a magnetoelectric half-space. For instance, as an immediate result of using the duality principle for the half-space example, we may conclude from Eqs. (3.43) and (3.44) that in the nonretarded limit a (para)magnetic atom is subject to a repulsive force proportional to z^{-2} in the presence of a purely electric half-space [$\mu(\omega)=1$] and experiences an attractive force proportional to z^{-4} in the presence of a purely magnetic half-space [$\varepsilon(\omega)=1$].

3.3.2 Homogeneous sphere

As a second example, we consider an isotropic atom A, possessing both electric and magnetic polarizabilities, in a distance r_A from the center of a homogeneous magnetoelectric sphere of permittivity $\varepsilon(\omega)$, permeability $\mu(\omega)$, and radius R ($r_A>R$). Choosing the coordinate system such that its origin coincides with the center of the sphere (Fig. 3.2), we may represent the scattering part of the Green tensor as [100]

$$\boldsymbol{G}^{(1)}(\mathbf{r},\mathbf{r}',\omega)=\frac{i\omega}{4\pi c}\sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)}\sum_{m=0}^{n}\frac{(n-m)!}{(n+m)!}(2-\delta_{0m})$$
$$\times\sum_{p=\pm1}\left[B_n^M(\omega)\mathbf{M}_{nm,p}(\mathbf{r},\omega/c)\mathbf{M}_{nm,p}(\mathbf{r}',\omega/c)+B_n^N(\omega)\mathbf{N}_{nm,p}(\mathbf{r},\omega/c)\mathbf{N}_{nm,p}(\mathbf{r}',\omega/c)\right], \quad (3.46)$$

where $\mathbf{M}_{nm,p}(\mathbf{r},q)$ and $\mathbf{N}_{nm,p}(\mathbf{r},q)$ are even ($p=+1$) and odd ($p=-1$) spherical wave vector functions. In spherical coordinates, they can be expressed in terms of spherical Hankel functions of the first kind, $h_n^{(1)}(x)$, and Legendre functions, $P_n^m(x)$, as follows:

$$\mathbf{M}_{nm,\pm1}(\mathbf{r},q)=\mp\frac{m}{\sin\theta}\,h_n^{(1)}(qr)P_n^m(\cos\theta)\begin{matrix}\sin\\\cos\end{matrix}(m\phi)\mathbf{e}_\theta-h_n^{(1)}(qr)\frac{\mathrm{d}P_n^m(\cos\theta)}{\mathrm{d}\theta}\begin{matrix}\cos\\\sin\end{matrix}(m\phi)\mathbf{e}_\phi, \quad (3.47)$$

$$\mathbf{N}_{nm,\pm1}(\mathbf{r},q)=\frac{n(n+1)}{qr}\,h_n^{(1)}(qr)P_n^m(\cos\theta)\begin{matrix}\cos\\\sin\end{matrix}(m\phi)\mathbf{e}_r$$
$$+\frac{1}{qr}\frac{\mathrm{d}[rh_n^{(1)}(qr)]}{\mathrm{d}r}\left[\frac{\mathrm{d}P_n^m(\cos\theta)}{\mathrm{d}\theta}\begin{matrix}\cos\\\sin\end{matrix}(m\phi)\mathbf{e}_\theta\mp\frac{m}{\sin\theta}\,P_n^m(\cos\theta)\begin{matrix}\sin\\\cos\end{matrix}(m\phi)\mathbf{e}_\phi\right], \quad (3.48)$$

with $\mathbf{e}_r$, $\mathbf{e}_\theta$, and $\mathbf{e}_\phi$ being the mutually orthogonal unit vectors pointing in the directions of radial distance r, polar angle θ, and azimuthal angle ϕ, respectively (Fig. 3.2). The spherical

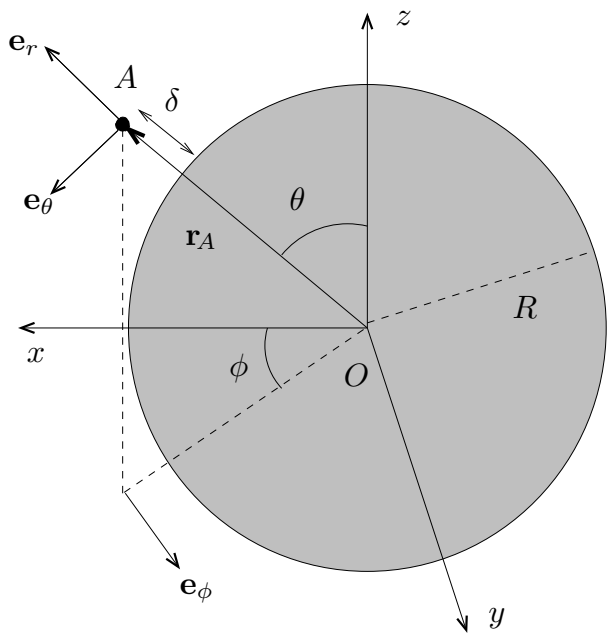

Figure 3.2: Atom A in the presence of a sphere.

wave vector functions are related to each other via

$$\boldsymbol{\nabla} \times \mathbf{M}_{nm,\pm1}(\mathbf{r}, q) = q\mathbf{N}_{nm,\pm1}(\mathbf{r}, q), \tag{3.49}$$

$$\boldsymbol{\nabla} \times \mathbf{N}_{nm,\pm1}(\mathbf{r}, q) = q\mathbf{M}_{nm,\pm1}(\mathbf{r}, q). \tag{3.50}$$

The coefficients $B_n^M(\omega)$ and $B_n^N(\omega)$ in Eq. (3.46) read

$$B_n^M(\omega) = -\frac{\mu(\omega)[z_0 j_n(z_0)]' j_n(z_1) - [z_1 j_n(z_1)]' j_n(z_0)}{\mu(\omega)[z_0 h_n^{(1)}(z_0)]' j_n(z_1) - [z_1 j_n(z_1)]' h_n^{(1)}(z_0)}, \tag{3.51}$$

$$B_n^N(\omega) = -\frac{\varepsilon(\omega)[z_0 j_n(z_0)]' j_n(z_1) - [z_1 j_n(z_1)]' j_n(z_0)}{\varepsilon(\omega)[z_0 h_n^{(1)}(z_0)]' j_n(z_1) - [z_1 j_n(z_1)]' h_n^{(1)}(z_0)}, \tag{3.52}$$

where $j_n(z)$ is the spherical Bessel function of the first kind, $z_0 = R\omega/c$, $z_1 = n(\omega)z_0$, and the prime denotes differentiation with respect to the argument.

Let us first focus on the electric part U_e of the vdW potential. This part, as given in Ref. [82], can be obtained by substituting the scattering part of the Green tensor (3.46) referring to equal positions (Appendix B),

$$\boldsymbol{G}^{(1)}(\mathbf{r}, \mathbf{r}, \omega) = \frac{i\omega}{8\pi c} \sum_{n=1}^{\infty} (2n+1) \left(\frac{2c^2 B_n^N}{r^2\omega^2} n(n+1)[h_n^{(1)}(r\omega/c)]^2 \mathbf{e}_r\mathbf{e}_r \right.$$
$$\left. + \left\{ B_n^M [h_n^{(1)}(r\omega/c)]^2 + \frac{c^2 B_n^N}{r^2\omega^2} \left[z h_n^{(1)}(z) \right]'^2_{z=r\omega/c} \right\} (\mathbf{e}_\theta\mathbf{e}_\theta + \mathbf{e}_\phi\mathbf{e}_\phi) \right), \tag{3.53}$$

into Eq. (3.11) that leads to

$$U_e(r_A) = \frac{-\hbar\mu_0}{8\pi^2 c}\int_0^\infty \mathrm{d}u\, u^3\alpha_A(iu)\sum_{n=1}^{\infty}(2n+1) \times\left(\left[B_n^M(iu)+\frac{n(n+1)}{z^2}B_n^N(iu)\right]\left[h_n^{(1)}(z)\right]^2+\frac{B_n^N(iu)}{z^2}\left[zh_n^{(1)}(z)\right]'^2\right)_{z=ir_Au/c}. \tag{3.54}$$

Further evaluation of Eq. (3.54) requires numerical method in general. However this equation can be further evaluated in the limiting cases of large and small sphere.

The limiting case of a large sphere may be defined by the condition

$$\delta \equiv r_A - R \ll R \tag{3.55}$$

(Fig. 3.2). By using exactly the same argument made for an electric sphere in Ref. [82], it can be shown that in the case where the sphere is magnetically as well as electrically polarizable, the main contribution to the sum on the right-hand side of Eq. (3.54) arises from $n \gg 1$. In this limit (Appendix B.2)

$$\mathrm{Tr}\boldsymbol{G}^{(1)}(\mathbf{r}_A,\mathbf{r}_A,iu) = -\frac{c^2}{8\pi u^2\delta^3}\left\{\frac{\varepsilon-1}{\varepsilon+1}+\frac{(3\varepsilon+1)(\varepsilon-1)}{(\varepsilon+1)^2}\frac{\delta}{R}+\frac{2}{(\varepsilon+1)^2}\left[\frac{\varepsilon(\varepsilon-1)^2}{\varepsilon+1}\right.\right. \left.\left.-\frac{(2\mu^2+3\mu-1)\varepsilon^2+\mu-4\varepsilon-1}{(\mu+1)}\left(\frac{Ru}{c}\right)^2-\frac{\varepsilon\mu(\varepsilon-1)}{4}\left(\frac{Ru}{c}\right)^4\right]\frac{\delta^2}{2R^2}+O\left(\frac{\delta}{R}\right)^3\right\} \tag{3.56}$$

[$\varepsilon=\varepsilon(iu)$, $\mu=\mu(iu)$]. Recalling Eq. (3.55), it can be seen that unless $|\varepsilon-1|\ll 1$, the second and third terms in the curly brackets in Eq. (3.56) can be approximately ignored. Only in the case of a very weak permittivity, the permeability of the sphere may have a significant contribution to the vdW potential. Therefore, the second term in the curly brackets is to be ignored anyway and in the third term ε can be set to 1. Substituting the resulting expression into Eq. (3.11) gives the vdW potential of an electric atom in the presence of a (very) large sphere as

$$U_e(r_A) = \frac{\hbar\mu_0}{16\pi^2}\int_0^\infty \mathrm{d}u\, u^2\alpha_A(iu)\left\{\frac{-c^2}{u^2\delta^3}\frac{\varepsilon(iu)-1}{\varepsilon(iu)+1}+\frac{1}{2\delta}\frac{[\mu(iu)+3][\mu(iu)-1]}{\mu(iu)+1}\right\}. \tag{3.57}$$

Comparing Eq. (3.57) to Eqs. (3.43) and (3.44), it is seen that the first(second) term in Eq. (3.57) corresponds to the nonretarded vdW potential in the presence of a purely electric(magnetic) half-space, as expected.

In the limiting case of a small sphere defined by the requirement $r_A \gg R$, it can be shown that the main contribution to the integral on the right-hand side of Eq. (3.54) is resulted effectively from the region where [82]

$$n(iu)Ru/c \ll 1. \tag{3.58}$$

In this region we may approximate the spherical Bessel and Hankel functions appearing in Eqs. (3.51) and (3.52) by their next-to-leading order expansions in z [101], i.e.,

$$j_n(z) = \frac{z^n}{(2n+1)!!}\left[1 - \frac{z^2}{4n+6}\right] \tag{3.59}$$

and

$$h_n^{(1)}(z) = -i\frac{(2n-1)!!}{z^{n+1}}\left[1 - \frac{z^2}{2-4n}\right], \tag{3.60}$$

so that Eqs. (3.51) and (3.52), respectively, approximate to

$$B_n^M(\omega) = i\frac{(n+1)(2n+1)[\mu(\omega)-1]}{[(2n+1)!!]^2[n\mu(\omega)+n+1]}\left(\frac{R\omega}{c}\right)^{2n+1} + O\left(\frac{R\omega}{c}\right)^{2n+3} \tag{3.61}$$

and

$$B_n^N(\omega) = i\frac{(n+1)(2n+1)[\varepsilon(\omega)-1]}{[(2n+1)!!]^2[n\varepsilon(\omega)+n+1]}\left(\frac{R\omega}{c}\right)^{2n+1} + O\left(\frac{R\omega}{c}\right)^{2n+3}. \tag{3.62}$$

Further, it can be seen that in contrast to the large sphere, in the sum in Eq. (3.54) the term with $n=1$ is the leading one [recall (3.58)] and hence, Eq. (3.54) for the limiting case of small sphere reduces to

$$U_e(r_A) = \frac{\hbar\mu_0^2}{16\pi^3 r_A^4}\int_0^\infty \mathrm{d}u\,\alpha_A(iu)\mathrm{e}^{-2r_A u/c}\left[u^2\beta_{\rm sp}(iu)\left(1 + 2\frac{r_A u}{c} + \frac{r_A^2u^2}{c^2}\right)\right.$$
$$\left. -\frac{c^4}{r_A^2}\alpha_{\rm sp}(iu)\left(3 + 6\frac{r_A u}{c} + 5\frac{r_A^2u^2}{c^2} + 2\frac{r_A^3u^3}{c^3} + \frac{r_A^4u^4}{c^4}\right)\right], \tag{3.63}$$

where

$$\alpha_{\rm sp}(\omega) = 4\pi\varepsilon_0 R^3\frac{\varepsilon(\omega)-1}{\varepsilon(\omega)+2}, \tag{3.64}$$

$$\beta_{\rm sp}(\omega) = \frac{4\pi R^3}{\mu_0}\frac{\mu(\omega)-1}{\mu(\omega)+2}. \tag{3.65}$$

Let us consider a sphere to which the Clausius-Mossotti relation applies, so that

$$\frac{\varepsilon(\omega)-1}{\varepsilon(\omega)+2} = \frac{1}{3\varepsilon_0}\sum_k n_k\alpha_k(\omega), \tag{3.66}$$

with n_k and $\alpha_k(\omega)$, respectively, being the number density and the polarizability of the atoms of type k. Denoting by N_k the number of atoms of type k of the sphere, Eq. (3.64) can be written as

$$\alpha_{\rm sp}(\omega) = \sum_k N_k\alpha_k(\omega), \tag{3.67}$$

Accordingly, the magnetic analog of Eq. (3.67) is

$$\beta_{\rm sp}(\omega) = \sum_k N_k\beta_k(\omega) \tag{3.68}$$

with $\beta_k(\omega)$ being the magnetizability of the atoms of type k. Hence we may replace in Eq. (3.63) the sphere parameters $\alpha_{\rm sp}$ and $\beta_{\rm sp}$, respectively, with the electric and magnetic polarizability of a single atom [say α_k and β_k], to obtain the vdW interaction potential between two atoms, one being polarizable while the one another being simultaneously polarizable and magnetizable. The first and second terms in the squared brackets in Eq. (3.63) are, respectively, in agreement with the findings in Refs. [24] and [19].

Let us now evaluate the magnetic part of the vdW potential of the atom for which the tensor $\boldsymbol{L}^{(1)}$ is required. This can be obtained by substituting $\boldsymbol{G}^{(1)}$ from Eq. (3.46) into Eq. (3.16), leading to

$$\boldsymbol{L}^{(1)}(\mathbf{r},\mathbf{r}',\omega)=\frac{-i\omega^3}{4\pi c^3}\sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)}\sum_{m=0}^{n}\frac{(n-m)!}{(n+m)!}(2-\delta_{0m})$$
$$\times\sum_{p=\pm1}\left[B_n^N(\omega)\mathbf{M}_{nm,p}(\mathbf{r},\omega/c)\mathbf{M}_{nm,p}(\mathbf{r}',\omega/c)+B_n^M(\omega)\mathbf{N}_{nm,p}(\mathbf{r},\omega/c)\mathbf{N}_{nm,p}(\mathbf{r}',\omega/c)\right], \quad (3.69)$$

where the relations (3.49) and (3.50) have been used. Similar to the multilayer example, the magnetic part of the potential can be obtained from its electric part. Comparing Eq. (3.17) [together with Eq. (3.69)] and Eq. (3.11) [together with Eq. (3.46)] it is seen that the magnetic part of the vdW potential can be found from the right-hand side of Eq. (3.54) by replacing α_A with β_A/c^2 and interchanging of B_n^M and B_n^N (or equivalently interchanging of ε and μ), in agreement with the electromagnetic duality principle [95, HS6].

It is worth noting that according to Eq. (3.63) the interaction between an electric atom and an atom with both electric and magnetic polarizabilities, can be expressed as the superposition of the interaction potential between two electric atoms and the one between an electric atom and a magnetic atom. Hence, making use of the duality properties mentioned above, Eq. (3.63) can be generalized easily to give the interaction between two atoms, both with electric and magnetic polarizabilities [24, 35, 105]. Note that in the case of atoms possessing crossed electric-magnetic polarizabilities, the right-hand side of Eq. (3.63) will be supplemented by a non-additive term (see, e.g., Ref. [25]), so that the interaction potential is no longer the superposition of the electric-electric and electric-magnetic interactions.

Chapter 4

Two-atom vdW interaction potential

The method used in the previous chapter to obtain the single-atom vdW potential can be used to find the potential for the cases including many atoms. In a many-atom case with the interatomic forces being disregarded comparing to the forces originated from the material bodies, e.g., in the case of sufficiently large(small) interatomic(atom-body) distances, the total vdW potential may be given as a sum over single-atom potentials and the force acting on each atom A is given by Eq. (3.1), independent of the other atomic positions. As the interatomic forces become more pronounced the total vdW force on each atom follows from a potential that depends on all atomic positions and requires higher order perturbative calculations. In what follows, we calculate the vdW interaction potential between two ground-state atoms with both electric and magnetic polarizabilities in the presence of arbitrary magnetoelectric environment.

4.1 General expression

The Hamiltonian for a system consisting of two atoms A and B with nonrelativistic center-of-mass motion and the medium assisted electromagnetic field in the long wave-length approximation can be given in the form

$$\hat{H} = \hat{H}_F + \sum_{A'=A,B} \hat{H}_{A'} + \sum_{A'=A,B} \hat{H}_{A'F}, \tag{4.1}$$

with $\hat{H}_F$, $\hat{H}_{A'}$, and $\hat{H}_{A'F}$ being given by Eqs. (2.92), (2.93), and (2.99), respectively. To describe the medium-assisted vdW interaction potential between two atoms by a perturbative approach, we can exploit an argument similar to the one in the beginning of Sec. 3.1 that suggests to treat the first two terms on the right-hand side of Eq. (4.1) as the unperturbed Hamiltonian and the sum over the atom-field interaction Hamiltonians as the perturbation

$$\hat{H}_{\rm int} = \hat{H}_{AF} + \hat{H}_{BF} = -\hat{\mathbf{d}}_A \cdot \hat{\mathbf{E}}(\mathbf{r}_A) - \hat{\mathbf{m}}_A \cdot \hat{\mathbf{B}}(\mathbf{r}_A) - \hat{\mathbf{d}}_B \cdot \hat{\mathbf{E}}(\mathbf{r}_B) - \hat{\mathbf{m}}_B \cdot \hat{\mathbf{B}}(\mathbf{r}_B). \tag{4.2}$$

Let us consider the two atoms and the medium-assisted electromagnetic field to be prepared in their ground state such that the (unperturbed) state of the overall system is given by $|0\rangle = |0_A\rangle|0_B\rangle|\{0\}\rangle$. Having the vdW potential of each individual atom processed in chapter 3, here we focus on the interatomic vdW potential. The leading-order energy shift

describing the interaction between the atoms is given by the fourth-order perturbation

$$\Delta^{(4)}E = -\sum_{I,II,III\neq 0}\frac{\langle 0|\hat{H}_{\rm int}|III\rangle\langle III|\hat{H}_{\rm int}|II\rangle\langle II|\hat{H}_{\rm int}|I\rangle\langle I|\hat{H}_{\rm int}|0\rangle}{(E_{III}-E_0)\,(E_{II}-E_0)\,(E_I-E_0)} + \sum_{I,II\neq 0}\frac{\langle 0|\hat{H}_{\rm int}|II\rangle\langle II|\hat{H}_{\rm int}|0\rangle\langle 0|\hat{H}_{\rm int}|I\rangle\langle I|\hat{H}_{\rm int}|0\rangle}{(E_I-E_0)^2\,(E_{II}-E_0)}, \tag{4.3}$$

while the first- and third-order energy shift vanish since the electric and magnetic dipole moments do not have diagonal matrix elements in the basis of atomic energy-eigenstates, and the second-order energy shift contributes only to the vdW potential of the atoms, individually. On the right-hand side of Eq. (4.3), each matrix element appearing in the numerators may be thought of as being associated with a virtual process, which consists of a photon exchange between one of the atoms and the electromagnetic field together with a transition in the same atom. Every single numerator thus is related to four photon exchanges (two emissions and two absorptions) and two mutually opposite transitions in each atom. Only the terms in which the photon emitted by one of the atoms is absorbed by the other one can be counted for the two-atom interaction and hence, the second term on the right-hand side of Eq. (4.3) does not contribute to the interaction potential and the energy shift associated with the two-atom interaction reduces to the first term on the right-hand side of Eq. (4.3)

$$\Delta E_{AB} = -\sum_{I,II,III\neq 0}\frac{\langle 0|\hat{H}_{\rm int}|III\rangle\langle III|\hat{H}_{\rm int}|II\rangle\langle II|\hat{H}_{\rm int}|I\rangle\langle I|\hat{H}_{\rm int}|0\rangle}{(E_{III}-E_0)\,(E_{II}-E_0)\,(E_I-E_0)}. \tag{4.4}$$

Further, it can be inferred that the summand on the right-hand side of Eq. (4.3) vanishes unless the intermediate states $|I\rangle$ and $|III\rangle$ are such that one of the atoms is excited and one medium-assisted field excitation is present, while the intermediate state $|II\rangle$ corresponds to one of the following three types: (i) both atoms in the ground state with two field excitation present, (ii) both atoms excited with no field excitation present, and (iii) both atoms excited with two field excitation present. All possible intermediate states together with the respective denominators are listed in Tab. 4.1.

Let us consider, e.g., case (1) in Tab. 4.1 for which the required matrix elements are found to be as follows:

$$\langle 0|\hat{H}_{\rm int}|I\rangle = -\left[\mathbf{d}_A^{0k}\cdot\boldsymbol{G}_{\lambda_1}(\mathbf{r}_A,\mathbf{r}_1,\omega_1)\right]_{i_1} + \frac{i}{\omega_1}\left[\mathbf{m}_A^{0k}\cdot\boldsymbol{\nabla}_A\times\boldsymbol{G}_{\lambda_1}(\mathbf{r}_A,\mathbf{r}_1,\omega_1)\right]_{i_1}, \tag{4.5}$$

$$\langle I|\hat{H}_{\rm int}|II\rangle = -\frac{\delta_{(13)}}{\sqrt{2}}\left[\mathbf{d}_A^{k0}\cdot\boldsymbol{G}_{\lambda_2}(\mathbf{r}_A,\mathbf{r}_2,\omega_2)\right]_{i_2} - \frac{\delta_{(12)}}{\sqrt{2}}\left[\mathbf{d}_A^{k0}\cdot\boldsymbol{G}_{\lambda_3}(\mathbf{r}_A,\mathbf{r}_3,\omega_3)\right]_{i_3} + \frac{i\delta_{(13)}}{\omega_2\sqrt{2}}\left[\mathbf{m}_A^{k0}\cdot\boldsymbol{\nabla}_A\times\boldsymbol{G}_{\lambda_2}(\mathbf{r}_A,\mathbf{r}_2,\omega_2)\right]_{i_2} + \frac{i\delta_{(12)}}{\omega_3\sqrt{2}}\left[\mathbf{m}_A^{k0}\cdot[\boldsymbol{\nabla}_A\times\boldsymbol{G}_{\lambda_3}(\mathbf{r}_A,\mathbf{r}_3,\omega_3)\right]_{i_3}, \tag{4.6}$$

Case	$\|I\rangle$	$\|II\rangle$	$\|III\rangle$	Denominator
(1)	$\|k_A\rangle\|0_B\rangle\|1_{(1)}\rangle$	$\|0_A\rangle\|0_B\rangle\|1_{(2)},1_{(3)}\rangle$	$\|0_A\rangle\|l_B\rangle\|1_{(4)}\rangle$	$D_{1a}=(\omega_A^k+\omega')(\omega'+\omega)(\omega_B^l+\omega')$,
				$D_{1b}=(\omega_A^k+\omega')(\omega'+\omega)(\omega_B^l+\omega)$
(2)	$\|k_A\rangle\|0_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|\{0\}\rangle$	$\|0_A\rangle\|l_B\rangle\|1_{(2)}\rangle$	$D_2=(\omega_A^k+\omega')(\omega_A^k+\omega_B^l)(\omega_B^l+\omega)$
(3)	$\|k_A\rangle\|0_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|\{0\}\rangle$	$\|k_A\rangle\|0_B\rangle\|1_{(2)}\rangle$	$D_3=(\omega_A^k+\omega')(\omega_A^k+\omega_B^l)(\omega_A^k+\omega)$
(4)	$\|k_A\rangle\|0_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|1_{(2)},1_{(3)}\rangle$	$\|0_A\rangle\|l_B\rangle\|1_{(4)}\rangle$	$D_4=(\omega_A^k+\omega')(\omega_A^k+\omega_B^l+\omega'+\omega)(\omega_B^l+\omega')$
(5)	$\|k_A\rangle\|0_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|1_{(2)},1_{(3)}\rangle$	$\|k_A\rangle\|0_B\rangle\|1_{(4)}\rangle$	$D_5=(\omega_A^k+\omega')(\omega_A^k+\omega_B^l+\omega'+\omega)(\omega_A^k+\omega)$
(6)	$\|0_A\rangle\|l_B\rangle\|1_{(1)}\rangle$	$\|0_A\rangle\|0_B\rangle\|1_{(2)},1_{(3)}\rangle$	$\|k_A\rangle\|0_B\rangle\|1_{(4)}\rangle$	$D_{6a}=(\omega_B^l+\omega')(\omega'+\omega)(\omega_A^k+\omega')$,
				$D_{6b}=(\omega_B^l+\omega')(\omega'+\omega)(\omega_A^k+\omega)$
(7)	$\|0_A\rangle\|l_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|\{0\}\rangle$	$\|k_A\rangle\|0_B\rangle\|1_{(2)}\rangle$	$D_7=(\omega_B^l+\omega')(\omega_A^k+\omega_B^l)(\omega_A^k+\omega)$
(8)	$\|0_A\rangle\|l_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|\{0\}\rangle$	$\|0_A\rangle\|l_B\rangle\|1_{(2)}\rangle$	$D_8=(\omega_B^l+\omega')(\omega_A^k+\omega_B^l)(\omega_B^l+\omega)$
(9)	$\|0_A\rangle\|l_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|1_{(2)},1_{(3)}\rangle$	$\|k_A\rangle\|0_B\rangle\|1_{(4)}\rangle$	$D_9=(\omega_B^l+\omega')(\omega_A^k+\omega_B^l+\omega'+\omega)(\omega_A^k+\omega')$
(10)	$\|0_A\rangle\|l_B\rangle\|1_{(1)}\rangle$	$\|k_A\rangle\|l_B\rangle\|1_{(2)},1_{(3)}\rangle$	$\|0_A\rangle\|l_B\rangle\|1_{(4)}\rangle$	$D_{10}=(\omega_B^l+\omega')(\omega_A^k+\omega_B^l+\omega'+\omega)(\omega_B^l+\omega)$

Table 4.1: The intermediate states contributing to the two-atom vdW interaction according to Eq. (4.4) together with the energy denominators are shown, where the short-hand notations $|1_{(\mu)}\rangle=|1_{\lambda_\mu i_\mu}(\mathbf{r}_\mu,\omega_\mu)\rangle$ and $|1_{(\mu)},1_{(\nu)}\rangle=|1_{\lambda_\mu i_\mu}(\mathbf{r}_\mu,\omega_\mu),1_{\lambda_\nu i_\nu}(\mathbf{r}_\nu,\omega_\nu)\rangle$ have been used.

$$\begin{aligned}\langle II|\hat{H}_{\rm int}|III\rangle=&-\frac{\delta_{(34)}}{\sqrt{2}}\left[\mathbf{d}_B^{0l}\cdot\boldsymbol{G}^*_{\lambda_2}(\mathbf{r}_B,\mathbf{r}_2,\omega_2)\right]_{i_2}-\frac{\delta_{(24)}}{\sqrt{2}}\left[\mathbf{d}_B^{0l}\cdot\boldsymbol{G}^*_{\lambda_3}(\mathbf{r}_B,\mathbf{r}_3,\omega_3)\right]_{i_3}\\&-\frac{i\delta_{(34)}}{\omega_2\sqrt{2}}\left[\mathbf{m}_B^{0l}\cdot\boldsymbol{\nabla}_B\times\boldsymbol{G}^*_{\lambda_2}(\mathbf{r}_B,\mathbf{r}_2,\omega_2)\right]_{i_2}-\frac{i\delta_{(24)}}{\omega_3\sqrt{2}}\left[\mathbf{m}_B^{0l}\cdot\boldsymbol{\nabla}_B\times\boldsymbol{G}^*_{\lambda_3}(\mathbf{r}_B,\mathbf{r}_3,\omega_3)\right]_{i_3},\end{aligned}\tag{4.7}$$

$$\langle III|\hat{H}_{\rm int}|0\rangle=-\left[\mathbf{d}_B^{l0}\cdot\boldsymbol{G}^*_{\lambda_4}(\mathbf{r}_B,\mathbf{r}_4,\omega_4)\right]_{i_4}-\frac{i}{\omega_4}\left[\mathbf{m}_B^{l0}\cdot\boldsymbol{\nabla}_B\times\boldsymbol{G}^*_{\lambda_4}(\mathbf{r}_B,\mathbf{r}_4,\omega_4)\right]_{i_4},\tag{4.8}$$

where

$$\delta_{(\alpha\beta)}=\delta_{i_\alpha i_\beta}\delta_{\lambda_\alpha\lambda_\beta}\delta(\mathbf{r}_\alpha-\mathbf{r}_\beta)\delta(\omega_\alpha-\omega_\beta).\tag{4.9}$$

By substituting these matrix elements into Eq. (4.3), we derive the contribution $\Delta E_{(1)}$ to the two-atom energy shift ΔE. Restricting the consideration to non-chiral atoms, since the selection rules for electric-dipole transitions differ (under parity) from those of magnetic-dipole transitions, the two mutually oposite transitions made by each atom must be either of electric- or magnetic-dipole type (for the interaction of two chiral molecules in free space, see Ref. [102]). Therefore, as in the single-atom case, we may distinguish different classes of contributions to the vdW interaction between two atoms A and B which are both electric and magnetic according to electric or magnetic nature of those transitions. The vdW interaction [potential $V(\mathbf{r}_A,\mathbf{r}_B)$] thus may be considered as the superposition of (i) an electric–electric interaction [potential $V_{ee}(\mathbf{r}_A,\mathbf{r}_B)$] where both atoms are electrically polarizable, (ii) an electric–magnetic interaction [potential $V_{em}(\mathbf{r}_A,\mathbf{r}_B)$] where atom A is electrically polarizable and atom B is magnetically polarizable, (iii) the reverse case [potential

$V_{me}(\mathbf{r}_A, \mathbf{r}_B)$], and (iv) a magnetic–magnetic interaction [potential $V_{mm}(\mathbf{r}_A, \mathbf{r}_B)$] where both atoms are magnetically polarizable:

$$V(\mathbf{r}_A, \mathbf{r}_B) = V_{ee}(\mathbf{r}_A, \mathbf{r}_B) + V_{em}(\mathbf{r}_A, \mathbf{r}_B) + V_{me}(\mathbf{r}_A, \mathbf{r}_B) + V_{mm}(\mathbf{r}_A, \mathbf{r}_B). \tag{4.10}$$

To calculate the electric-electric part of the vdW potential, let us consider again case (1) in Tab. 4.1. The corresponding matrix elements in the numerator of Eq. (4.4) can be obtained from Eqs. (4.5)–(4.8) by ignoring the terms associated with magnetic dipole moments of the atoms. In this way we derive the contribution $\Delta E^{ee}_{AB(1)}$ to the two-atom energy shift ΔE^{ee}_{AB} to be

$$\begin{aligned}\Delta E^{ee}_{AB(1)} = -\frac{1}{\hbar^3}\sum_{k,l}\sum_{j=1,2}\sum_{\lambda_1,\lambda_2}\int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \int_0^\infty \mathrm{d}\omega_1 \int_0^\infty \mathrm{d}\omega_2 \, \frac{1}{(\omega_A^k+\omega_1)(\omega_1+\omega_2)(\omega_B^l+\omega_j)} \\ \times \Big\{ \delta_{j1}\mathbf{d}_A^{0k}\cdot \boldsymbol{G}_{\lambda_1}(\mathbf{r}_A,\mathbf{r}_1,\omega_1)\cdot \boldsymbol{G}^{*\mathsf{T}}_{\lambda_1}(\mathbf{r}_B,\mathbf{r}_1,\omega_1)\cdot \mathbf{d}_B^{l0}\mathbf{d}_A^{k0}\cdot \boldsymbol{G}_{\lambda_2}(\mathbf{r}_A,\mathbf{r}_2,\omega_2)\cdot \boldsymbol{G}^{*\mathsf{T}}_{\lambda_2}(\mathbf{r}_B,\mathbf{r}_2,\omega_2)\cdot \mathbf{d}_B^{0l} \\ + \delta_{j2}\mathbf{d}_A^{0k}\cdot \boldsymbol{G}_{\lambda_1}(\mathbf{r}_A,\mathbf{r}_1,\omega_1)\cdot \boldsymbol{G}^{*\mathsf{T}}_{\lambda_1}(\mathbf{r}_B,\mathbf{r}_1,\omega_1)\cdot \mathbf{d}_B^{0l}\mathbf{d}_A^{k0}\cdot \boldsymbol{G}_{\lambda_2}(\mathbf{r}_A,\mathbf{r}_2,\omega_2)\cdot \boldsymbol{G}^{*\mathsf{T}}_{\lambda_2}(\mathbf{r}_B,\mathbf{r}_2,\omega_2)\cdot \mathbf{d}_B^{l0} \Big\}.\end{aligned} \tag{4.11}$$

Using the integral relation (2.35) we may perform the volume integrals in Eq. (4.11) to simplify it to

$$\begin{aligned}\Delta E^{ee}_{AB(1)} = -\frac{\mu_0^2}{\hbar\pi^2}\sum_{n,m}\int_0^\infty \mathrm{d}\omega \int_0^\infty \mathrm{d}\omega' \, \omega^2\omega'^2\left(\frac{1}{D_{1a}}+\frac{1}{D_{1b}}\right) \\ \times \left[\mathbf{d}_A^{0k}\cdot \mathrm{Im}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega)\cdot \mathbf{d}_B^{0l}\right]\left[\mathbf{d}_A^{0k}\cdot \mathrm{Im}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega')\cdot \mathbf{d}_B^{0l}\right],\end{aligned} \tag{4.12}$$

where D_{1a} and D_{1b} are, respectively, the first and second denominators in Tab. 4.1, and without loss of generality we have assumed that the matrix elements of the electric-dipole operators are real. The contributions $\Delta E^{ee}_{AB(i)}$ to ΔE^{ee}_{AB} which correspond to the cases (2)–(10) in Tab. 4.1 can be calculated analogously. It turns out that they differ from Eq. (4.12) only in the energy denominators. Therefore, ΔE^{ee}_{AB} can be found from the right-hand side of Eq. (4.12) by replacing the brackets in the first line by a sum over all denominators, that can be replaced by

$$\frac{4(\omega_A^k+\omega_B^l+\omega)}{(\omega_A^k+\omega_B^l)(\omega_A^k+\omega)(\omega_B^l+\omega)}\left(\frac{1}{\omega+\omega'}-\frac{1}{\omega-\omega'}\right) \tag{4.13}$$

under double frequency integral in (4.12), where we have exploited the fact that the remaning integrand is symmetric with respect to an exchange of ω and ω' (Appendix C). Hence, the two-atom contributions $\Delta E^{ee}_{AB(k)}$ to the fourth-order energy shift lead to the vdW potential

$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)=\sum_i \Delta E_{AB(i)}$ as follows:

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)=-\frac{4\mu_0^2}{\hbar\pi^2}\sum_{k,l}\frac{1}{\omega_A^k+\omega_B^l}\int_0^\infty \mathrm{d}\omega\int_0^\infty \mathrm{d}\omega'\frac{\omega^2\omega'^2(\omega_A^k+\omega_B^l+\omega)}{(\omega_A^k+\omega)(\omega_B^l+\omega)}\left(\frac{1}{\omega+\omega'}-\frac{1}{\omega-\omega'}\right)$$
$$\times[\mathbf{d}_A^{0k}\cdot\mathrm{Im}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega)\cdot\mathbf{d}_B^{0l}][\mathbf{d}_A^{0k}\cdot\mathrm{Im}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega')\cdot\mathbf{d}_B^{0l}]. \quad (4.14)$$

The integral over ω', upon using the identity $\mathrm{Im}\,\boldsymbol{G}=(\boldsymbol{G}-\boldsymbol{G}^*)/(2i)$ and relation (2.25) can be written as

$$\int_0^\infty \mathrm{d}\omega'\left(\frac{1}{\omega+\omega'}-\frac{1}{\omega-\omega'}\right)\omega'^2\mathrm{Im}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega')$$
$$=\frac{1}{2i}\int_{-\infty}^\infty \mathrm{d}\omega'\left(\frac{1}{\omega+\omega'}-\frac{1}{\omega-\omega'}\right)\omega'^2\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega'), \quad (4.15)$$

where the poles at $\omega'=-\omega$ and $\omega'=\omega$ are to be treated as principal values. The Green tensor is analytic in the upper half of the complex frequency plane including the real axis, apart from a possible pole at the origin. We may therefore replace the integral on the right-hand side of Eq. (4.15) by contour integrals along infinitely small half-circles surrounding $\pm\omega$, and an infinitely large half-circle in the upper complex half-plane. The integral along the infinitely large half-circle vanishes and collecting the contributions from the infinitely small half-circles, we end up with

$$\int_0^\infty \mathrm{d}\omega'\left(\frac{1}{\omega+\omega'}-\frac{1}{\omega-\omega'}\right)\omega'^2\mathrm{Im}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega')=\frac{\pi}{2}\omega^2[\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega)+\boldsymbol{G}^*(\mathbf{r}_A,\mathbf{r}_B,\omega)], \quad (4.16)$$

where we have again made use of the relation (2.25). Substitution of Eq. (4.16) into Eq. (4.14) leads to

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)=-\frac{\mu_0^2}{i\hbar\pi}\sum_{k,l}\frac{1}{\omega_A^k+\omega_B^l}\left\{\int_0^\infty \mathrm{d}\omega\frac{\omega^4(\omega_A^k+\omega_B^l+\omega)}{(\omega_A^k+\omega)(\omega_B^l+\omega)}\right.$$
$$\left.+\int_0^{-\infty} \mathrm{d}\omega\frac{\omega^4(\omega_A^k+\omega_B^l-\omega)}{(\omega_A^k-\omega)(\omega_B^l-\omega)}\right\}[\mathbf{d}_A^{0k}\cdot\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega)\cdot\mathbf{d}_B^{0l}]^2. \quad (4.17)$$

It can be seen that the integrands in Eq. (4.17) are analytic in the upper half of the complex frequency plane, including the positive real axis. Therefore, this equation can be further simplified by using a contour-integral techniques analogous to the one below Eq. (3.14), which transforms the integrals on the right-hand side to the ones over the imaginary axis. Combining the contributions from the two integrals leads to

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)=-\frac{2\mu_0^2}{\hbar\pi}\sum_{k,l}\int_0^\infty\frac{\mathrm{d}u\,u^4\omega_A^k\omega_B^l}{[(\omega_A^k)^2+u^2][(\omega_B^l)^2+u^2]}[\mathbf{d}_A^{0k}\cdot\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\mathbf{d}_B^{0l}]^2. \quad (4.18)$$

An expression of this type was first given in Ref. [32] on the basis of a heuristic generalization of the respective free-space result. We may rewrite Eq. (4.18) in terms of electric polarizabilities of the atoms defined by Eq. (3.8) as

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B) = -\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}u\, u^4\,\mathrm{Tr}\big[\boldsymbol{\alpha}_A(iu)\cdot\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\boldsymbol{\alpha}_B(iu)\cdot\boldsymbol{G}(\mathbf{r}_B,\mathbf{r}_A,iu)\big], \tag{4.19}$$

where Eq. (2.35) is used. In particular for isotropic atoms Eq. (4.19) becomes

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B) = -\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}u\, u^4\alpha_A(iu)\alpha_B(iu)\,\mathrm{Tr}\big[\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\boldsymbol{G}(\mathbf{r}_B,\mathbf{r}_A,iu)\big]. \tag{4.20}$$

Now, we calculate the electric-magnetic vdW potential V_{em}, which is due to contribution of atom A undergoing electric transitions and B undergoing magnetic transitions. Each of the possible intermediate-state combinations listed in Tab. 4.1 contributes to V_{em}, where again we begin with the intermediate states of case (1). The respective matrix elements in the numerator of Eq. (4.4) can be obtained from Eqs. (4.5)–(4.8) by ignoring the terms associated with either magnetic dipole moment of atom A or electric dipole moment of atom B. Substituting the results in Eq. (4.4) the contribution $\Delta E^{em}_{AB(1)}$ to the two atom energy shift ΔE^{em}_{AB} is found to be

$$\begin{aligned}\Delta E^{em}_{AB(1)} = \frac{\mu_0^2}{\hbar\pi^2}\sum_{k,l}\int_0^\infty \mathrm{d}\omega\,\omega\int_0^\infty \mathrm{d}\omega'\,\omega'\left(\frac{1}{D_{1a}}+\frac{1}{D_{1b}}\right)\\ \times\Big\{\Big[\mathbf{d}_A^{0k}\cdot\mathrm{Im}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega)\times\overleftarrow{\boldsymbol{\nabla}}_B\cdot\mathbf{m}_B^{0l}\Big]\big[\mathbf{d}_A^{0k}\cdot\boldsymbol{\nabla}_B\times\mathrm{Im}\boldsymbol{G}(\mathbf{r}_B,\mathbf{r}_A,\omega')\cdot\mathbf{m}_B^{0l}\big]\Big\},\end{aligned} \tag{4.21}$$

where the integral relation (2.35) is used. One can then easily find that the contributions $\Delta E^{em}_{AB(k)}$ ($k\in\{2,3,\ldots,10\}$) from the other possible intermediate-state combinations differ from Eq. (4.21) only with respect to their energy denominators and signs. Case (6) leads to two terms with different energy denominators $1/D_{6a}+1/D_{6b}$, just like case (1), while all other cases only give rise to a single term each. Furthermore, the contributions from cases (3)–(5), (8)–(10) differ in sign from Eq. (4.21). The electric–magnetic vdW potential can be found as the sum of all contributions $V_{em}(\mathbf{r}_A,\mathbf{r}_B)=\sum_k \Delta E^{em}_{AB(k)}$. It can be seen that the denominator sum

$$\begin{aligned}&\frac{1}{D_{1a}}+\frac{1}{D_{1b}}+\frac{1}{D_2}-\frac{1}{D_3}-\frac{1}{D_4}-\frac{1}{D_5}+\frac{1}{D_{6a}}+\frac{1}{D_{6b}}\\&+\frac{1}{D_7}-\frac{1}{D_8}-\frac{1}{D_9}-\frac{1}{D_{10}}\end{aligned} \tag{4.22}$$

can be replaced by

$$\frac{4(\omega_A^k+\omega_B^l+\omega)}{(\omega_A^k+\omega_B^l)(\omega_A^k+\omega)(\omega_B^l+\omega)}\left(\frac{1}{\omega+\omega'}+\frac{1}{\omega-\omega'}\right), \tag{4.23}$$

under the double frequency integral in Eq. (4.21) (Appendix C). Hence the interaction potential $V_{em}(\mathbf{r}_A, \mathbf{r}_B)$ can be obtained from the right-hand side of Eq. (4.21) by replacing the brackets in the first line with (4.23) as

$$V_{em}(\mathbf{r}_A, \mathbf{r}_B) = -\frac{4\mu_0^2}{\hbar\pi^2} \sum_{k,l} \frac{1}{\omega_A^k + \omega_B^l} \int_0^\infty \mathrm{d}\omega \int_0^\infty \mathrm{d}\omega' \frac{\omega\omega'(\omega_A^k + \omega_B^l + \omega)}{(\omega_A^k + \omega)(\omega_B^l + \omega)} \left(\frac{1}{\omega + \omega'} + \frac{1}{\omega - \omega'}\right)$$
$$\times \left\{ \left[\mathbf{d}_A^{0k} \cdot \mathrm{Im}\, \boldsymbol{G}(\mathbf{r}_A, \mathbf{r}_B, \omega) \times \overleftarrow{\boldsymbol{\nabla}}_B \cdot \mathbf{m}_B^{0l} \right] \left[\mathbf{m}_B^{0l} \cdot \boldsymbol{\nabla}_B \times \mathrm{Im}\, \boldsymbol{G}(\mathbf{r}_B, \mathbf{r}_A, \omega') \cdot \mathbf{d}_A^{0k} \right] \right\}. \quad (4.24)$$

Finally, following a procedure similar to the one for converting Eq. (4.14) to (4.19), we will end up with

$$V_{em}(\mathbf{r}_A, \mathbf{r}_B) = \frac{\hbar\mu_0^2}{2\pi} \int_0^\infty \mathrm{d}u\, u^2 \mathrm{Tr} \left[\boldsymbol{\alpha}_A(iu) \cdot \boldsymbol{K}^{\mathsf{T}}(\mathbf{r}_B, \mathbf{r}_A, iu) \cdot \boldsymbol{\beta}_B(iu) \cdot \boldsymbol{K}(\mathbf{r}_B, \mathbf{r}_A, iu) \right]$$
$$= \frac{\hbar\mu_0^2}{2\pi} \int_0^\infty \mathrm{d}u\, u^2 \alpha_A(iu)\beta_B(iu) \mathrm{Tr} \left[\boldsymbol{K}^{\mathsf{T}}(\mathbf{r}_B, \mathbf{r}_A, iu) \cdot \boldsymbol{K}(\mathbf{r}_B, \mathbf{r}_A, iu) \right], \quad (4.25)$$

where

$$\boldsymbol{K}(\mathbf{r}, \mathbf{r}', \omega) = \boldsymbol{\nabla} \times \boldsymbol{G}(\mathbf{r}, \mathbf{r}', \omega), \quad (4.26)$$

and the second equality holds for isotropic atoms. Obviously, the magnetic–electric potential $V_{me}(\mathbf{r}_A, \mathbf{r}_B)$, which is due to all contributions of atom A undergoing magnetic transitions and atom B undergoing electric transitions, can be obtained from Eq. (4.25) by interchanging the subscripts A and B on the right-hand side of Eq. (4.25).

The magnetic–magnetic potential V_{mm}, associated with magnetic transitions of both atoms, can be found in a procedure analogous to the one outlined above for deriving Eq. (4.25), resulting in

$$V_{mm}(\mathbf{r}_A, \mathbf{r}_B) = -\frac{\hbar\mu_0^2}{2\pi} \int_0^\infty \mathrm{d}u \mathrm{Tr} \left[\boldsymbol{\beta}_A(iu) \cdot \boldsymbol{L}(\mathbf{r}_A, \mathbf{r}_B, iu) \cdot \boldsymbol{\beta}_B(iu) \cdot \boldsymbol{L}(\mathbf{r}_B, \mathbf{r}_A, iu) \right]$$
$$= -\frac{\hbar\mu_0^2}{2\pi} \int_0^\infty \mathrm{d}u\, \beta_A(iu)\beta_B(iu) \mathrm{Tr} \left[\boldsymbol{L}(\mathbf{r}_A, \mathbf{r}_B, iu) \cdot \boldsymbol{L}(\mathbf{r}_B, \mathbf{r}_A, iu) \right], \quad (4.27)$$

where the tensor $\boldsymbol{L}$ is given by Eq. (3.16) and again the second equality holds for isotropic atoms.

The total two-atom vdW potential of two polarizable and (para)magnetizable atoms placed within an arbitrary environment of magnetoelectric bodies is given by Eq. (4.10) together with Eqs. (4.19), (4.25) and (4.27) (the diamagnetic contribution to the dispersion potential of two atoms in free space is discussed in Refs. [102, 103, 104]). Having obtained the single-atom and two-atom vdW potentials, the total vdW force on atom A can be deduced from the potential $U(\mathbf{r}_A, \mathbf{r}_B)$

$$U(\mathbf{r}_A, \mathbf{r}_B) = U_A(\mathbf{r}_A) + U_B(\mathbf{r}_B) + V(\mathbf{r}_A, \mathbf{r}_B), \quad (4.28)$$

according to

$$\mathbf{F}_A(\mathbf{r}_A,\mathbf{r}_B) = -\boldsymbol{\nabla}_A U(\mathbf{r}_A,\mathbf{r}_B) = -\boldsymbol{\nabla}_A U_A(\mathbf{r}_A) + \mathbf{F}_{AB}(\mathbf{r}_A,\mathbf{r}_B), \tag{4.29}$$

with $\mathbf{F}_{AB}$ being the interatomic force on atom A

$$\mathbf{F}_{AB}(\mathbf{r}_A,\mathbf{r}_B) = -\boldsymbol{\nabla}_A V(\mathbf{r}_A,\mathbf{r}_B). \tag{4.30}$$

4.2 Local-field corrections

The two-atom interaction potentials given in Sec. 4.1 refer to two atoms placed in empty regions. As in the single-atom case, the potential formulae are to be corrected when one or both atoms are embedded in a magnetoelectric medium. Again, to treat the local field corrections we may apply the real-cavity model; each atom can be considered to be surrounded by small spherical free-space cavities of radius R_c. The local field corrected form of the Green tensor $\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega)$ is found in Ref. [64] to be

$$\boldsymbol{G}_{\rm loc}(\mathbf{r}_A,\mathbf{r}_B,\omega) = \frac{3\varepsilon_A}{2\varepsilon_A+1}\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,\omega)\frac{3\varepsilon_B}{2\varepsilon_B+1}\,, \tag{4.31}$$

where $\varepsilon_{A(B)} = \varepsilon(\mathbf{r}_{A(B)},\omega)$ and $\mu_{A(B)} = \mu(\mathbf{r}_{A(B)},\omega)$ are, respectively, the permittivity and permeability of the unperturbed medium at the position of the guest atom $A(B)$.

It may be instructive to compare Eq. (4.31) with the local-field corrected Green tensor for equal positions, Eq. (3.21). The position-independent first term on the right-hand side of Eq. (3.21), describes the electromagnetic field reaching the point $\mathbf{r}_A$, where it originated, after (multiple) scattering at the inner surface of the cavity surrounding atom A, and hence, a similar term does not exist in Eq. (4.31), in which A and B refer to two separate points ($\mathbf{r}_A \neq \mathbf{r}_B$).

Inserting the corrected Green tensor into Eq. (3.25), one obtains the local-field corrected form of the vdW interaction potential as [64]

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B) = -\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}u\, u^4 \left[\frac{3\varepsilon_A(iu)}{2\varepsilon_A(iu)+1}\right]^2 \left[\frac{3\varepsilon_B(iu)}{2\varepsilon_B(iu)+1}\right]^2 \times \mathrm{Tr}\big[\boldsymbol{\alpha}_A(iu)\cdot\boldsymbol{G}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\boldsymbol{\alpha}_B(iu)\cdot\boldsymbol{G}(\mathbf{r}_B,\mathbf{r}_A,iu)\big], \tag{4.32}$$

Following the method used in Ref. [64] in obtaining Eq. (4.32), the respective local-field corrected tensors for electric-magnetic and magnetic-magnetic vdW interaction potentials can be found in term of the uncorrected ones, respectively, as [HS5]

$$\boldsymbol{K}_{\rm loc}(\mathbf{r}_A,\mathbf{r}_B,\omega) = \frac{3}{2\mu_A+1}\boldsymbol{K}(\mathbf{r}_A,\mathbf{r}_B,\omega)\frac{3\varepsilon_B}{2\varepsilon_B+1}\,, \tag{4.33}$$

$$\boldsymbol{L}_{\rm loc}(\mathbf{r}_A,\mathbf{r}_B,\omega)=\frac{3}{2\mu_A+1}\boldsymbol{L}(\mathbf{r}_A,\mathbf{r}_B,\omega)\frac{3}{2\mu_B+1}\,. \tag{4.34}$$

The latter is almost a trivial consequent of having Eq. (3.30) obtained and a comparison between Eqs. (3.21) and (4.31). Replacing the uncorrected tensors in Eqs. (4.25), and (4.27) with the corrected ones leads to their local-field corrected form

$$V_{em}(\mathbf{r}_A,\mathbf{r}_B)=\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}u\,u^2\left[\frac{3}{2\mu_A(iu)+1}\right]^2\left[\frac{3\varepsilon_B(iu)}{2\varepsilon_B(iu)+1}\right]^2 \times \mathrm{Tr}\left[\boldsymbol{\alpha}_A(iu)\cdot\boldsymbol{K}^{\rm T}(\mathbf{r}_B,\mathbf{r}_A,iu)\cdot\boldsymbol{\beta}_B(iu)\cdot\boldsymbol{K}(\mathbf{r}_B,\mathbf{r}_A,iu)\right], \tag{4.35}$$

$$V_{mm}(\mathbf{r}_A,\mathbf{r}_B)=-\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}u\left[\frac{3}{2\mu_A(iu)+1}\right]^2\left[\frac{3}{2\mu_B(iu)+1}\right]^2 \times \mathrm{Tr}\left[\boldsymbol{\beta}_A(iu)\cdot\boldsymbol{L}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\boldsymbol{\beta}_B(iu)\cdot\boldsymbol{L}(\mathbf{r}_B,\mathbf{r}_A,iu)\right]. \tag{4.36}$$

Recall that $V_{me}(\mathbf{r}_A,\mathbf{r}_B)$ can be obtained from Eq. (4.35) by interchanging subscripts A and B on the right-hand side of this equation. Needless to say that Eqs. (4.32),(4.35), and (4.36) reduce to Eqs. (4.19), (4.25), and (4.27), respectively, when the atoms are situated in free space so that $\varepsilon_{A(B)}=\varepsilon_{A(B)}=1$.

4.3 Applications

Further process on the potential formulae, Eqs. (4.32), (4.35), and (4.36), is possible by substituting the explicit form of the respective tensors, $\boldsymbol{G}$, $\boldsymbol{K}$, and $\boldsymbol{L}$. This requires that the electromagnetic and geometric properties of the material environment be specified. In this section, considering various material systems we present the vdW potential formulae in explicit forms with respect to electric permittivities, magnetic permeabilities, and geometric properties of the systems. In order to illustrate the effect of the bodies on the interactions, the examples are supported by numerical results.

4.3.1 Bulk medium

Let us, for example, consider the two atoms embedded in an infinitely extended bulk medium of permittivity $\varepsilon(\omega)$ and permeability $\mu(\omega)$. To illustrate the relevance of the local-field corrections, let us first consider the uncorrected two-atom potential and begin with the contributions (4.19) and (4.27), which by making use of the bulk-material tensors as given in Eqs. (3.25) and (3.29) take the form

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar}{16\pi^3\varepsilon_0^2 l^6}\int_0^\infty \mathrm{d}u\,\alpha_A(iu)\alpha_B(iu)\,\frac{h_1[n(iu)ul/c]}{\varepsilon^2(iu)} \tag{4.37}$$

and

$$V_{mm}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar\mu_0^2}{16\pi^3 l^6}\int_0^\infty \mathrm{d}u\,\beta_A(iu)\beta_B(iu)\mu^2(iu)h_1[n(iu)ul/c] \tag{4.38}$$

$[\mathbf{l}=\mathbf{r}_B-\mathbf{r}_A,\ l=|\mathbf{l}|]$, where

$$h_1(x)=\mathrm{e}^{-2x}(3+6x+5x^2+2x^3+x^4). \tag{4.39}$$

We see that, due to the factors $\varepsilon^{-2}(iu)$ and $\mu^2(iu)$, the uncorrected quantities V_{ee} and V_{mm} do not transform into each other under the duality transformation $\varepsilon\leftrightarrow\mu$, $c^2\alpha\leftrightarrow\beta$. As a consequence, the uncorrected total two-atom potential violates the duality symmetry.

By contrast, the local-field corrected two-atom potential obeys the duality symmetry. From Eqs. (4.32) and (4.36) together with Eqs. (3.25) and (3.29), respectively, we find that

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar}{16\pi^3\varepsilon_0^2 l^6}\int_0^\infty \mathrm{d}u\,\alpha_A(iu)\alpha_B(iu)\,\frac{81\varepsilon^2(iu)}{[2\varepsilon(iu)+1]^4}\,h_1[n(iu)ul/c], \tag{4.40}$$

$$V_{mm}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar\mu_0^2}{16\pi^3 l^6}\int_0^\infty \mathrm{d}u\,\beta_A(iu)\beta_B(iu)\,\frac{81\mu^2(iu)}{[2\mu(iu)+1]^4}\,h_1[n(iu)ul/c]. \tag{4.41}$$

The needed tensor $\boldsymbol{K}_{\mathrm{bulk}}$ for calculating the interaction potentials V_{em} and V_{me}, can be obtained by substituting the bulk Green tensor (3.25) into Eq. (4.26) as

$$\boldsymbol{K}_{\mathrm{bulk}}(\mathbf{r}_B,\mathbf{r}_A,\omega)=-\boldsymbol{K}_{\mathrm{bulk}}^{\mathsf{T}}(\mathbf{r}_B,\mathbf{r}_A,\omega)=\frac{-\mu(\omega)\mathrm{e}^{ikl}}{4\pi l^2}\,(1-ikl)\mathbf{e}_l\times\boldsymbol{I} \tag{4.42}$$

($\mathbf{e}_l=\mathbf{l}/l$). We find that Eq. (4.35) takes the form

$$V_{em}(\mathbf{r}_A,\mathbf{r}_B)=\frac{\hbar\mu_0^2}{16\pi^3 l^4}\int_0^\infty \mathrm{d}u\,u^2\alpha_A(iu)\beta_B(iu)\,\frac{81\varepsilon^2(iu)\mu^2(iu)}{[2\varepsilon(iu)+1]^2[2\mu(iu)+1]^2}\,h_2[n(iu)ul/c], \tag{4.43}$$

where

$$h_2(x)=\mathrm{e}^{-2x}(1+2x+x^2), \tag{4.44}$$

from which $V_{me}(\mathbf{r}_A,\mathbf{r}_B)$ can be obtained by simply interchanging subscripts A and B on the right-hand side. Inspection of Eqs. (4.40), (4.41), and (4.43) immediately reveals that the duality transformation $\varepsilon\leftrightarrow\mu$, $c^2\alpha\leftrightarrow\beta$ results in

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)\leftrightarrow V_{mm}(\mathbf{r}_A,\mathbf{r}_B), \tag{4.45}$$

$$V_{em}(\mathbf{r}_A,\mathbf{r}_B)\leftrightarrow V_{me}(\mathbf{r}_A,\mathbf{r}_B), \tag{4.46}$$

so the total potential $V(\mathbf{r}_A,\mathbf{r}_B)$, Eq. (4.10), is invariant under the duality transformation. The result clearly shows that (i) the inclusion in the calculation of local-field effects is essential for obtaining duality-consistent results and that (ii) the real-cavity model is an appropriate tool for achieving this.

It may be instructive to have a look at the nonretarded and retarded limits of Eqs. (4.40), (4.41), and (4.43). In the nonretarded limit where the atom–atom separation is small in comparison with the characteristic atomic and medium wavelengths, the integrals in Eqs. (4.40), (4.41), and (4.43) are effectively limited to a region where $\mathrm{e}^{-2n(iu)ul/c} \simeq 1$, and the approximations $h_1[n(iu)ul/c] \simeq h_1(0)$ and $h_2[n(iu)ul/c] \simeq h_2(0)$ result in

$$V_{ee}(\mathbf{r}_A, \mathbf{r}_B) = \frac{-3\hbar}{16\pi^3\varepsilon_0^2 l^6} \int_0^\infty \mathrm{d}u\, \alpha_A(iu)\alpha_B(iu) \frac{81\varepsilon^2(iu)}{[2\varepsilon(iu)+1]^4}\,, \tag{4.47}$$

$$V_{mm}(\mathbf{r}_A, \mathbf{r}_B) = \frac{-3\hbar\mu_0^2}{16\pi^3 l^6} \int_0^\infty \mathrm{d}u\, \beta_A(iu)\beta_B(iu) \frac{81\mu^2(iu)}{[2\mu(iu)+1]^4}\,, \tag{4.48}$$

$$V_{em}(\mathbf{r}_A, \mathbf{r}_B) = \frac{\hbar\mu_0^2}{16\pi^3 l^4} \int_0^\infty \mathrm{d}u\, u^2 \alpha_A(iu)\beta_B(iu) \frac{81\varepsilon^2(iu)\mu^2(iu)}{[2\varepsilon(iu)+1]^2[2\mu(iu)+1]^2}\,. \tag{4.49}$$

In the opposite limit, i.e., retarded limit, due to the presence of the exponential factor in the integrands in Eqs. (4.40), (4.41), and (4.43), only small values of u significantly contribute. Hence we may approximately replace the atomic polarizabilities and magnetizabilities and the permittivity and permeability of the medium by their respective static values,

$$\alpha_{A(B)}(iu) = \alpha_{A(B)}(0), \quad \beta_{A(B)}(iu) = \beta_{A(B)}(0), \quad \varepsilon(iu) = \varepsilon(0), \quad \mu(iu) = \mu(0), \tag{4.50}$$

and perform the integrals in the closed form to yield

$$V_{ee}(\mathbf{r}_A, \mathbf{r}_B) = -\frac{23\hbar c\alpha_A(0)\alpha_B(0)}{64\pi^3\varepsilon_0^2 l^7} \frac{81\varepsilon^2(0)}{n(0)[2\varepsilon(0)+1]^4}\,, \tag{4.51}$$

$$V_{mm}(\mathbf{r}_A, \mathbf{r}_B) = -\frac{23\hbar c\mu_0^2\beta_A(0)\beta_B(0)}{64\pi^3 l^7} \frac{81\mu^2(0)}{n(0)[2\mu(0)+1]^4}\,, \tag{4.52}$$

$$V_{em}(\mathbf{r}_A, \mathbf{r}_B) = \frac{7\hbar c\mu_0\alpha_A(0)\beta_B(0)}{64\pi^3\varepsilon_0 l^7} \frac{81n(0)}{[2\varepsilon(0)+1]^2[2\mu(0)+1]^2}\,. \tag{4.53}$$

Comparing with the case of the two atoms being in free space $\varepsilon = \mu = 1$, we see that the medium modifies the magnitude of the interatomic potential contributions, but does not change their signs. Since $\varepsilon(iu) > 1$ and $\mu(iu) > 1$, inspection of Eqs. (4.40) and (4.41) reveals that the medium always leads to a reduction of V_{ee} and V_{mm}. In particular in the nonretarded limit, V_{ee} is only influenced by the electric properties of the medium and V_{mm} only by the magnetic ones, cf. Eqs. (4.47) and (4.48). On the contrary, V_{em} and V_{me} are reduced by the medium in the retarded limit, Eq. (4.53), but are enhanced by a factor of up to 81/16 [for $\varepsilon(iu) \gg 1$ and $\mu(iu) \gg 1$] in the nonretarded limit, Eq. (4.49).

In the retarded limit, the influence of the medium on all four types of potential contributions is very similar. The coupling of each atom to the field is screened by a factor $9\varepsilon(0)/[2\varepsilon(0)+1]^2$ for polarizable atoms, and a factor $9\mu(0)/[2\mu(0)+1]^2$ for magnetizable

atoms. In addition, the reduced speed of light in the medium leads to a further reduction of the potential by a factor $n(0)$.

It should be pointed out that the uncorrected potentials V_{mm} and V_{em} as given by Eqs. (4.41) and (4.43) differ from the corresponding results given in Ref. [105] by factors of μ^{-4} and μ^{-2}, respectively. The discrepancy is due to the different atom–field couplings employed; While our calculation is based on a magnetic coupling of the form $\mathbf{m}\cdot\hat{\mathbf{B}}$, a $\mathbf{m}\cdot\hat{\mathbf{H}}$ coupling is used in Ref. [105], which is valid only in free space (in Gaussian units) and hence throws some doubt on whether the results found therein are correct. The potentials derived therein thus do not follow from a Hamiltonian that is demonstrably consistent with the Maxwell equations and generates the correct equations of motion for the charged particles inside the atoms, whereas both of these requirements have been verified for the Hamiltonian (2.91) together with (2.92), (2.93) and (2.94) employed in this work. Furthermore, in spite of the use of a $\mathbf{m}\cdot\hat{\mathbf{H}}$ coupling, the contribution due to the noise magnetization contained in $\hat{\mathbf{H}}$ (cf. Ref. [42, 90]) was not discussed.

4.3.2 Planar multilayer system

Let us consider two isotropic atoms A and B placed respectively at the positions $\mathbf{r}_A$ and $\mathbf{r}_B$ in front of the planar multilayer medium described in Sec. 3.3.1. Further, let us restrict our considerations to atoms being only electrically polarizable where the interatomic vdW potential is given by Eq. (4.20). We choose the coordinate system as in Sec. 3.3.1 with the x axis chosen such that the two atoms lie in the xz plane (Fig. 4.1). The Green tensor can

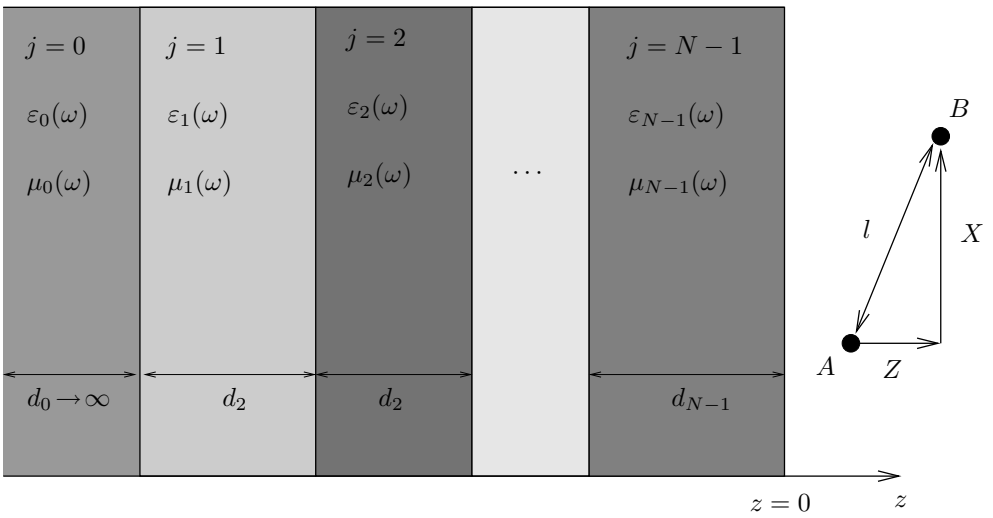

Figure 4.1: Two atoms in the presence of the planar multilayer medium.

be given by Eq. (3.9) with

$$\boldsymbol{G}^{(0)}(\mathbf{r},\mathbf{r}',\omega) = -\frac{c^2}{4\pi\omega^2 l^3}\left[f(-il\omega/c)\boldsymbol{I} - g(-il\omega/c)\frac{\mathbf{ll}}{l^2}\right]\mathrm{e}^{il\omega/c} \tag{4.54}$$

[with $f(x)$ and $g(x)$ being defined by Eq. (3.26)] and the scattering part $\boldsymbol{G}^{(1)}$ being given by Eq. (3.32) together with Eqs. (3.33)–(3.36). The polarization vectors defined by Eq. (3.34) may be written in terms of the Cartesian unit vectors as

$$\mathbf{e}_s^{\pm} = \sin\phi\,\mathbf{e}_x - \cos\phi\,\mathbf{e}_y, \tag{4.55}$$

$$\mathbf{e}_p^{\pm} = \mp\frac{b_N}{k_N}(\cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y) - \frac{iq}{k_N}\,\mathbf{e}_z \tag{4.56}$$

with ϕ being the angle between $\mathbf{e}_q$ and $\mathbf{e}_x$, i.e., $\mathbf{e}_q = \cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y$. Equations (4.55) and (4.56) imply that

$$\mathbf{e}_s^{+}\mathbf{e}_s^{-} = \begin{pmatrix} \sin^2\phi & -\sin\phi\cos\phi & 0 \\ -\sin\phi\cos\phi & \cos^2\phi & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{4.57}$$

$$\mathbf{e}_p^{+}\mathbf{e}_p^{-} = \frac{-1}{k_N^2}\begin{pmatrix} b_N^2\cos^2\phi & b_N^2\sin\phi\cos\phi & -ib_N q\cos\phi \\ b_N^2\sin\phi\cos\phi & b_N^2\sin^2\phi & -ib_N q\sin\phi \\ ib_N q\cos\phi & ib_N q\sin\phi & q^2 \end{pmatrix}. \tag{4.58}$$

Substituting these results into Eq. (3.32) and performing the ϕ-integrals by means of [101]

$$\int_0^{2\pi}\mathrm{d}\phi\, e^{ix\cos\phi}\cos(\nu\phi) = 2\pi i^{\nu}J_{\nu}(x) \tag{4.59}$$

[$J_\nu(x)$ denoting Bessel function], the nonzero matrix elements of the scattering-Green tensor, in the coordinate system chosen above, are found to be as follows:

$$G^{(1)}_{xx(yy)}(\mathbf{r},\mathbf{r}',\omega) = \frac{1}{8\pi}\int_0^{\infty}\mathrm{d}q\, q\mathrm{e}^{-b_N Z_+} \times\left\{\frac{1}{b_N}\left[J_0(qX)\underset{(-)}{\pm}J_2(qX)\right]r_N^s + \frac{c^2 b_N}{\omega^2}\left[J_0(qX)\underset{(+)}{\mp}J_2(qX)\right]r_N^p\right\}, \tag{4.60}$$

$$G^{(1)}_{xz(zx)}(\mathbf{r},\mathbf{r}',\omega) = \underset{(-)}{\pm}\frac{c^2}{4\pi}\int_0^{\infty}\mathrm{d}q\, q^2\mathrm{e}^{-b_N Z_+}\frac{1}{\omega^2}J_1(qX)r_N^p, \tag{4.61}$$

$$G^{(1)}_{zz}(\mathbf{r},\mathbf{r}',\omega) = \frac{c^2}{4\pi}\int_0^{\infty}\mathrm{d}q\, q^3\mathrm{e}^{-b_N Z_+}\frac{J_0(qX)}{b_N\omega^2}\,r_N^p, \tag{4.62}$$

where $Z_+ = z_A + z_B$, $X = x_B - x_A$.

According to the decomposition (3.9) of the Green tensor, the two-atom potential V_{ee}, Eq. (4.20), can be decomposed into bulk part $V_{ee}^{(0)}$ and body-induced part $V_{ee}^{(b)}$,

$$V_{ee}(\mathbf{r}_A,\mathbf{r}_B)=V_{ee}^{(0)}(\mathbf{r}_A,\mathbf{r}_B)+V_{ee}^{(b)}(\mathbf{r}_A,\mathbf{r}_B), \tag{4.63}$$

where the bulk part of the interaction potential reads

$$V_{ee}^{(0)}(\mathbf{r}_A,\mathbf{r}_B)=-\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}u\, u^4\alpha_A(iu)\alpha_B(iu)\mathrm{Tr}\big[\boldsymbol{G}^{(0)}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\boldsymbol{G}^{(0)}(\mathbf{r}_B,\mathbf{r}_A,iu)\big], \tag{4.64}$$

and the body-induced part can be written as

$$V_{ee}^{(b)}(\mathbf{r}_A,\mathbf{r}_B)=V_{ee}^{(1)}(\mathbf{r}_A,\mathbf{r}_B)+V_{ee}^{(2)}(\mathbf{r}_A,\mathbf{r}_B), \tag{4.65}$$

with

$$V_{ee}^{(1)}(\mathbf{r}_A,\mathbf{r}_B)=-\frac{\hbar\mu_0^2}{\pi}\int_0^\infty \mathrm{d}u\, u^4\alpha_A(iu)\alpha_B(iu)\mathrm{Tr}\big[\boldsymbol{G}^{(0)}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\boldsymbol{G}^{(1)}(\mathbf{r}_B,\mathbf{r}_A,iu)\big] \tag{4.66}$$

coming from the cross term of bulk and scattering parts, and

$$V_{ee}^{(2)}(\mathbf{r}_A,\mathbf{r}_B)=-\frac{\hbar\mu_0^2}{2\pi}\int_0^\infty \mathrm{d}u\, u^4\alpha_A(iu)\alpha_B(iu)\mathrm{Tr}\big[\boldsymbol{G}^{(1)}(\mathbf{r}_A,\mathbf{r}_B,iu)\cdot\boldsymbol{G}^{(1)}(\mathbf{r}_B,\mathbf{r}_A,iu)\big] \tag{4.67}$$

is the scattering-part contribution. The bulk part of the interaction potential can be found from Eq. (4.40) [$\varepsilon(iu)=1=n(iu)$] as

$$V_{ee}^{(0)}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar}{16\pi^3\varepsilon_0^2 l^6}\int_0^\infty \mathrm{d}u\,\alpha_A(iu)\alpha_B(iu)h_1(lu/c) \tag{4.68}$$

with $h_1(x)$ being given by (4.39). Equations. (4.66) and (4.67) together with Eqs. (4.54)–(4.62) leads to

$$\begin{aligned}V_{ee}^{(1)}(\mathbf{r}_A,\mathbf{r}_B)=&-\frac{\hbar\mu_0^2c^2}{32\pi^3l^5}\int_0^\infty \mathrm{d}u\, u^2\alpha_A(iu)\alpha_B(iu)\,e^{-lu/c}\int_0^\infty \mathrm{d}q\, q\, e^{-b_NZ_+}\\
&\times\Bigg\{\left[2f(lu/c)l^2-g(lu/c)X^2\right]\left(\frac{r_N^s}{b_N}-\frac{c^2b_N}{u^2}\,r_N^p\right)J_0(qX)-2\left[f(lu/c)l^2-g(lu/c)Z^2\right]\\
&\times\frac{c^2q^2r_N^p}{b_Nu^2}\,J_0(qX)-g(lu/c)X^2\left[\frac{r_N^s}{b_N}+\frac{c^2b_N}{u^2}\,r_N^p\right]J_2(qX)\Bigg\},\end{aligned} \tag{4.69}$$

$$\begin{aligned}V_{ee}^{(2)}(\mathbf{r}_A,\mathbf{r}_B)=&-\frac{\hbar\mu_0^2}{64\pi^3}\int_0^\infty \mathrm{d}u\, u^4\alpha_A(iu)\alpha_B(iu)\int_0^\infty \mathrm{d}q\, q\int_0^\infty \mathrm{d}q'\, q'\, e^{-(b_N+b'_N)Z_+}\Bigg\{\Bigg[\frac{r_N^sr_N^{s\prime}}{b_Nb'_N}\\
&-\frac{c^2b'_Nr_N^sr_N^{p\prime}}{b_Nu^2}-\frac{c^2b_Nr_N^{s\prime}r_N^p}{b'_Nu^2}+\frac{c^4r_N^pr_N^{p\prime}}{u^4}\left(b_Nb'_N+\frac{2q^2q'^2}{b_Nb'_N}\right)\Bigg]J_0(qX)J_0(q'X)+\frac{4c^4qq'r_N^pr_N^{p\prime}}{u^4}\\
&\times J_1(qX)J_1(q'X)+\left[\frac{r_N^sr_N^{s\prime}}{b_Nb'_N}+\frac{c^4b_Nb'_Nr_N^pr_N^{p\prime}}{u^4}+\frac{c^2b'_Nr_N^sr_N^{p\prime}}{b_Nu^2}+\frac{c^2b_Nr_N^{s\prime}r_N^p}{b'_Nu^2}\right]J_2(qX)J_2(q'X)\Bigg\}\end{aligned} \tag{4.70}$$

[$Z=z_B-z_A$, $b'_N=b_N(q',u)$, $r_N^{s\prime}=r_N^s(q',u)$, and $r_N^{p\prime}=r_N^p(q',u)$]. Equations (4.69) and (4.70) generalize results presented in Refs. [33, 34, 37] for two atoms in front of a metalic or dielectric half-space, respectively to arbitrary magnetodielectric multilayer systems. Since, in this example, $V=V_{ee}$ we drop the subscripts ee in the rest of this section.

Perfectly reflecting plate

As the simplest example of a planar system, let us consider the limiting case of a perfectly reflecting plate,

$$N = 1, \quad r_p = r_1^p = \pm 1, \quad r_s = r_1^s = \mp 1, \tag{4.71}$$

where the upper(lower) sign corresponds to a perfectly conducting(permeable) plate. In the retarded limit, where $l, z_A, z_B \gg c/\omega_{\min}$ $[\omega_{\min} = \min(\{\omega_{A'}^n | A' = A, B;\, n = 1, 2, \ldots\})]$, $V^{(0)}$ is given by Eq. (4.51) with $n(0) \equiv 1 \equiv \varepsilon(0)$,

$$V^{(0)} = -\frac{23\hbar c \alpha_A(0)\alpha_B(0)}{64\pi^3 \varepsilon_0^2 l^7}, \tag{4.72}$$

whereas $V^{(1)}$ [Eq. (4.69)] and $V^{(2)}$ [Eq. (4.70)] can be given in closed form in some special cases. In this limit it is convenient to replace the integration variable q in Eqs. (4.60)–(4.62) in favour of $v = bc/u$ with b being defined by Eq. (3.40), i.e., $q = \sqrt{v^2 - 1}u/c$, and hence

$$\int_0^\infty \mathrm{d}q \, \frac{q}{b_1} \cdots \;\mapsto\; \int_1^\infty \mathrm{d}v \, \frac{u}{c} \cdots . \tag{4.73}$$

In the case where $X \ll Z_+$ (cf. Fig. 4.1), the exponential terms in Eqs. (4.60)–(4.62) effectively limits the integrals to the region where $qX \ll 1$, hence we can approximate $J_\nu(qX)$ by $J_\nu(0) = \delta_{\nu 0}$, such that the nonzero scattering-Green tensor components read

$$G_{xx}^{(1)}(\mathbf{r}_A, \mathbf{r}_B, iu) = G_{yy}^{(1)}(\mathbf{r}_A, \mathbf{r}_B, iu) = \frac{1}{8\pi Z_+}\left[r_s - \left(1 + 2\frac{c}{Z_+ u} + 2\frac{c^2}{Z_+^2 u^2}\right) r_p\right] e^{-Z_+ u/c}, \tag{4.74}$$

$$G_{zz}^{(1)}(\mathbf{r}_A, \mathbf{r}_B, iu) = -\frac{1}{2\pi Z_+}\left(\frac{c}{Z_+ u} + \frac{c^2}{Z_+^2 u^2}\right) r_p \, e^{-Z_+ u/c}, \tag{4.75}$$

leading to

$$V^{(1)} = \pm \frac{\hbar c \alpha_A(0)\alpha_B(0)}{2\pi^3 \varepsilon_0^2} \frac{X^2 + 6l^2}{l^3 Z_+ (l + Z_+)^5}, \tag{4.76}$$

$$V^{(2)} = -\frac{23\hbar c \alpha_A(0)\alpha_B(0)}{64\pi^3 \varepsilon_0^2 Z_+^7}. \tag{4.77}$$

Thus the interaction potential (4.63) reads

$$V = \frac{23\hbar c \alpha_A(0)\alpha_B(0)}{64\pi^3 \varepsilon_0^2}\left[-\frac{1}{l^7} \pm \frac{32}{23}\frac{X^2 + 6l^2}{l^3 Z_+ (l + Z_+)^5} - \frac{1}{Z_+^7}\right], \tag{4.78}$$

which is in agreement with Ref. [38] in the case of a conducting plate. In particular, if $z_A \ll z_B$, or equivalently $Z_+ \simeq Z \simeq l$, from Eqs. (4.76) and (4.77) it follows that

$$V^{(1)} = \mp \frac{6}{23} V^{(0)}, \tag{4.79}$$

$$V^{(2)} = V^{(0)}, \tag{4.80}$$

so the interaction potential V, Eq. (4.63), is enhanced by the presence of the perfectly reflecting plate:

$$V = \begin{cases} \frac{40}{23} V^{(0)} & \text{for } r_{p(s)} = \overset{+}{(-)} 1, \\ \\ \frac{52}{23} V^{(0)} & \text{for } r_{p(s)} = \overset{-}{(+)} 1. \end{cases} \tag{4.81}$$

Next, we discuss the behavior of V in the case where the condition $z_A \ll z_B$ is not valid. Since the bulk part $V^{(0)}$ [first term in the square brackets in Eq. (4.78)] is negative, the interaction potential is enhanced(reduced) by the plate if the scattering part $V^{(1)} + V^{(2)}$ [second and third terms in the square brackets in Eq. (4.78)] is negative(positive). In the case of a perfectly conducting plate, it is seen that especially for $Z = 0$, briefly referred to as the parallel case, $V^{(1)} + V^{(2)}$ is positive, and hence the interaction potential is reduced by the plate, whereas for $X = 0$, briefly referred to as the vertical case, $V^{(1)} + V^{(2)}$ is positive and the interaction potential is reduced iff

$$z_B / z_A \lesssim 4.90, \tag{4.82}$$

where, without loss of generality, atom A is assumed to be closer to the plate than atom B. It is apparent from Eq. (4.78) that for a perfectly permeable plate $V^{(1)} + V^{(2)}$ is always negative, and hence the interaction potential is always enhanced by the plate.

Let us now turn to the nonretarded limit, where $l, z_A, z_B \ll c/\omega_{\max}$ [$\omega_{\max} = \max(\{\omega^n_{A'} | A' = A, B;\, n = 1, 2, \ldots\})$], and $V^{(0)}$ can be found from Eq. (4.47) [$\varepsilon(iu) \equiv 1$]

$$V^{(0)} = -\frac{C_{\rm nr}}{l^6}\,, \tag{4.83}$$

where

$$C_{\rm nr} = \frac{3\hbar}{16\pi^3 \varepsilon_0^2} \int_0^\infty \mathrm{d}u\, \alpha_A(iu) \alpha_B(iu). \tag{4.84}$$

It can be inferred that in this limit, the main contribution to the frequency integrals in Eqs. (4.69) and (4.70) comes from the region where $u/(cb) \ll 1$ (compare with the single atom case given in Ref. [97]). In this region we have

$$q = b\sqrt{1 - \frac{u^2}{b^2 c^2}} \simeq b. \tag{4.85}$$

Therefore, we may use this approximation in Eqs. (4.60)–(4.62) from which, by changing the integration variable q according to

$$\int_0^\infty \mathrm{d}q\, \frac{q}{b_1} \ldots \;\mapsto\; \int_{u/c}^\infty \mathrm{d}b \;\ldots \tag{4.86}$$

and performing a Taylor expansion in u/c, we find the nonzero elements of the scattering Green tensor as

$$G^{(1)}_{xx}(\mathbf{r}_A,\mathbf{r}_B,iu)=\frac{c^2}{4\pi u^2 l_+^5}\left(2X^2-Z_+^2\right)\,r_p, \tag{4.87}$$

$$G^{(1)}_{yy}(\mathbf{r}_A,\mathbf{r}_B,iu)=-\frac{c^2}{4\pi u^2 l_+^3}\,r_p, \tag{4.88}$$

$$G^{(1)}_{xz(zx)}(\mathbf{r}_A,\mathbf{r}_B,iu)=\overset{-}{(+)}\frac{3c^2XZ_+}{4\pi u^2 l_+^5}\,r_p, \tag{4.89}$$

$$G^{(1)}_{zz}(\mathbf{r}_A,\mathbf{r}_B,iu)=\frac{c^2}{4\pi u^2 l_+^5}\left(X^2-2Z_+^2\right)\,r_p, \tag{4.90}$$

with $l_+=\sqrt{X^2+Z_+^2}$, leading to

$$V^{(1)}=\pm\frac{4X^4-2Z^2Z_+^2+X^2(Z_+^2+Z^2)}{3l^5l_+^5}\,C_{\rm nr}, \tag{4.91}$$

$$V^{(2)}=-\frac{C_{\rm nr}}{l_+^6}\,. \tag{4.92}$$

Hence, the interaction potential (4.63), reads, on recalling Eq. (4.63),

$$V=\left(-\frac{1}{l^6}\pm\frac{3X^4-3Z^2Z_+^2+l^2l_+^2}{3l^5l_+^5}-\frac{1}{l_+^6}\right)C_{\rm nr}\,. \tag{4.93}$$

Let us again consider the effect of the plate on the interaction potential for the parallel and vertical cases. In the parallel case, Eq. (4.93) takes the form

$$V=\left[-\frac{1}{l^6}\pm\frac{4l^2+Z_+^2}{3l^3(l^2+Z_+^2)^{\frac{5}{2}}}-\frac{1}{(l^2+Z_+^2)^3}\right]C_{\rm nr}\,, \tag{4.94}$$

which in the on-surface limit $Z_+\to 0$ approaches

$$V=\begin{cases}\frac{2}{3}V^{(0)} & \text{for } r_{p(s)}=\overset{+}{(-)}1,\\[2ex] \frac{10}{3}V^{(0)} & \text{for } r_{p(s)}=\overset{-}{(+)}1,\end{cases} \tag{4.95}$$

in agreement with the corresponding result found in Refs. [31, 49] for the case of conducting plate. It can be seen easily that the term $V^{(1)}$ [second term in the square brackets in Eq. (4.94)] dominates the term $V^{(2)}$ [third term in the square brackets in Eq. (4.94)], so $V^{(1)}+V^{(2)}$ is positive(negative) for a perfectly conducting(permeable) plate, and hence the interaction potential is reduced(enhanced) due to the presence of the plate.

In the vertical case, from Eq. (4.93) the interaction potential is obtained to be

$$V=\left[-\frac{1}{l^6}\mp\frac{2}{3Z_+^3l^3}-\frac{1}{Z_+^6}\right]C_{\rm nr}\,. \tag{4.96}$$

It is obvious that $V^{(1)}+V^{(2)}$ [second and third terms in Eq. (4.96)] is negative when the plate is perfectly conducting, thereby enhancing the interaction potential since $V^{(0)}$ [first

term in Eq. (4.96)] is negative. In the case of a perfectly permeable plate, $V^{(1)}+V^{(2)}$ is positive iff

$$\frac{z_B}{z_A} < 1 + \frac{2}{(\frac{3}{2})^{\frac{1}{3}}-1} \simeq 14.82, \tag{4.97}$$

where atom A is again assumed to be closer to the plate than atom B.

Semi-infinite magnetoelectric half-space

Let us now abandon the assumption of perfect reflectivity and consider again the thick magnetoelectric plate for which the single-atom potential is evaluated in chapter 3, applying the model of half-space. The body-assisted part of the two-atom potential is given by Eq. (4.65) together with Eqs. (4.69) and (4.70), where $N=1$ and the reflection coefficients r_s and r_p are given by Eq. (3.39).

In the retarded limit, $l, z_A, z_B \gg c/\omega_{\min}$ [with $\omega_{\min}$ being defined as above Eq. (3.41)] we may again replace the atomic polarizability and the permittivity and permeability of the plate by their static values. Replacing the integration variable q in Eq. (4.69) by $v=b_1 c/u$ [see Eq. (4.73)] leads to

$$\begin{aligned} V^{(1)}(\mathbf{r}_A,\mathbf{r}_B) = \frac{\hbar c}{32\pi^3 l^3 \varepsilon_0^2}\alpha_A(0)\alpha_B(0)\int_1^\infty \mathrm{d}v\, \Bigg\{ v^2 \Bigg[Z^2 A_{5-} + (Z^2-2X^2)\left(\frac{A_{4-}}{l}+\frac{A_{3-}}{l^2}\right) \\ + l^2 A_{5+} + l A_{4+} + A_{3+} \Bigg] r_p(v) + 2(v^2-1)\left[X^2 B_5 + \left(X^2-2Z^2\right)\left(\frac{B_4}{l}+\frac{B_3}{l^2}\right)\right] r_p(v) \\ + \left[Z^2 A_{5+} + \left(Z^2-2X^2\right)\left(\frac{A_{4+}}{l}+\frac{A_{3+}}{l^2}\right) + l^2 A_{5-} + l A_{4-} + A_{3-} \right] r_s(v) \Bigg\}, \end{aligned} \tag{4.98}$$

with $r_s(v)$ and $r_p(v)$ being defined by Eq. (3.42), and

$$A_{n\pm} = \frac{1}{c^{n+1}}\int_0^\infty \mathrm{d}u\, u^n\, e^{-au/c}\big[J_0(\beta u/c) \pm J_2(\beta u/c)\big], \tag{4.99}$$

$$B_n = \frac{1}{c^{n+1}}\int_0^\infty \mathrm{d}u\, u^n e^{-au/c} J_0(\beta u/c), \tag{4.100}$$

with $\beta = X\sqrt{v^2-1}$ and $a = l + vZ_+$. By performing the u integrals in (4.99) and (4.100), the explicit expressions of $A_{n\pm}$ and B_n will be found as follows:

$$\begin{aligned} A_{3+} &= \frac{6a}{\left(a^2+\beta^2\right)^{\frac{5}{2}}}, \quad A_{4+} = \frac{6\left(4a^2-\beta^2\right)}{\left(a^2+\beta^2\right)^{\frac{7}{2}}}, \quad A_{5+} = \frac{30\left(4a^3-3a\beta^2\right)}{\left(a^2+\beta^2\right)^{\frac{9}{2}}}, \quad A_{3-} = \frac{6\left(a^3-4a\beta^2\right)}{\left(a^2+\beta^2\right)^{\frac{7}{2}}}, \\ A_{4-} &= \frac{6\left(4a^4-27a^2\beta^2+4\beta^4\right)}{\left(a^2+\beta^2\right)^{\frac{9}{2}}}, \quad A_{5-} = \frac{30\left(4a^5-41a^3\beta^2+18a\beta^4\right)}{\left(a^2+\beta^2\right)^{\frac{11}{2}}}, \\ B_3 &= \frac{3a\left(2a^2-3\beta^2\right)}{\left(a^2+\beta^2\right)^{\frac{7}{2}}}, \quad B_4 = \frac{3\left(8a^4-24a^2\beta^2+3\beta^4\right)}{\left(a^2+\beta^2\right)^{\frac{9}{2}}}, \quad B_5 = \frac{15a\left(8a^4-40a^2\beta^2+15\beta^4\right)}{\left(a^2+\beta^2\right)^{\frac{11}{2}}}. \end{aligned} \tag{4.101}$$

Similarly, Eq. (4.70) reduces to

$$V^{(2)}(\mathbf{r}_A,\mathbf{r}_B) = -\frac{\hbar\mu_0^2}{64\pi^3c^2}\,\alpha_A(0)\alpha_B(0)\int_1^\infty \mathrm{d}v\int_1^\infty \mathrm{d}v'\Big\{\Big(r_pr'_p\big[3v^2v'^2-2(v^2+v'^2)+2\big] + r_sr'_s - r_sr'_pv'^2 - r_pr'_sv^2\Big)M_0 + 4vv'\sqrt{v^2-1}\sqrt{v'^2-1}r_pr'_pM_1 + \big(r_sr'_s + r_pr'_pv^2v'^2 + r_sr'_pv'^2 + r_pr'_sv^2\big)M_2\Big\} \quad (4.102)$$

$[r_\sigma = r_\sigma(v),\ r'_\sigma = r_\sigma(v')]$, where

$$M_n = \int_0^\infty \mathrm{d}u\,u^6e^{-(v+v')Z_+u/c}J_n(\beta u/c)J_n(\beta' u/c) \quad (4.103)$$

($\beta' = X\sqrt{v'^2-1}$), which can be evaluated analytically only in some special cases. In particular, when $X \ll Z_+$ (cf. Fig. 4.1), then approximately

$$M_n = J_n^2(0)\int_0^\infty \mathrm{d}u\,u^6e^{-(v+v')Z_+u/c} = \frac{720c^7}{(v+v')^7Z_+^7}\,\delta_{n0}. \quad (4.104)$$

In the nonretarded limit, $l, z_A, z_B \ll c/[n(0)\omega_{\max}]$ [with $\omega_{\max}$ being defined as above Eq. (3.43)], we apply a similar procedure to the one below Eq. (4.84) and expand the reflection coefficients r_s and r_p, Eq. (3.39), in terms of $u/(bc)$

$$r_s = \frac{\mu(iu)-1}{\mu(iu)+1} - \frac{\mu(iu)[\varepsilon(iu)\mu(iu)-1]}{[\mu(iu)+1]^2}\,\frac{u^2}{b^2c^2}\,, \quad (4.105)$$

$$r_p = \frac{\varepsilon(iu)-1}{\varepsilon(iu)+1} - \frac{\varepsilon(iu)[\varepsilon(iu)\mu(iu)-1]}{[\varepsilon(iu)+1]^2}\,\frac{u^2}{b^2c^2}. \quad (4.106)$$

That leads, in the case of a magnetoelectric half-space, to

$$V^{(1)} = \big(3X^4 - 3Z^2Z_+^2 + l^2l_+^2\big)\,\frac{C_{\rm nr}^{(1)}}{l^5l_+^5} + \big[Z^2 - 2X^2 + 3Z_+\,(l_+ - Z_+)\big]\,\frac{C_{\rm nr}^{(2)}}{l^5l_+}, \quad (4.107)$$

$$V^{(2)} = -\frac{C_{\rm nr}^{(3)}}{l_+^6}, \quad (4.108)$$

where

$$C_{\rm nr}^{(1)} = \frac{\hbar}{16\pi^3\varepsilon_0^2}\int_0^\infty \mathrm{d}u\,\alpha_A(iu)\alpha_{\rm B}(iu)\frac{\varepsilon(iu)-1}{\varepsilon(iu)+1}\,, \quad (4.109)$$

$$C_{\rm nr}^{(2)} = \frac{\hbar}{64\pi^3\varepsilon_0^2c^2}\int_0^\infty \mathrm{d}u\,u^2\,\alpha_A(iu)\alpha_B(iu)\frac{[\mu(iu)-1][\mu(iu)-3]}{\mu(iu)+1}\,, \quad (4.110)$$

$$C_{\rm nr}^{(3)} = \frac{3\hbar}{16\pi^3\varepsilon_0^2}\int_0^\infty \mathrm{d}u\,\alpha_A(iu)\alpha_B(iu)\left[\frac{\varepsilon(iu)-1}{\varepsilon(iu)+1}\right]^2. \quad (4.111)$$

In the case of a purely electric half-space ($\mu = 1$), the second term in the right-hand side of Eq. (4.107) vanishes and the vdW interaction potential becomes

$$V = -\frac{C_{\rm nr}}{l^6} + \big(3X^4 - 3Z^2Z_+^2 + l^2l_+^2\big)\,\frac{C_{\rm nr}^{(1)}}{l^5l_+^5} - \frac{C_{\rm nr}^{(3)}}{l_+^6}\,, \quad (4.112)$$

with $C_{\rm nr}$ being defined by Eq. (4.84). Equation (4.112) together with Eqs. (4.109) and (4.111) is in agreement with the results obtained in Refs. [33, 37, 34]. In particular in the limiting case when $l \ll Z_+$, Eq. (4.112) reduces to

$$V = -\frac{C_{\rm nr}}{l^6} + \frac{\big(X^2 - 2Z^2\big)C_{\rm nr}^{(1)}}{l^5 Z_+^3}\,. \tag{4.113}$$

It is seen that the second term on the right-hand side of this equation is positive(negative) in the parallel(vertical) case, so the vdW potential is reduced(enhanced) by the presence of the dielectric half-space.

In the case of a purely magnetic half-space ($\varepsilon = 1$) $V^{(2)}$, Eq. (4.108), does not contribute to the vdW interaction potential and vanishes as well as the first term in the right hand side of Eq. (4.107), resulting in

$$V = -\frac{C_{\rm nr}}{l^6} + \big[Z^2 - 2X^2 + 3Z_+(l_+ - Z_+)\big]\frac{C_{\rm nr}^{(2)}}{l^5 l_+}\,. \tag{4.114}$$

In particular in the limiting case when $X \ll Z_+$, Eq. (4.114) reduces to

$$V = -\frac{C_{\rm nr}}{l^6} + \frac{\big(2Z^2 - X^2\big)C_{\rm nr}^{(2)}}{2l^5 Z_+}\,. \tag{4.115}$$

It is seen that the second term on the right-hand side of this equation is negative(positive) in the parallel(vertical) case, so the vdW potential is enhanced(reduced) due to the presence of the magnetic half-space.

It should be pointed out that the nonretarded limit for the magnetoelectric half-space [Eq. (4.63) together with Eqs. (4.65), (4.83), and (4.107)–(4.111)] is in general incompatible with the limit of perfect reflectivity [$\varepsilon(iu) \to \infty$ or $\mu(iu) \to \infty$] given by Eq. (4.93), as is clearly seen from the condition given above Eq. (4.107) [cf. also the expansions (4.105) and (4.106), which are not well-behaved in the limit of perfect reflectivity]. As a consequence, Eq. (4.114) does not reduce to Eq. (4.93) via the limit $\mu(iu) \to \infty$. It is therefore remarkable that the result for a purely electric half-space, Eq. (4.112), does reduce to Eq. (4.93) in the limit $\varepsilon(iu) \to \infty$, as already noted in Ref. [106] in the case of the single-atom potential.

Figures 4.2–4.4 show the results of exact (numerical) calculation of the vdW interaction between two identical two-level atoms near a semi-infinite half-space, as given by Eq. (4.63) together with Eqs. (4.68), (4.65), (4.69), and (4.70). In the figures the potentials and the forces are normalized with respect to their values in free space, $V^{(0)}$. In the calculations, we have used single-resonance Drude–Lorenz-type electric and magnetic susceptibilities of the half-space,

$$\varepsilon(\omega) = 1 + \frac{\omega_{{\rm P}e}^2}{\omega_{{\rm T}e}^2 - \omega^2 - i\omega\gamma_e}\,, \tag{4.116}$$

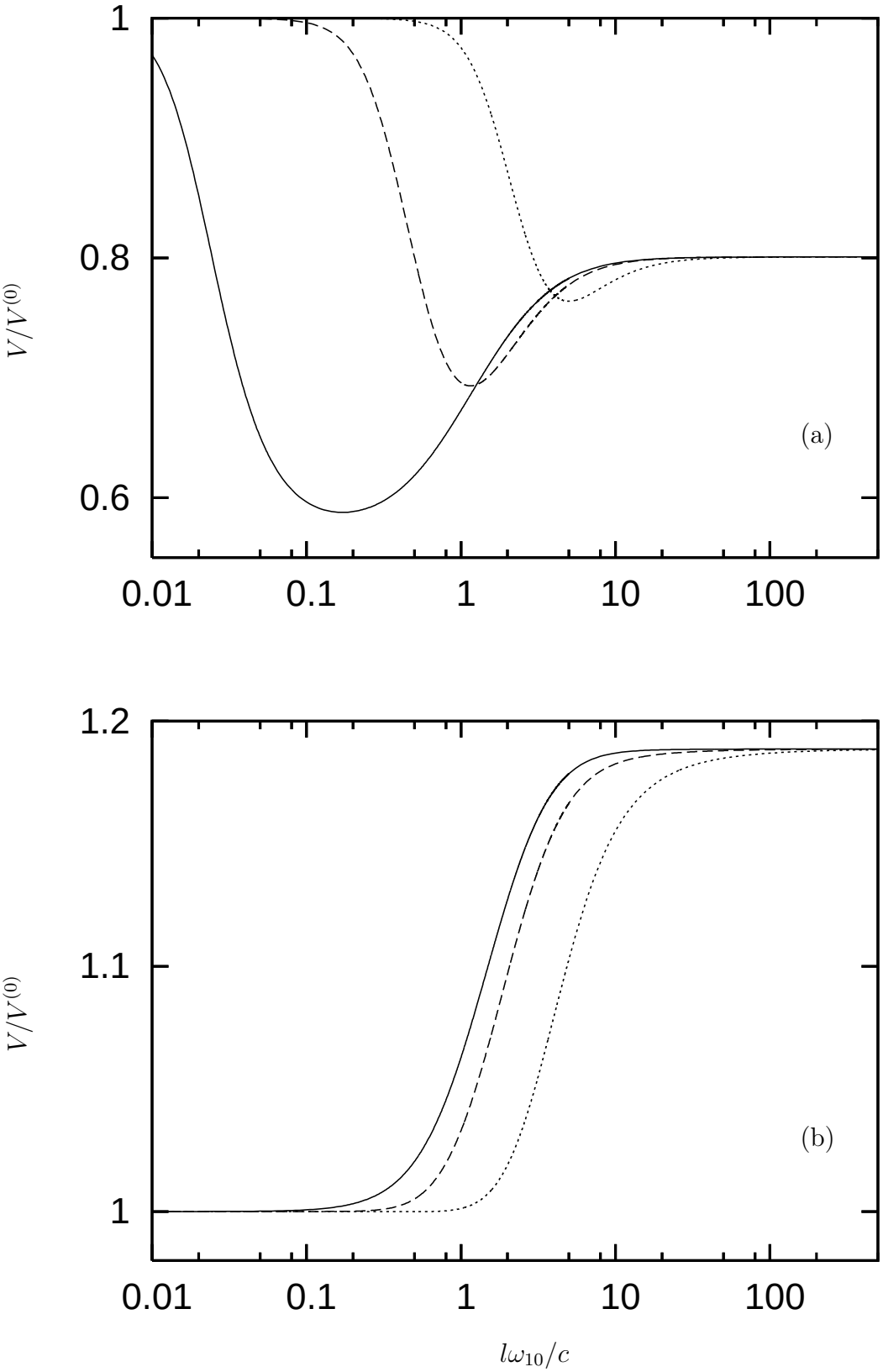

Figure 4.2: The vdW potential for two identical two-level atoms in the parallel case in presence of (a) a purely electric half-space with $\omega_{\mathrm{P}e}/\omega_{10}=3$, $\omega_{\mathrm{T}e}/\omega_{10}=1$, and $\gamma_e/\omega_{10}=0.001$ (b) a purely magnetic half-space with $\omega_{\mathrm{P}m}/\omega_{10}=3$, $\omega_{\mathrm{T}m}/\omega_{10}=1$, and $\gamma_m/\omega_{10}=0.001$ is shown as a function of the atom–atom separation l [ω_{10} is the atomic transition frequency, and $V^{(0)}$ is the potential in free space]. The atom–half-space separations are $z_A=z_B=0.01c/\omega_{10}$ (solid line), $0.2c/\omega_{10}$ (dashed line), and c/ω_{10} (dotted line).

$$\mu(\omega) = 1 + \frac{\omega_{\mathrm{P}m}^2}{\omega_{\mathrm{T}m}^2 - \omega^2 - i\omega\gamma_m}\,. \tag{4.117}$$

From the figures it is seen that the vdW interaction is unaffected by the presence of the half-space for atom–half-space separations that are much greater than the interatomic separations, while an asymptotic enhancement or reduction of the interaction is observed in the opposite limit.

Figure 4.2(a) shows the dependence of the normalized interaction potential V on the atom–atom separation l in the parallel case ($Z = 0$) for different values of the distance $z_A\,(= z_B)$ of the atoms from a purely electric half-space. The ratio of the interatomic force along the connecting line of the two atoms, F_{ABx} [Eq. (4.30)] to the corresponding force in free space, $F_{ABx}^{(0)}$, follows closely the ratio $V/V^{(0)}$, so that, within the resolution of the figures, the curves for $F_{ABx}/F_{ABx}^{(0)}$ (not shown) would coincide with those for $V/V^{(0)}$. The figure reveals that due to the presence of the electric half-space the attractive interaction potential and force are reduced, in agreement with the predictions from the nonretarded limit, Eq. (4.113). The relative reduction of the potential and the force are not monotonic, there is a value of the atom–atom separation where the reduction is strongest. The l-dependence of $V/V^{(0)}$ in the presence of a purely magnetic half-space in the parallel case is shown in Figs. 4.2(b). Again, the corresponding force ratio $F_{ABx}/F_{ABx}^{(0)}$ (not shown) behaves like $V/V^{(0)}$. The figure indicates that the presence of a purely magnetic half-space enhances the vdW interaction between the two atoms, with the enhancement increasing with the atom-atom separation, in agreement with the nonretarded limit, Eq. (4.115).

Figure 4.3 shows $V/V^{(0)}$ in the vertical case ($X = 0$) when the half-space is purely electric [Fig. 4.3(a)] or purely magnetic [Fig. 4.3(b)]. In the figure, atom A is assumed to be closer to the surface of the half-space than atom B, and the graphs show the variation of the interaction potential with the atom–atom separation l for different distances z_A of atom A from the surface of the half-space. It is seen that for a purely electric half-space the potential is enhanced compared to the one observed in the free-space case—in agreement with Eq. (4.113). Note that there are values of the atom–atom separation at which the enhancement is strongest. For a purely magnetic half-space, the potential is seen to be typically enhanced although for very small atom–atom separations a reduction appears [inset in Fig. 4.3(b)]—in agreement with Eq. (4.115). Whereas the force $F_{BAz}/F_{BAz}^{(0)}$ for the force acting on atom B (not shown) again follows closely the potential ratio $V/V^{(0)}$, the ratio $F_{ABz}/F_{ABz}^{(0)}$, for the force acting on atom A noticeably differs from $V/V^{(0)}$, as can be seen from comparing Figs. 4.3 and 4.4. Clearly, the reason must be seen in the different

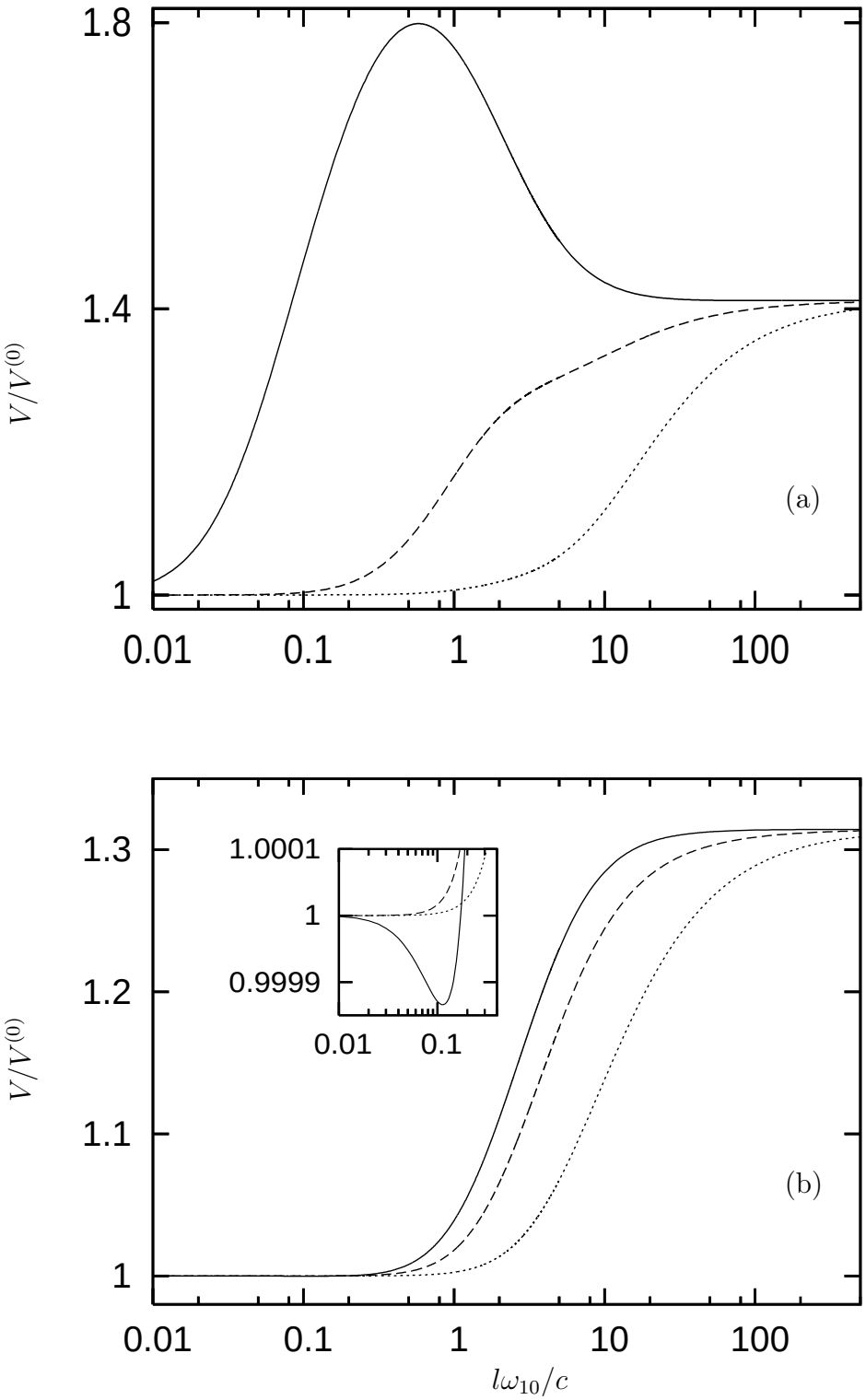

Figure 4.3: The vdW potential for two two-level atoms in the vertical case in the presence of (a) a purely electric half-space and (b) a purely magnetic half-space is shown as a function of the atom–atom separation l. The distance between atom A (which is closer to the surface of the half-space than atom B) and the surface is $z_A = 0.01c/\omega_{10}$ (solid line), $0.2c/\omega_{10}$ (dashed line), and c/ω_{10} (dotted line). All other parameters are the same as in Fig. 4.2.

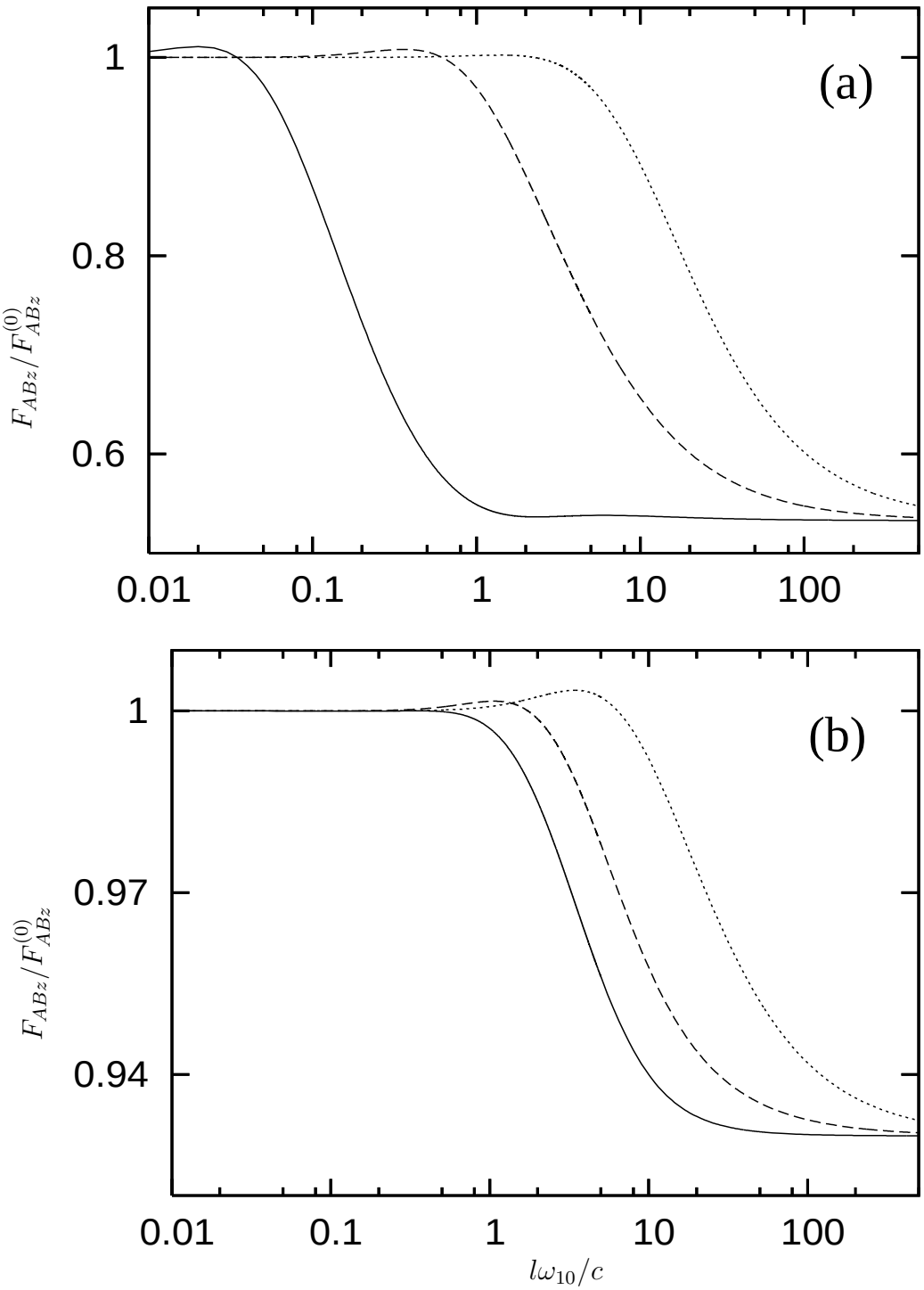

Figure 4.4: The vdW force acting on atom A (which is closer to the surface of the half-space than atom B) in the presence of (a) a purely electric half-space and (b) a purely magnetic half-space is shown as a function of the atom–atom separation l. All parameters are the same as in Fig. 4.3.

atom–atom and atom–half-space directions in the two cases.

Figures 4.2(a) and 4.3(a) showing the interaction potential of two atoms in the presence of a purely electric half-space in the parallel and vertical cases, respectively, confirm the results shown in Ref. [34]. The results here are more complete because they show that the relative potential does not have the monotonic behavior suggested by the figures in Ref. [34].

4.3.3 Homogeneous sphere

So far, the theoretical studies of medium-assisted interatomic vdW interactions have concentrated on bulk media and infinitely extended planar bodies. Here we shall consider the vdW interaction between two ground-state atoms located near a finite-size body, namely, a sphere. Let us consider two ground-state isotropic atoms A and B, being polarizable as well as magnetizable, in the presence of a homogeneous magnetoelectric sphere of permittivity $\varepsilon(\omega)$, permeability $\mu(\omega)$, and radius R. The vdW interaction potential V can be found using Eq. (4.10) with V_{ee}, V_{em}, and V_{mm} being calculated from Eqs. (4.20), (4.25), and (4.27), respectively, recalling that V_{me} can be found from V_{em} by interchanging A and B. According to the decomposition of the Green tensor, Eq. (3.9), the tensors $\boldsymbol{K}$ and $\boldsymbol{L}$ also can be decomposed into bulk and scattering parts and hence, V_{em} and V_{mm} can be broken down into bulk and body-induced parts just the same as V_{ee}, Eq. (4.63). Needless to say that again the bulk-part contribution $V_{ee}^{(0)}$ is given by Eq. (4.68), and the contributions $V_{em}^{(0)}$, and $V_{mm}^{(0)}$ can be found from Eqs. (4.43) and (4.41), respectively as

$$V_{em}^{(0)}(\mathbf{r}_A,\mathbf{r}_B)=\frac{\hbar\mu_0^2}{16\pi^3 l^4}\int_0^\infty \mathrm{d}u\, u^2\alpha_A(iu)\beta_B(iu)\, h_2(ul/c), \tag{4.118}$$

$$V_{mm}^{(0)}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar\mu_0^2}{16\pi^3 l^6}\int_0^\infty \mathrm{d}u\, \beta_A(iu)\beta_B(iu) h_1(ul/c), \tag{4.119}$$

with $h_1(x)$ and $h_2(x)$ being defined by Eqs. (4.39) and (4.44). We are hence left with the calculation of the body-induced part of the potential.

Calculation of $V_{ee}^{(b)}$ and $V_{mm}^{(b)}$

To calculate $V_{ee}^{(b)}$ we first need to determine the scattering part of the Green tensor, $\boldsymbol{G}^{(1)}$. Choosing a spherical coordinate system such that its origin coincides with the center of the sphere, $\boldsymbol{G}^{(1)}$ can be given by Eq. (3.46) together with Eqs. (3.47), (3.48), (3.51), and (3.52). Without loss of generality, we assume that the two atoms are located in the xz plane (Fig. 4.5),

$$\mathbf{r}_A=(r_A,\theta_A,0),\quad \mathbf{r}_B=(r_B,\theta_B,\pi). \tag{4.120}$$

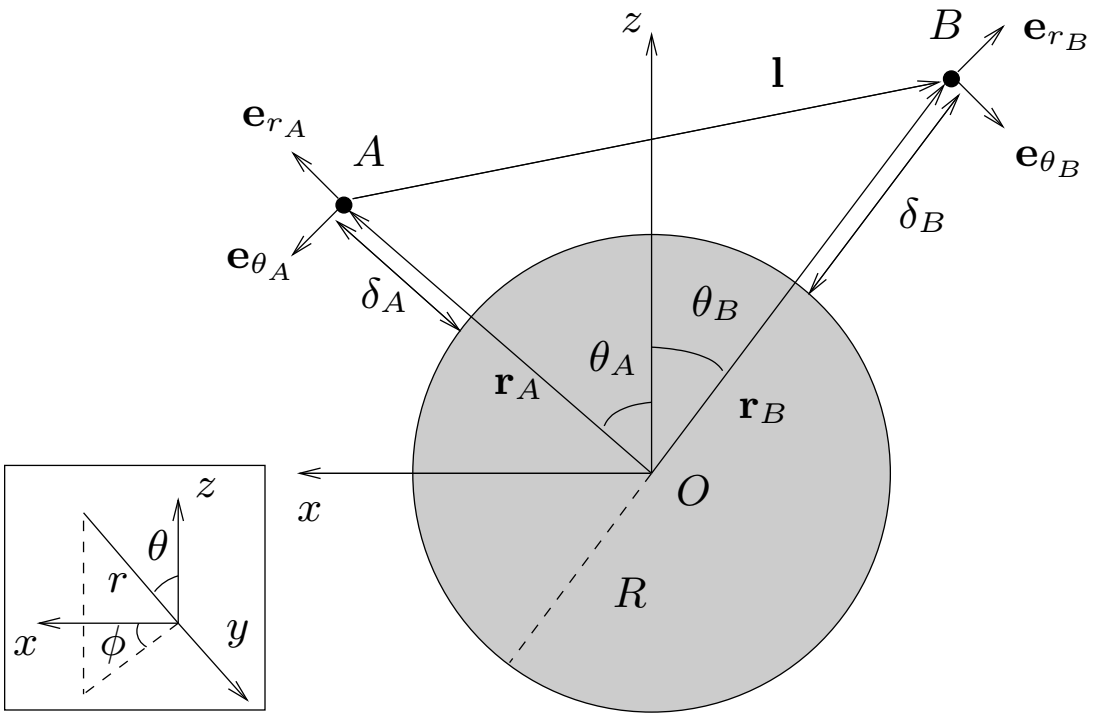

Figure 4.5: Two atoms A and B in the presence of a sphere ($\theta_A + \theta_B = \Theta$).

Substituting $\mathbf{r}_A$ and $\mathbf{r}_B$ from Eq. (4.120) into Eqs. (3.47) and (3.48), making use of the results in Eq. (3.46), and performing the summation over m and p in Eq. (3.46) leads to (Appendix B)

$$\boldsymbol{G}^{(1)}(\mathbf{r}_A, \mathbf{r}_B, \omega) = \frac{ic}{4\pi\omega r_A r_B} \sum_{n=1}^{\infty}(2n+1)\Big\{ n(n+1)B_n^N P_n(\gamma) Q_n \mathbf{e}_{r_A}\mathbf{e}_{r_B} - \sin\Theta\, B_n^N P_n'(\gamma)$$
$$\times \left(Q_n^B \mathbf{e}_{r_A}\mathbf{e}_{\theta_B} + Q_n^A \mathbf{e}_{\theta_A}\mathbf{e}_{r_B}\right) - \frac{1}{n(n+1)}\left[\frac{r_A r_B \omega^2}{c^2} B_n^M P_n'(\gamma) Q_n + B_n^N F_n(\gamma) L_n\right] \mathbf{e}_{\theta_A}\mathbf{e}_{\theta_B}$$
$$-\frac{1}{n(n+1)}\left[\frac{r_A r_B \omega^2}{c^2} B_n^M F_n(\gamma) Q_n + B_n^N P_n'(\gamma) L_n\right] \mathbf{e}_{\phi_A}\mathbf{e}_{\phi_B}\Big\}, \tag{4.121}$$

where $r_{A(B)} = |\mathbf{r}_{A(B)}|$, $\gamma = \cos\Theta$, $\Theta = \theta_A + \theta_B$ is angular separation between two atoms with respect to the sphere center,

$$Q_n = h_n^{(1)}(ir_A u/c) h_n^{(1)}(ir_B u/c), \tag{4.122}$$

$$Q_n^A = h_n^{(1)}(ir_B u/c)[y h_n^{(1)}(y)]'_{y=ir_A u/c}, \tag{4.123}$$

$$Q_n^B = h_n^{(1)}(ir_A u/c)[z h_n^{(1)}(z)]'_{z=ir_B u/c}, \tag{4.124}$$

$$L_n = [y h_n^{(1)}(y)]'_{y=ir_A u/c}[z h_n^{(1)}(z)]'_{z=ir_B u/c}, \tag{4.125}$$

$$F_n(x) = n(n+1)P_n(x) - xP_n'(x). \tag{4.126}$$

In order to facilitate further evaluations, it is convenient to represent the free-space Green tensor (4.54) in the same spherical coordinate system as the scattering part, so that it reads

$$\boldsymbol{G}^{(0)}(\mathbf{r}_A,\mathbf{r}_B,\omega)=\frac{c^2\mathrm{e}^{il\omega/c}}{4\pi\omega^2 l^5}\Big\{\left[-l^2 f(-il\omega/c)\cos\Theta-l_A l_B\, g(-il\omega/c)\right]\mathbf{e}_{r_A}\mathbf{e}_{r_B}$$
$$+\sin\Theta\big[l^2 f(-il\omega/c)+r_A l_A\, g(-il\omega/c)\big]\mathbf{e}_{r_A}\mathbf{e}_{\theta_B}+\sin\Theta\big[l^2 f(-il\omega/c)+r_B l_B\, g(-il\omega/c)\big]\mathbf{e}_{\theta_A}\mathbf{e}_{r_B}$$
$$+\big[l^2 f(-il\omega/c)\cos\Theta-r_A r_B\, g(-il\omega/c)\sin^2\Theta\big]\mathbf{e}_{\theta_A}\mathbf{e}_{\theta_B}+l^2 f(-il\omega/c)\mathbf{e}_{\phi_A}\mathbf{e}_{\phi_B}\Big\} \quad (4.127)$$

($l=|\mathbf{l}|$, $\mathbf{l}=\mathbf{r}_B-\mathbf{r}_A$), where $l_A(l_B)$ is the component of $\mathbf{l}$ in the direction of $\mathbf{r}_A(-\mathbf{r}_B)$,

$$l_A=r_B\cos\Theta-r_A,\quad l_B=r_A\cos\Theta-r_B. \quad (4.128)$$

The contributions $V_{ee}^{(1)}$ and $V_{ee}^{(2)}$ to the body-induced potential $V_{ee}^{(b)}$, Eq. (4.65), can be calculated by using $\boldsymbol{G}^{(0)}$ and $\boldsymbol{G}^{(1)}$ from Eqs. (4.127) and (4.121) in Eqs. (4.66) and (4.67), which leads to

$$V_{ee}^{(1)}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar\mu_0^2c^3}{16\pi^3 l^5 r_A r_B}\sum_{n=1}^{\infty}\frac{(2n+1)}{n(n+1)}\int_0^\infty \mathrm{d}u\, u\alpha_A(iu)\alpha_B(iu)\mathrm{e}^{-\xi}$$
$$\times\Bigg(B_n^N\Big\{n^2(n+1)^2P_n(\gamma)Q_n\big[\gamma\, l^2 f(\xi)+g(\xi)l_A l_B\big]+n(n+1)\sin^2\Theta P_n'(\gamma)\left[l^2 f(\xi)\left(Q_n^A+Q_n^B\right)\right.$$
$$\left.+g(\xi)\big(r_A l_A Q_n^B+r_B l_B Q_n^A\big)\big]+l^2 f(\xi)L_n\big[\gamma F_n(\gamma)+P_n'(\gamma)\big]-r_A r_B g(\xi)\sin^2\Theta L_n F_n(\gamma)\Big\}$$
$$+r_A r_B\frac{u^2}{c^2}B_n^M Q_n\Big[g(\xi)r_A r_B\sin^2\Theta P_n'(\gamma)-n(n+1)l^2 f(\xi)P_n(\gamma)\Big]\Bigg), \quad (4.129)$$

$$V_{ee}^{(2)}(\mathbf{r}_A,\mathbf{r}_B)=\frac{-\hbar\mu_0^2c^2}{32\pi^3 r_A^2 r_B^2}\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}\frac{(2n+1)(2n'+1)}{n(n+1)n'(n'+1)}\int_0^\infty \mathrm{d}u\, u^2\alpha_A(iu)\alpha_B(iu)$$
$$\times\Bigg\{B_n^N B_{n'}^N\big[n^2(n+1)^2n'^2(n'+1)^2P_n(\gamma)P_{n'}(\gamma)Q_nQ_{n'}+n(n+1)n'(n'+1)\sin^2\Theta\, P_n'(\gamma)P_{n'}'(\gamma)$$
$$\times\left(Q_n^AQ_{n'}^A+Q_n^BQ_{n'}^B\right)\big]+\Big(r_A^2r_B^2\frac{u^4}{c^4}B_n^MB_{n'}^MQ_nQ_n'+B_n^NB_{n'}^NL_nL_{n'}\Big)\big[F_n(\gamma)F_{n'}(\gamma)+P_n'(\gamma)P_{n'}'(\gamma)\big]$$
$$-2r_Ar_B\frac{u^2}{c^2}B_n^MB_{n'}^NQ_nL_{n'}\left[P_n'(\gamma)F_{n'}(\gamma)+F_n(\gamma)P_{n'}'(\gamma)\right]\Bigg\}, \quad (4.130)$$

where $\xi=lu/c$. Further evaluation of Eqs. (4.129) and (4.130) requires numerical methods in general. Before doing so, let us consider the limiting cases of large and small spheres.

The limiting case of a large sphere may be defined by the requirement that

$$\delta_{A'}\equiv r_{A'}-R\ll R,\quad (A'=A,B) \quad (4.131)$$

and

$$l\ll R\Rightarrow\Theta\ll 1 \quad (4.132)$$

(cf. Fig. 4.5). In this limit, the body-induced part of the interaction potential is found to be (Appendix B.2)

$$V_{ee}^{(b)} = \frac{1}{l^5 l_+^5}\Big\{\left(3X^4 - 3\delta_-^2\delta_+^2 + l^2 l_+^2\right) I_{011} - \frac{l_+^2}{R}\left[3l_+^2(l_+ - \delta_+) + \delta_+(2\delta_-^2 - X^2)\right] I_{012}$$
$$+ l_+^4\left[\delta_-^2 - 2X^2 + 3\delta_+(l_+ - \delta_+)\right] C_{\rm nr}^{(2)} - \frac{3l^5}{l_+} I_{022} - \frac{l^5}{Rl_+^3}\left[2l_+^2\delta_+ + 3\left(\delta_+^3 - l_+^3\right)\right] I_{023}$$
$$- \frac{l^5\delta_+}{Rl_+^3}\left(5\delta_+^2 + 2X^2\right) I_{123}\Big\}, \tag{4.133}$$

with $X = -R\Theta$, $\delta_\pm = \delta_B - \delta_A$, $l_+ = \left(X^2 + \delta_+^2\right)^{1/2}$,

$$I_{ijk} = \frac{\hbar}{16\pi^3\varepsilon_0^2}\int_0^\infty \mathrm{d}u\, \alpha_A(iu)\alpha_B(iu)\varepsilon^i(iu)\frac{[\varepsilon(iu)-1]^j}{[\varepsilon(iu)+1]^k}, \tag{4.134}$$

and $C_{\rm nr}^{(2)}$ being given by Eq. (4.110). The case of a purely electric sphere can be simply obtained by setting $\mu(iu) = 1$ in Eq. (4.133). For a purely magnetic sphere [$\varepsilon(iu) = 1$], Eq. (4.133) reduces, under the conditions (4.131) and (4.132), to

$$V_{ee}^{(b)} = [\delta_-^2 - 2X^2 + 3\delta_+(l_+ - \delta_+)]\frac{C_{\rm nr}^{(2)}}{l^5 l_+}, \tag{4.135}$$

that is the body-induced interaction potential in the presence of a purely magnetic half-space [cf. Eq. (4.114)]. As expected, Eq. (4.133) for $l_+/R \to 0$ reduces to the body-assisted potential found for a half-space, Eq. (4.65) together with (4.107) and (4.108).

In the opposite limit of small sphere, where

$$R \ll r_{A'} \quad (A' = A, B), \tag{4.136}$$

the body-induced part of the interaction potential yield the form (Appendix B.2)

$$V_{ee}^{(b)} = \frac{\hbar}{64\pi^4\varepsilon_0^3 r_A^3 r_B^3 l^3}\int_0^\infty \mathrm{d}u\alpha_A(iu)\alpha_B(iu)e^{-(r_A+r_B+l)u/c}$$
$$\times\Bigg(\alpha_{\rm sp}(iu)\Big\{\left[2(1+a) - g(a)\sin^2\Theta\right]g(b)f(\xi) + 2a^2 f(b)f(\xi) + \left[(2l^2 - r_A r_B\cos\Theta)f(a)f(b)\right.$$
$$\left. + 2a^2 f(b)r_A l_A - 2b^2 f(a)r_B l_B\right]\frac{g(\xi)}{l^2}\sin^2\Theta - 4(1+a)(1+b)\frac{g(\xi)}{l^2}l_A l_B\cos\Theta\Big\}$$
$$+ \frac{ab}{c^2}(1+a)(1+b)\beta_{\rm sp}(iu)\left[g(\xi)\frac{r_A r_B}{l^2}\sin^2\Theta - 2f(\xi)\cos\Theta\right]\Bigg) \tag{4.137}$$

($a = r_A u/c$, $b = r_B u/c$), where $\alpha_{\rm sp}$ and $\beta_{\rm sp}$ are defined by Eqs. (3.64) and (3.65), respectively. As in the case of singl-atom potential Eq. (3.63), we may replace the sphere parameters $\alpha_{\rm sp}$ and $\beta_{\rm sp}$, respectively with the electric and magnetic polarizability of an atom, to obtain the non-additive interaction potential of three atoms, two of which being purely electric whereas the third atom being simultaneously electrically and magnetically polarizable. Indeed, after

a straightforward but lengthy calculation, it can be shown that in the case of a purely electric sphere, Eq. (4.137) [$\beta_{\rm sp}(iu)=0$] leads to the interaction potential between three electric atoms, as derived in Refs. [55, 57, 59, 107].

In the retarded limit where l,r_A,$r_B \gg c/\omega_{\rm min}$ ($\omega_{\rm min}$ denoting the minimum frequency among the relevant atomic and medium transition frequencies), due to the presence of the exponential term in the integral in Eq. (4.137), only small values of u significantly contribute to the integral. Therefore, the electric and magnetic polarizabilities can be approximately replaced with their static values. After performing the remaining integral and expressing all the geometric parameters in terms of r_A, r_B, and l, we arrive at

$$V_{ee}^{(b)} = \frac{\hbar c \alpha_A(0)\alpha_B(0)}{32\pi^4\varepsilon_0^3 r_A^5 r_B^5 l^5 (r_A+r_B+l)^7}\Bigg[\alpha_{\rm sp}(0)\big\{\mathcal{S}[h_3(r_A,r_B,l)] + \mathcal{S}[h_3(r_B,l,r_A)] + \mathcal{S}[h_3(l,r_A,r_B)]\big\} + \frac{r_A^2 r_B^2}{c^2}\beta_{\rm sp}(0)\mathcal{S}[h_4(r_A,r_B,l)]\Bigg], \quad (4.138)$$

where

$$h_3(x,y,z) = 3x^6y^2(y-x)(x+y+7z)(x^2+7xy+11y^2) - x^4y^2z^2(53x^4+280x^3y-137x^2y^2 - 329xy^3-623xy^2z-192y^2z^2), \quad (4.139)$$

$$h_4(x,y,z) = 3x^4(y-x)(x+y+7z)(x^2+7xy+11y^2) - 2x^3z^2(x+y)(26x^2+93xy-133y^2) - 7x^2z^5(3x-2y) - 14x^3z^3(2x^2-3xy-13y^2) - x^3z^4(17x+161y) + 2xz^6(31x+105y) + 5z^7(14x+z), \quad (4.140)$$

and $\mathcal{S}[f(x,y,z)] = f(x,y,z)+f(y,x,z)$.

In the nonretarded limit where l,r_A,$r_B \ll c/[n(0)\omega_{\rm max}]$ ($\omega_{\rm max}$ denoting the maximum frequency among the relevant atomic and medium transition frequencies), the leading contribution to the integral in Eq. (4.137) comes from the region where $e^{-(r_A+r_B+l)u/c} \simeq 1$, so Eq. (4.137) reduces to

$$V_{ee}^{(b)} = \frac{3\hbar}{64\pi^4\varepsilon_0^3 r_A^3 r_B^3 l^3}\left\{\left[1+\frac{1}{l^2}(4l_Al_B - r_Ar_B\sin^2\Theta)\cos\Theta+\cos^2\Theta\right]J_1 + \frac{r_Ar_B}{c^4}\left(\frac{r_Ar_B}{l^2}\sin^2\Theta-\frac{2}{3}\cos\Theta\right)J_2\right\}, \quad (4.141)$$

where

$$J_1 = \int_0^\infty {\rm d}u\, \alpha_A(iu)\alpha_B(iu)\alpha_{\rm sp}(iu), \quad (4.142)$$

$$J_2 = \int_0^\infty {\rm d}u\, u^2\alpha_A(iu)\alpha_B(iu)\beta_{\rm sp}(iu). \quad (4.143)$$

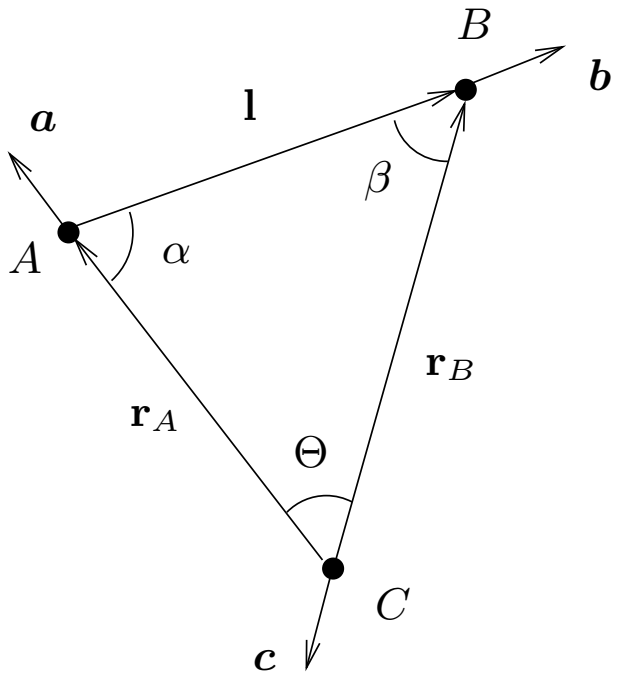

Figure 4.6: The triangle formed by the two atoms (at the corners A and B) and the sphere (at the corner C) is shown for the small-sphere limit. It is seen that the vector products $\boldsymbol{a}\cdot\boldsymbol{b}$, $\boldsymbol{b}\cdot\boldsymbol{c}$ and $\boldsymbol{c}\cdot\boldsymbol{a}$ in the Axilrod and Teller's formula [55, 57] are equal to $-\cos\alpha$, $-\cos\beta$, and $-\cos\Theta$, respectively.

In particular, in the case of a purely electric sphere ($J_2=0$), Eq. (4.141) can be written in a very symmetric form. For this purpose we introduce the unit vectors $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ pointing in the directions of $\mathbf{r}_A$, $\mathbf{l}$, and $-\mathbf{r}_B$, respectively (see Fig. 4.6). Noting that l_A and l_B defined by Eq. (4.128) can be written as $l(\boldsymbol{a}\cdot\boldsymbol{b})$ and $l(\boldsymbol{b}\cdot\boldsymbol{c})$, respectively, we see that

$$\frac{1}{l^2}(4l_Al_B - r_Ar_B\sin^2\Theta) + \cos\Theta = 3(\boldsymbol{a}\cdot\boldsymbol{b})(\boldsymbol{b}\cdot\boldsymbol{c}) \tag{4.144}$$

and can rewrite Eq. (4.141) as

$$V_{ee}^{(b)} = \frac{3\hbar}{64\pi^4\varepsilon_0^3 r_A^3 r_B^3 l^3}\left[1 - 3(\boldsymbol{a}\cdot\boldsymbol{b})(\boldsymbol{b}\cdot\boldsymbol{c})(\boldsymbol{c}\cdot\boldsymbol{a})\right] J_1. \tag{4.145}$$

If $\alpha_{sp}(iu)$ in Eq. (4.142) is again identified with the electric polarizability of a single atom, Eq. (4.145) is nothing but the formula for the nonretarded three-atom interaction potential, which was first given by Axilrod and Teller [55, 57].

Based on numerical calculations, the effect of a medium-sized magnetoelectric sphere on the mutual vdW interaction of two identical, electric, two-level atoms is illustrated in Figs. 4.7 and 4.8 showing the ratio $V_{ee}/V_{ee}^{(0)}$. The results have been found by exact numerical evaluation of Eqs. (4.129), (4.130), and (4.68), where the permittivity and permeability of the sphere have been described by the same model used for the half-space, Eqs. (4.116) and (4.117).

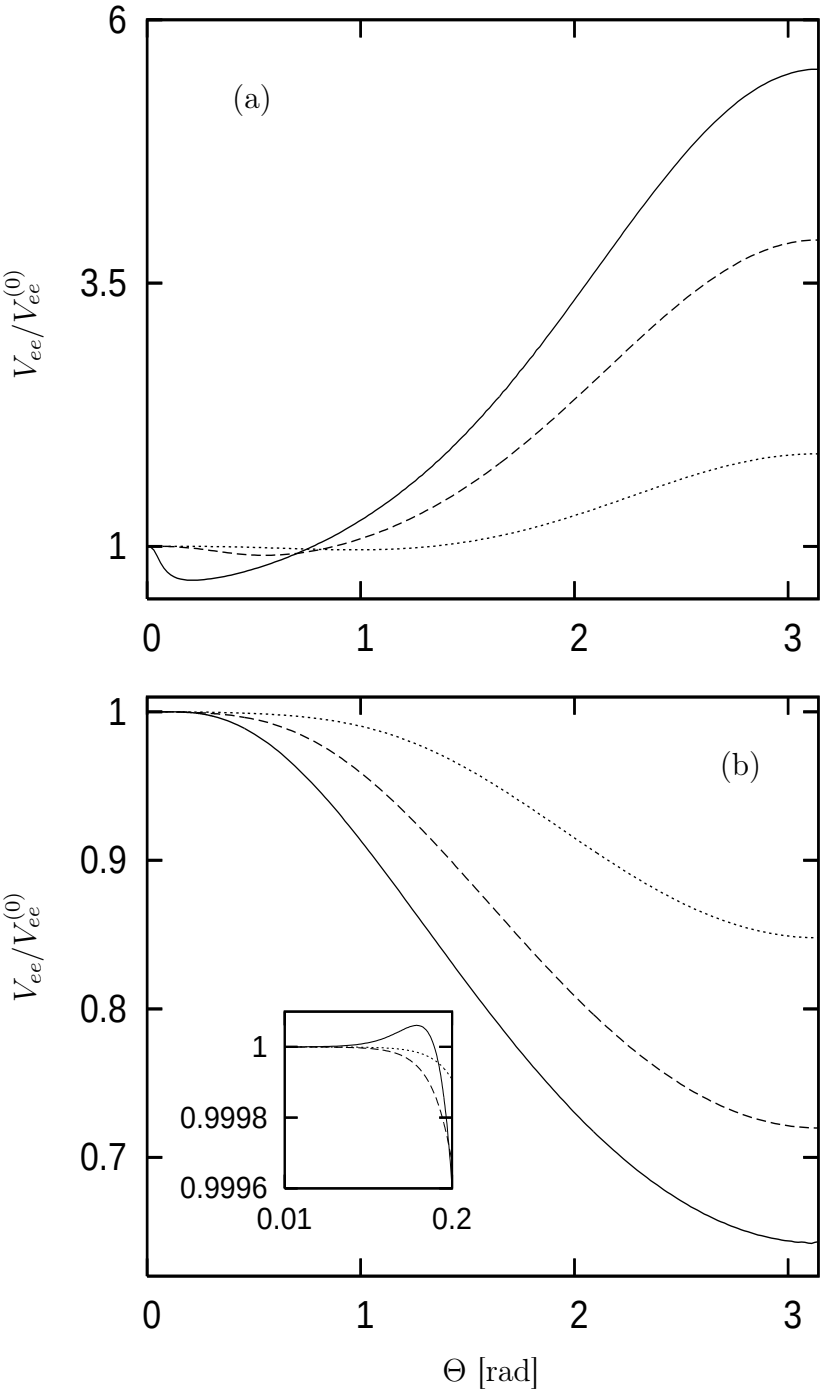

Figure 4.7: The mutual vdW potential of two identical two-level atoms in a triangular configuration with (a) a purely electric sphere with $\omega_{\mathrm{P}e}/\omega_{10}=3$, $\omega_{\mathrm{T}e}/\omega_{10}=1$, and $\gamma_e/\omega_{10}=0.001$ and (b) a purely magnetic sphere with $\omega_{\mathrm{P}m}/\omega_{10}=3$, $\omega_{\mathrm{T}m}/\omega_{10}=1$, and $\gamma_m/\omega_{10}=0.001$ is shown as a function of the atom–atom angular separation Θ (ω_{10} is the atomic transition frequency). The sphere radius is $R=c/\omega_{10}$ and the distances between the atoms and the center of the sphere are $r_A=r_B=1.03\,c/\omega_{10}$ (solid line), $1.3\,c/\omega_{10}$ (dashed line), and $2\,c/\omega_{10}$ (dotted line). $V_{ee}^{(0)}$ is the potential observed in free space.

In Fig. 4.7, a configuration is considered where the two atoms are positioned at equal distances from the sphere, $r_A{=}r_B$, briefly referred to as triangular configuration, and $V_{ee}/V_{ee}^{(0)}$ is shown as a function of the angular separation Θ for three different values of the atom–sphere separation. For a purely electric sphere [Fig. 4.7(a)], depending on the separation angle between the atoms, a (compared to the free-space case) relative reduction or enhancement of the vdW potential is possible, while for a purely magnetic sphere [Fig. 4.7(b)], the potential is typically reduced [note that for very small angular separations, a slight enhancement is possible, as can be seen from the inset in Fig. 4.7(b)], and the reduction increases with the angular separation. In both cases, the sphere-induced modification is strongest when the atoms are at opposite sides of the sphere ($\Theta = \pi$). Note that for small atom–sphere separations (solid curves) and small angular separations, the potential qualitatively agrees with the potential obtained for two atoms placed in parallel alignment near a semi-infinite half-space, Fig. 4.2, as expected from the results in the limiting case of a large sphere.

In Fig. 4.8, a configuration is considered where the two atoms and the sphere center are aligned on a straight line, briefly referred to as linear configuration, and $V_{ee}/V_{ee}^{(0)}$ is shown as a function of the interatomic distance for three different values of the position r_A of atom A which is positioned between the sphere and atom B ($\Theta = 0$). Unless both atoms are very close to the sphere, the sphere gives always rise to a (compared to the free-space case) relative enhancement of the vdW potential between the atoms; only for very small atom–sphere separations the potential can be reduced if the sphere is purely magnetic [inset in Fig. 4.8(b)]. Figure 4.8(a) shows that in the presence of a purely electric sphere the relative enhancement of the potential increases with the interatomic separation l and approaches a limit for larger interatomic separations, which depends on the separation distance between atom A and the sphere. From Fig. 4.8(b) it is seen that in the presence of a purely magnetic sphere the relative enhancement of the potential increases with the interatomic separation l, reaches a maximum, and decreases with a further increase of l. In agreement with the results of a large sphere, the potential observed for small atom sphere separations (solid curves) and small interatomic separations qualitatively agrees with the potential obtained for two atoms placed in vertical alignment near a semi-infinite half-space, Fig. 4.3.

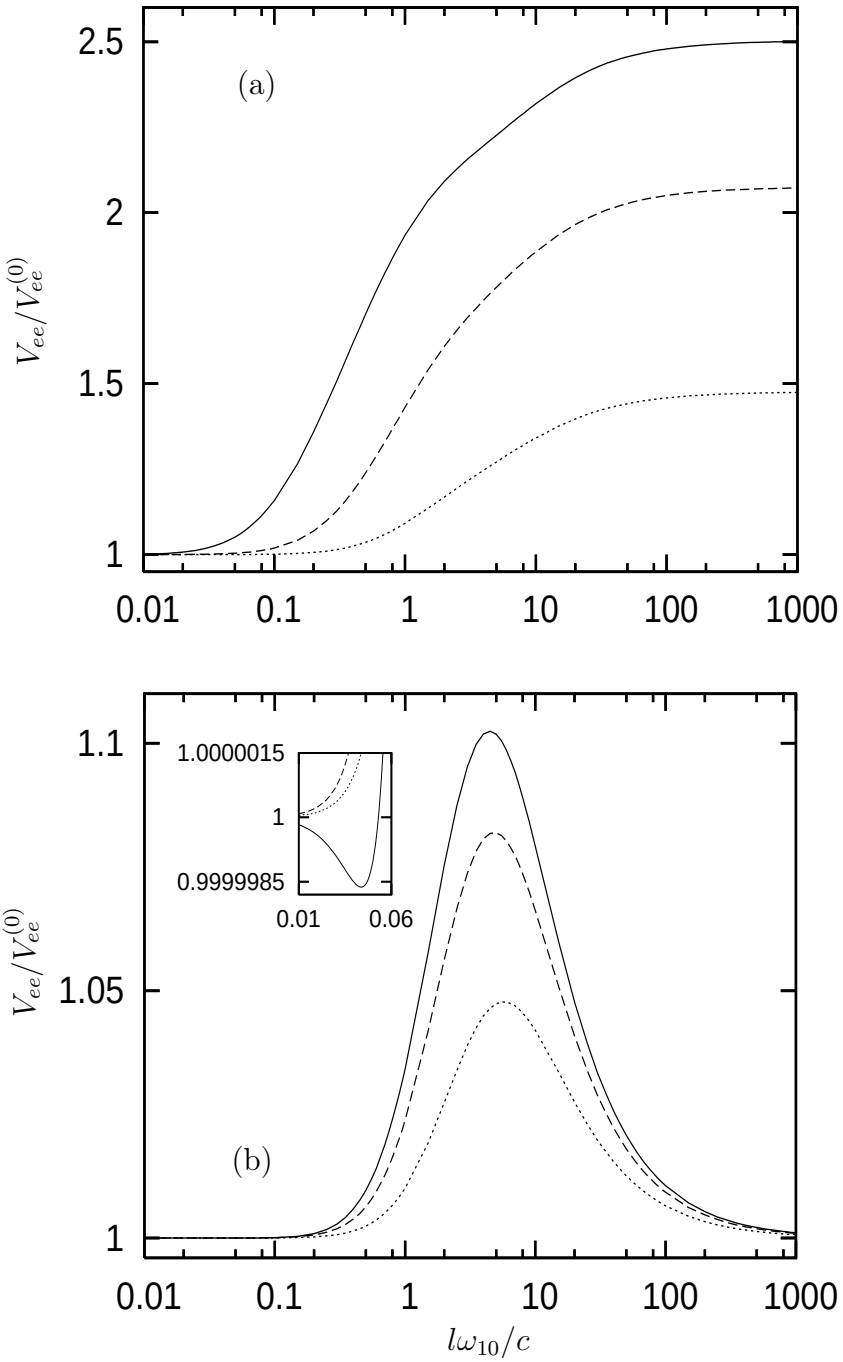

Figure 4.8: The mutual vdW potential of two identical two-level atoms in a linear configuration with (a) a purely electric sphere and (b) a purely magnetic sphere is shown as a function of the interatomic distance l. Atom A is held at a fixed position between atom B and the sphere center with $r_A = 1.03\, c/\omega_{10}$ (solid line), $1.1\, c/\omega_{10}$ (dashed line), and $1.3\, c/\omega_{10}$ (dotted line). All other parameters are the same as in Fig. 4.7.

Let us now evaluate the magnetic-magnetic part of the vdW potential, $V_{mm}^{(b)}$, for which the tensor $\boldsymbol{L}$ is required. The bulk part of the tensor $\boldsymbol{L}$ is given by Eq. (3.29), where $\varepsilon_A = \mu_A = k = 1$. Comparing Eq. (3.29) with (3.25), it can be found easily that

$$\boldsymbol{L}^{(0)}(\mathbf{r}_A, \mathbf{r}_B, \omega) = -\frac{\omega^2}{c^2}\boldsymbol{G}^{(0)}(\mathbf{r}_A, \mathbf{r}_B, \omega). \tag{4.146}$$

On the other hand, the scattering part of the tensor $\boldsymbol{L}$ can be obtained by replacing $\boldsymbol{G}$ on the right-hand side of Eq. (3.16) with $\boldsymbol{G}^{(1)}$ from Eq. (3.46). This leads, after making use of Eqs. (3.49) and (3.50), to

$$\begin{aligned}\boldsymbol{L}^{(1)}(\mathbf{r}, \mathbf{r}', \omega) = \frac{-i\omega^3}{4\pi c^3}\sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)}\sum_{m=0}^{n}\frac{(n-m)!}{(n+m)!}(2-\delta_{0m}) \\ \times\sum_{p=\pm 1}\left[B_n^M(\omega)\mathbf{N}_{nm,p}(\mathbf{r}, \omega/c)\mathbf{N}_{nm,p}(\mathbf{r}', \omega/c) + B_n^N(\omega)\mathbf{M}_{nm,p}(\mathbf{r}, \omega/c)\mathbf{M}_{nm,p}(\mathbf{r}', \omega/c)\right].\end{aligned} \tag{4.147}$$

By a comparison between Eqs. (4.147) and (3.46) it can be seen that $\boldsymbol{L}^{(1)}$ can be given as $-\omega^2\boldsymbol{G}^{(1)}/c^2$ after interchanging $B_n^M \leftrightarrow B_n^N$ [or, equaivalently, interchanging $\varepsilon \leftrightarrow \mu$; see Eqs. (3.51) and (3.52)]. Having these relations between the tensors $\boldsymbol{L}$ and $\boldsymbol{G}$, a comparison between Eqs. (4.19) and (4.27) leads directly to obtain $V_{mm}^{(b)}$ from $V_{ee}^{(b)}$ [Eq. (4.65) together with Eqs. (4.66) and (4.67)] by the transformation $\alpha \to \beta/c^2$, $\varepsilon \leftrightarrow \mu$ [95, HS6]. Hence, all various limiting cases treated for the potential $V_{ee}^{(b)}$, can be transformed easily to give the counterpart results for the potential $V_{mm}^{(b)}$. Therefore, we are intentionally refraining from presenting them here to avoid repetitions.

Calculation of $V_{em}^{(b)}$ and $V_{me}^{(b)}$

The body-induced part of the electric-magnetic interaction potential can be considered, similar to the electric-electric part, in the form

$$V_{em}^{(b)}(\mathbf{r}_A, \mathbf{r}_B) = V_{em}^{(1)}(\mathbf{r}_A, \mathbf{r}_B) + V_{em}^{(2)}(\mathbf{r}_A, \mathbf{r}_B) \tag{4.148}$$

with $V_{em}^{(1)}$ and $V_{em}^{(2)}$ being given as

$$V_{em}^{(1)}(\mathbf{r}_A, \mathbf{r}_B) = \frac{\hbar\mu_0^2}{\pi}\int_0^{\infty}\mathrm{d}u\, u^2\alpha_A(iu)\beta_B(iu)\mathrm{Tr}\left[\boldsymbol{K}^{(0)\mathsf{T}}(\mathbf{r}_B, \mathbf{r}_A, iu)\cdot\boldsymbol{K}^{(1)}(\mathbf{r}_B, \mathbf{r}_A, iu)\right], \tag{4.149}$$

$$V_{em}^{(2)}(\mathbf{r}_A, \mathbf{r}_B) = \frac{\hbar\mu_0^2}{2\pi}\int_0^{\infty}\mathrm{d}u\, u^2\alpha_A(iu)\beta_B(iu)\mathrm{Tr}\left[\boldsymbol{K}^{(1)\mathsf{T}}(\mathbf{r}_B, \mathbf{r}_A, iu)\cdot\boldsymbol{K}^{(1)}(\mathbf{r}_B, \mathbf{r}_A, iu)\right]. \tag{4.150}$$

Here, we use the same coordinate system chosen for deriving Eqs. (4.129) and (4.130) in which the bulk part of the tensor $\boldsymbol{K}$ given by Eq. (4.42) [$\mu(\omega) = 1 = k$] takes the form

$$\boldsymbol{K}^{(0)}(\mathbf{r}_B, \mathbf{r}_A, \omega) = \frac{\mathrm{e}^{il\omega/c}}{4\pi l^3}(1 - il\omega/c)(r_A\sin\Theta\,\mathbf{e}_{r_B}\mathbf{e}_{\phi_A} + l_B\mathbf{e}_{\theta_B}\mathbf{e}_{\phi_A} + r_B\sin\Theta\,\mathbf{e}_{\phi_B}\mathbf{e}_{r_A} + l_A\mathbf{e}_{\phi_B}\mathbf{e}_{\theta_A}) \tag{4.151}$$

and the scattering part can be found by substituting $\boldsymbol{G}^{(1)}(\mathbf{r}, \mathbf{r}', \omega)$ from Eq. (3.46) into (4.26) and setting $\mathbf{r}$ and $\mathbf{r}'$, respectively, to $\mathbf{r}_B$ and $\mathbf{r}_A$ given by Eq. (4.120), that results in (Appendix B)

$$\boldsymbol{K}^{(1)}(\mathbf{r}_B, \mathbf{r}_A, \omega) = \frac{i\omega}{4\pi r_A r_B}\sum_{n=1}^{\infty}(2n+1)\Big\{ r_A B_n^M Q_n P_n'(\gamma)\sin\Theta\, \mathbf{e}_{r_B}\mathbf{e}_{\phi_A} + \frac{1}{n(n+1)}\big[r_A B_n^M Q_n^B F_n(\gamma) - r_B B_n^N Q_n^A P_n'(\gamma)\big]\mathbf{e}_{\theta_B}\mathbf{e}_{\phi_A} + r_B B_n^N Q_n P_n' \sin\Theta\, \mathbf{e}_{\phi_B}\mathbf{e}_{r_A} + \frac{1}{n(n+1)}\left[r_B B_n^N Q_n^A F_n(\gamma) - r_A B_n^M Q_n^B P_n'(\gamma)\right]\mathbf{e}_{\phi_B}\mathbf{e}_{\theta_A}\Big\}. \quad (4.152)$$

Using Eqs. (4.151) and (4.152) in Eqs. (4.149) and (4.150), we find

$$V_{em}^{(1)} = \frac{-\hbar\mu_0^2}{16\pi^3 c l^3 r_A r_B}\sum_{n=1}^{\infty}\frac{(2n+1)}{n(n+1)}\int_0^{\infty}\mathrm{d}u\, u^3\alpha_A(iu)\beta_B(iu)\mathrm{e}^{-lu/c}\left(1+\frac{lu}{c}\right) \times\Big\{ n(n+1)\sin^2\Theta\left[r_A^2 B_n^M + r_B^2 B_n^N\right]Q_n P_n'(\gamma) + r_A B_n^M Q_n^B\left[l_B F_n(\gamma) - l_A P_n'(\gamma)\right] + r_B B_n^N Q_n^A\left[l_A F_n(\gamma) - l_B P_n'(\gamma)\right]\Big\}, \quad (4.153)$$

$$V_{em}^{(2)} = \frac{\hbar\mu_0^2}{32\pi^3 c^2 r_A^2 r_B^2}\sum_{n,n'=1}^{\infty}\frac{(2n+1)(2n'+1)}{n(n+1)n'(n'+1)}\int_0^{\infty}\mathrm{d}u\, u^4\alpha_A(iu)\beta_B(iu) \times\Big\{ n(n+1)n'(n'+1)Q_n Q_{n'}\sin^2\Theta P_n'(\gamma)P_{n'}'(\gamma)\left[r_A^2 B_n^M B_{n'}^M + r_B^2 B_n^N B_{n'}^N\right] + \left[r_B^2 B_n^N B_{n'}^N Q_n^A Q_{n'}^A + r_A^2 B_n^M B_{n'}^M Q_n^B Q_{n'}^B\right]\left[F_n(\gamma)F_{n'}(\gamma) + P_n'(\gamma)P_{n'}'(\gamma)\right] - 2r_A r_B B_n^M B_{n'}^N Q_n^B Q_{n'}^A\left[P_n'(\gamma)F_{n'}(\gamma) + P_{n'}'(\gamma)F_n(\gamma)\right]\Big\}. \quad (4.154)$$

Let us, as in the case of electric-electric potential, consider the limiting cases of large and small sphere. In the case of a large sphere, provided by the conditions (4.131) and (4.132), we obtain (Appendix B.2)

$$V_{em}^{(b)} = \frac{\hbar\mu_0^2}{32\pi^3 l^3 l_+^4 (l_+ + \delta_+)^2}\big\{2l_+(l_+ + \delta_+)^2\big[\left(X^2 - \delta_-\delta_+\right)J_{10} + \left(X^2 + \delta_-\delta_+\right)J_{01}\big] + l^3(2l_+^2 + X^2)(J_{20} + J_{02}) + 4l^3\left(X^2 - l_+\delta_+\right)J_{11}\big\}, \quad (4.155)$$

where X, $\delta_\pm$, and l_+ are defined as below Eq. (4.133), and

$$J_{kl} = \int_0^{\infty}\mathrm{d}u\, u^2\alpha_A(iu)\beta_B(iu)\left[\frac{\varepsilon(iu)-1}{\varepsilon(iu)+1}\right]^k\left[\frac{\mu(iu)-1}{\mu(iu)+1}\right]^l. \quad (4.156)$$

In the opposite limiting case of a small sphere, where the condition (4.136) comes true, $V_{em}^{(b)}$

can be approximated to (Appendix B.2)

$$V_{em}^{(b)} = \frac{\hbar\mu_0^3 c^2}{64\pi^4 l^3 r_A^3 r_B^3}\int_0^\infty \mathrm{d}u\, u^2 \alpha_A(iu)\beta_B(iu)e^{-(r_A+r_B+l)u/c}\left(1+l\frac{u}{c}\right)\Big\{\big[2r_B(1+a)\sin^2\Theta + (l_B - l_A\cos\Theta)f(a)\big](1+b)r_B\alpha_{\rm sp}(iu) + \big[2r_A(1+b)\sin^2\Theta + (l_A - l_B\cos\Theta)f(b)\big] \times (1+a)r_A\frac{\beta_{\rm sp}(iu)}{c^2}\Big\} \quad (4.157)$$

with a and b being defined below Eq. (4.137), and $\alpha_{\rm sp}$ and $\beta_{\rm sp}$ being given by Eqs. (3.64) and (3.65). It is worth mentioning that the non-additive interaction potential of three atoms (polarizable atom A, magnetizable atom B, and a simultaneously polarizable and magnetizable third atom) in free space may be obtained from Eq. (4.157) by the same approach used below Eq. (4.137) to obtain the non-additive three-atom potential for two polarizable atoms A and B, and a third simultaneously polarizable and magnetizable atom. It should be pointed out that these results together with the duality principle may be used to obtain the non-additive potential between three atoms, each being simultaneously polarizable and magnetizable.

Let us now present some numerical results illustrating the effect of a medium-sized magnetoelectric sphere on the electric-magnetic vdW interaction potential between two two-level atoms with equal transition frequencies. We again focus on the case where atom A is electric and atom B is magnetic. The results for two magnetic atoms can be found from that of two electric atoms, Figs. 4.7 and 4.8, by the duality. Figures 4.9 and 4.10 show the ratio $V_{em}/V_{em}^{(0)}$ obtained by exact numerical computation of Eqs. (4.118), (4.153), and (4.154), with the permittivity and permeability of the sphere being described by Eqs. (4.116) and (4.117), respectively.

Figure 4.9 shows the ratio $V_{em}/V_{em}^{(0)}$ as a function of the angular separation Θ of the atoms in triangular configuration ($r_A = r_B$), for three different values of the atom–sphere separation. It is seen that, dependent upon Θ, enhancement or reduction of $V_{em}/V_{em}^{(0)}$ can be observed. To be more specific, $V_{em}/V_{em}^{(0)}$ first increases with Θ, attains a maximum, and then decreases with increasing Θ to eventually become minimal at $\Theta = \pi$ when the atoms are positioned at opposite sides of the sphere. Whereas the position of the maximum shifts with the atom–sphere separation, the minimum is always at $\Theta = \pi$ observed. Note that when the electric sphere is replaced with an analogous magnetic sphere, the same behavior is found, because of duality.

Figure 4.10 illustrates the dependence of the ratio $V_{em}/V_{em}^{(0)}$ on the separation distance l between the two atoms in linear configuration, with atom A being closer to the sphere than

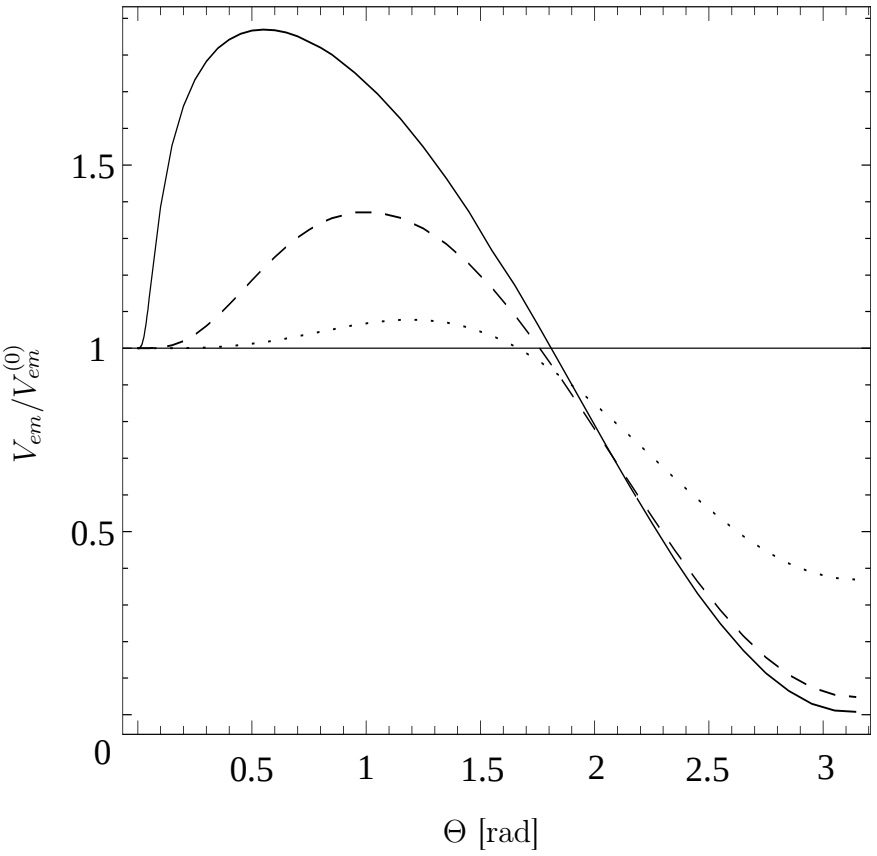

Figure 4.9: The (normalized) vdW interaction potential between two two-level atoms of transition frequency ω_{10} in the presence of an electric sphere is shown as a function of the atom–atom angular separation Θ. The sphere parameters are the same as in Fig. 4.7(a). Atom A is electrically and atom B is magnetically polarizable. The values of $r_A = r_B$ are $1.03\,c/\omega_{10}$ (solid line), $1.3\,c/\omega_{10}$ (dashed line), and $2\,c/\omega_{10}$ (dotted line).

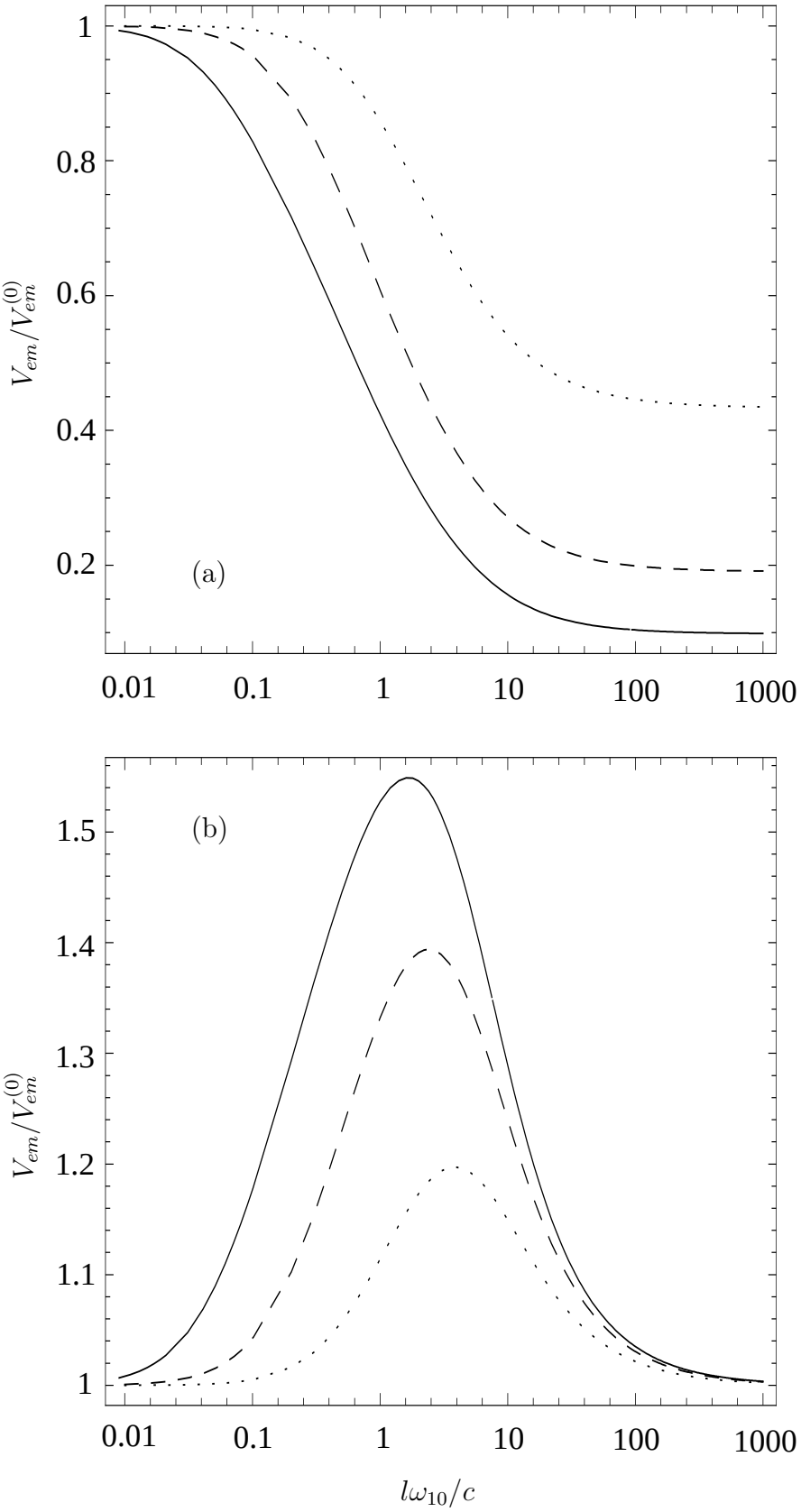

Figure 4.10: The vdW interaction potential between the same two atoms as in Fig. 4.9 in the presence of (a) an electric sphere and (b) an analogous magnetic sphere is shown as a function of atom–atom distance l for $\Theta = 0$ and $r_B = r_A + l$. The sphere parameters are the same as in Fig. 4.8. The values of r_A are $1.03\, c/\omega_{10}$ (solid line), $1.1\, c/\omega_{10}$ (dashed line), $1.3\, c/\omega_{10}$ (dotted line).

atom B. From Fig. 4.10(a) it is seen that in the case of an electric sphere the interaction potential is reduced compared to its value in free space; the ratio $V_{em}/V_{em}^{(0)}$ decreases with increasing l and approaches an asymptotic limit that depends to the distance between atom A and the sphere. On the contrary, from Fig. 4.10(b) it is seen that in the case of the analogous magnetic sphere the interaction potential is enhanced compared to its value in free space, with a pronounced maximum of the ratio $V_{em}/V_{em}^{(0)}$ being observed. For large atom–atom distances, $V_{em}/V_{em}^{(0)}$ approaches an asymptotic limit that is independent of the distance between atom A and the sphere.

4.4 Method of image charges

Many features of the vdW potential observed in Figs. 4.2–4.4, 4.7, and 4.8 can be subject to a physical interpretation via the method of image charges. Although being strictly valid only for sufficiently small atom–atom and atom–surface distances (such that retardation is negligible) and being most easily applicable in the perfect conductor limit, this approach yields qualitative predictions for the body-induced enhancement and reduction of the potential which apply beyond this case. According to this method, the effect of the boundaries is simulated by suitably placed image charges of appropriate magnitudes, so that the two-atom vdW potential effectively consists of interactions between fluctuating dipoles A and B and their images A' and B' in the body, with

$$\hat{H}_{\rm int} = \hat{V}_{AB} + \hat{V}_{AB'} + \hat{V}_{BA'} \tag{4.158}$$

being the corresponding interaction Hamiltonian. Here, $\hat{V}_{AB}$ denotes the direct interaction between dipole A and dipole B, while $\hat{V}_{AB'}$ and $\hat{V}_{BA'}$ denote the indirect interaction between each dipole and the image induced by the other one in the body. The leading contribution to the energy shift is of second order in $\hat{H}_{\rm int}$,

$$\Delta E_{AB} = -\sum_{k,l\neq 0} \frac{\langle 0_A, 0_B|\hat{H}_{\rm int}|k_A, l_B\rangle}{\hbar(\omega_A^k + \omega_B^l)} \langle k_A, l_B|\hat{H}_{\rm int}|0_A, 0_B\rangle. \tag{4.159}$$

In this approach, $V^{(0)}$ corresponds to the product of two direct interactions, so it is negative because of the minus sign on the right-hand side of Eq. (4.159). Accordingly, $V^{(2)}$ is due to the product of two indirect interactions and is also negative. Hence the realization of enhancement or reduction of the interaction potential depends only on the sign of $V^{(1)}$ and its magnitude compared to that of $V^{(2)}$. The terms containing one direct and one indirect interaction are contained in $V^{(1)}$ and determine its sign. The orientations of the dipoles

A and B are random and independent of each other, so that strictly speaking the signs of all dipole–dipole interactions has to be obtained by averaging over all possible orientations. The effect of such averaging on the sign of the interactions can be reproduced by restricting the attention to the maximally attractive case of both dipoles pointing in the same direction parallel to their connecting line, with the dipole–dipole interaction $\hat{V}_{AB}$ being negative in this case. The image dipoles A' and B' are constructed by appropriate reflection of the dipoles A and B. The resulting signs of the interactions $\hat{V}_{AB'}$ and $\hat{V}_{BA'}$ between dipoles and image dipoles are negative/positive if the respective dipole moments are parallel/antiparallel. We can hence predict the sign of $V^{(1)}$ from a graphical construction of the image charges.

4.4.1 perfectly reflecting plate

Let us begin with the case of two atoms in the presence of a perfectly reflecting plate, for which the sign of $V^{(1)}$, Eq. (4.91), is summarized in Tab. 4.2, and the graphical construction of the image charges are sketched in Figs. 4.11 and 4.12.

	conducting plate	permeable plate
parallel case	+	−
vertical case	−	+

Table 4.2: Sign of $V^{(1)}$ for a perfectly reflecting plate.

Figure 4.11(a) shows two electric dipoles in front of a perfectly conducting plate in the parallel case. The configuration of the dipoles and images indicates repulsion between dipole $A(B)$ and dipole $B'(A')$, so $V^{(1)}$ is positive, in agreement with Tab. 4.2. On the contrary, in the vertical case from Fig. 4.11(b) an attraction is indicated, i.e., negative $V^{(1)}$, which is also in agreement with Tab. 4.2.

The case of two electric dipoles in front of a perfectly permeable plate can be treated by considering two magnetic dipoles in front of a perfectly conducting plate, as the two situations are equivalent due to the duality between electric and magnetic fields in the absence of free charges or currents. From Figs. 4.12(a) (parallel case) and 4.12(b) (vertical case) it is apparent that the interaction between dipole $A(B)$ and dipole $B'(A')$ is attractive in the parallel case and repulsive in the vertical case, again confirming the sign of $V^{(1)}$ as given in Tab. 4.2. When the dipole–dipole separation in Fig. 4.12(b) is sufficiently small compared with the dipole–surface separations, then the direct interaction between the two dipoles is expected to be stronger than their indirect interaction via the image dipoles. As

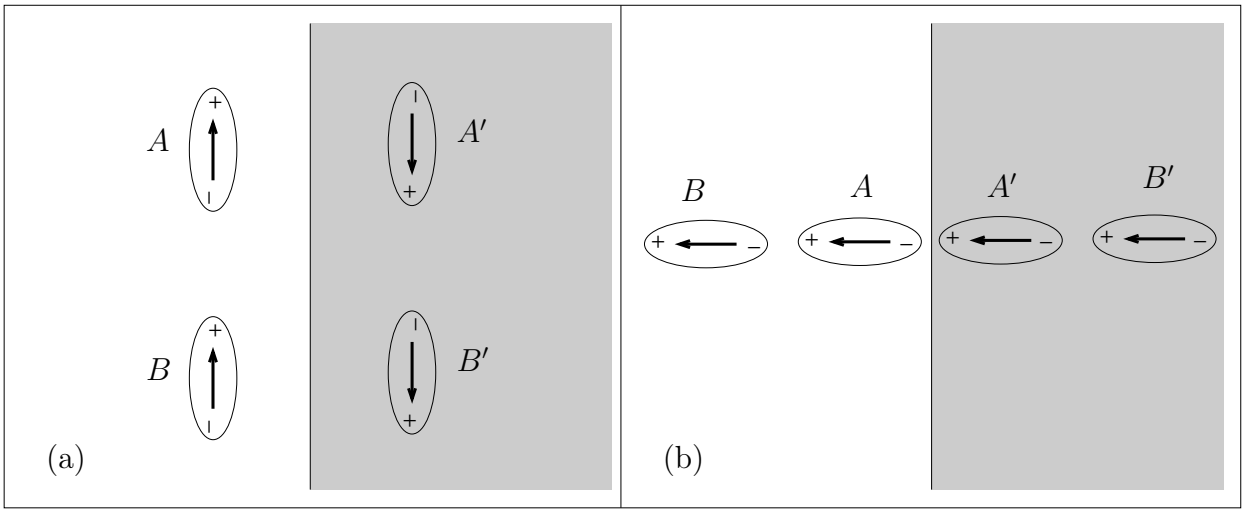

Figure 4.11: Two electric dipoles near a perfectly conducting plate are shown in (a) a parallel case (b) a vertical case.

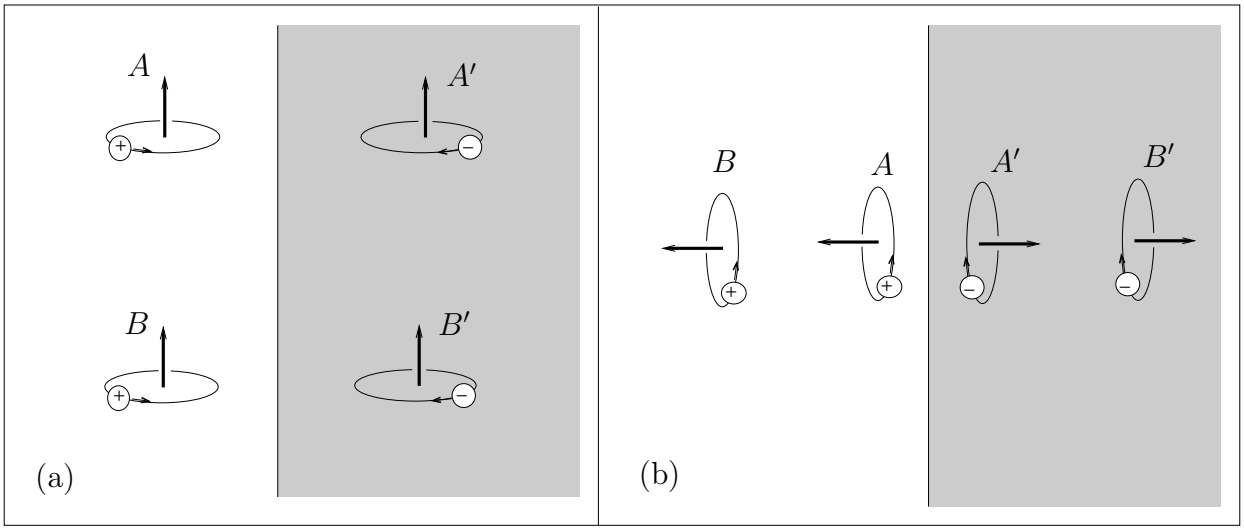

Figure 4.12: Two magnetic dipoles near a perfectly conducting plate are shown in (a) a parallel case (b) a vertical case.

a result, $V^{(1)}$ will be the dominant term in $V^{(1)}+V^{(2)}$ and $V^{(1)}+V^{(2)}$ becomes positive. However, when the dipole–dipole separation exceeds the dipole–surface separations, then the indirect interaction may become comparable to the direct one, and $V^{(2)}$ may be the dominant term, leading to negative $V^{(1)}+V^{(2)}$. The image dipole model hence gives also a qualitative explanation of the condition (4.97).

4.4.2 Homogeneous sphere

Let us now turn to the case of two electric atoms in the presence of a sphere. Figure 4.13 and 4.14 show, respectively, two electric dipoles and two magnetic dipoles near a purely

electric sphere in a triangular configuration, together with their images in the sphere. As in the case of a perfectly reflecting plate, the case of two electric dipoles in the presence of a purely magnetic body (i.e., the sphere) is replaced by two magnetic dipoles in the presence of a purely electric body, on the basis of utilizing the electromagnetic duality properties.

In a triangular configuration, when the inter-dipole angular separation is very small, the curvature of the spherical surface can be disregarded and the sphere can be approximately replaced by a half-space as in Figs. 4.13(a) and 4.14(a). Hence, for small angular separations, the interpretation of the sphere-induced enhancement or reduction of the two-atom interaction potential is the same as the case where the atoms are in the presence of a perfectly reflecting plate. That means, in small angular separations, a purely electric sphere suppresses the two-atom interaction potential whereas a purely magnetic sphere enhances the potential. This confirms the numerical results for short distances presented in Fig. 4.7. The case of two atoms located at the opposite ends of a sphere diameter

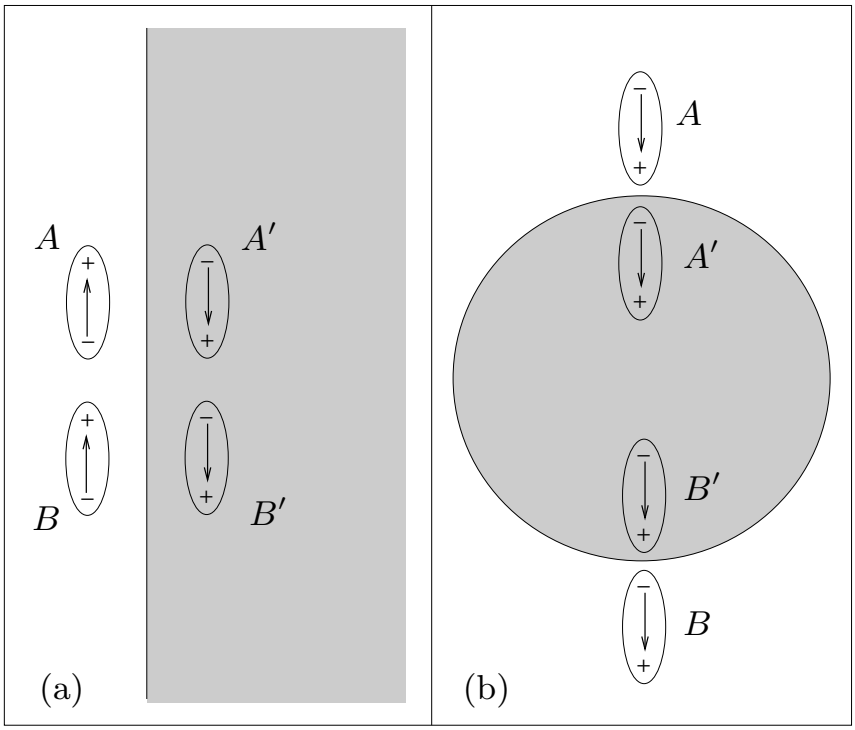

Figure 4.13: Two electric dipoles near a purely electric sphere are shown in a triangular configuration where the dipole-dipole angular separation (a) is small enough to replace the sphere, approximately, by a half-space and (b) is equal to π.

is sketched in Figs. 4.13(b) and 4.14(b), which, respectively, correspond to the cases of a purely electric sphere and a purely magnetic sphere, where in the latter the electromagnetic duality principle is invoked. It can be inferred from the figures that, in the case of a purely electric(magnetic) sphere $V_{ee}^{(1)}$ is negative(positive), and as a consequence, V_{ee} is

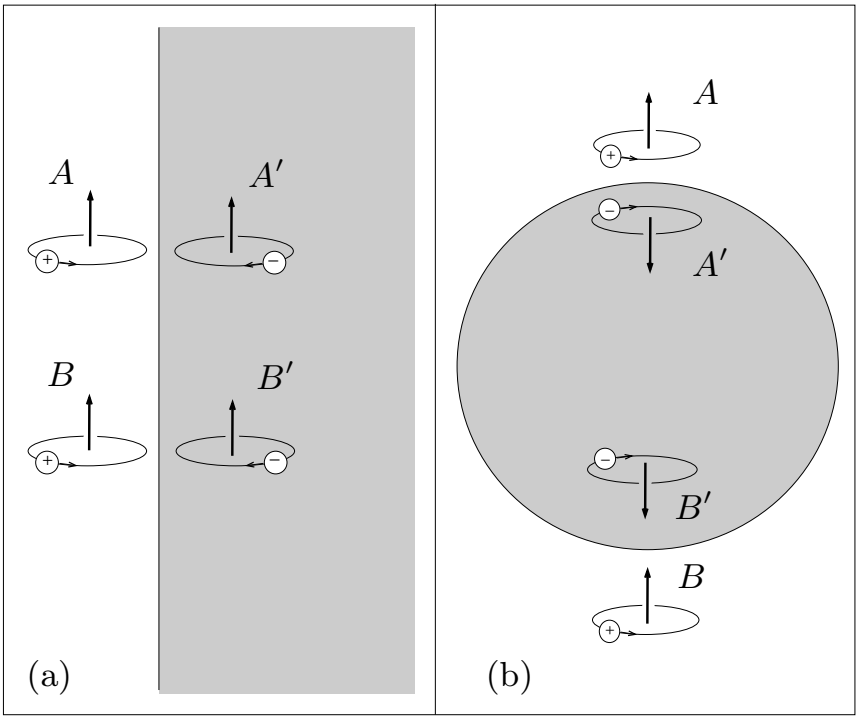

Figure 4.14: Two magnetic dipoles near a purely electric sphere are shown in a triangular configuration for a (a) very small angular separation (b) maximal angular separation.

enhanced(reduced) in agreement with the curves in Fig. 4.7 ($\Theta = \pi$).

We turn now to the linear configuration. For dipoles situated near a purely electric sphere [Fig. 4.15(a)], $V_{ee}^{(1)}$ is negative resulting in an enhancement of the total interaction potential for all distance regimes as visible in Fig. 4.8(a). For a purely magnetic sphere, we again invoke the duality principle to replace it by a purely electric one, and the electric dipoles by magnetic ones as shown in Fig. 4.15(b). It can be inferred from the sketch that $V_{ee}^{(1)}$ is positive for all distances. In order to be conclusive about the body-induced effects, one hence has to compare the magnitudes of the competing $V_{ee}^{(1)}$ and $V_{ee}^{(2)}$. For small atom–atom separations, the direct interaction dominates, so $V_{ee}^{(1)}$ is stronger than $V_{ee}^{(2)}$ and the potential is reduced as shown in Fig. 4.14(b), inset. As the interatomic separation increases, the indirect interaction gains in relevance and hence $V_{ee}^{(2)}$ may become dominant leading to an enhancement of the total vdW potential, in agreement with the curves presented in Fig. 4.8(b).

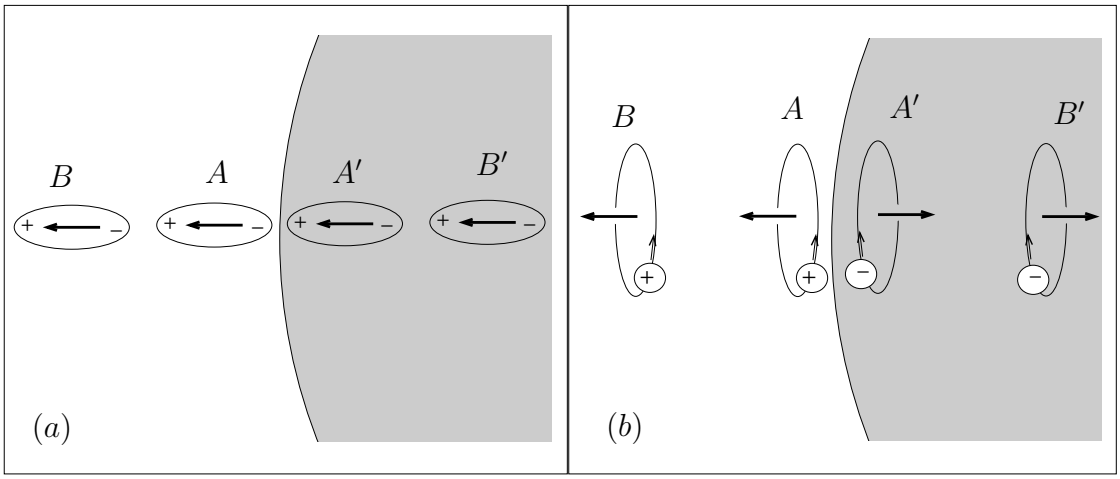

Figure 4.15: Two dipoles near a purely electric sphere are shown in a linear configuration. Figure 4.15(a) is showing two electric dipoles while in Fig. 4.15(b) two magnetic dipoles are shown.

Chapter 5

Summary and outlook

In this work the formulae of single-atom van der Waals (vdW) potential and two-atom vdW interaction potential of ground-state electric atoms in the presence of an arbitrary arrangement of linear magnetoelectric bodies have been generalized to atoms with both electric and magnetic polarizabilities within the framework of macroscopic quantum electrodynamics (QED). To this end, starting with the macroscopic Maxwell equations, we have extended an existing quantization scheme for a system consisting of a medium-assisted electromagnetic field and an atom with spinless constituents to a many-atom case, where in order to account for the paramagnetic atom-field interactions correctly, the spin of the constituents of the atoms are involved, leading to a spin-induced term in the magnetic dipole moment of the atoms. The quantization is followed by introducing a Hamiltonian whose consistency is examined by showing that it leads to the dynamical Maxwell equations and Newton equation of motion as the equations of motion for the electromagnetic field and for the charged particles, respectively. By transforming the Hamiltonian to the multipolar-coupling form, using the long wave-length approximation, and ignoring the diamagnetic properties of the atom, the atom-field interaction part of the Hamiltonian is written as a sum over the interactions of the electric and (transformed) magnetic dipoles with the (transformed) electric and (magnetic) induction fields, respectively, where the center-of-mass motion of the atoms are assumed to be sufficiently slow.

The single-atom vdW potential has been calculated using second-order perturbation theory. It is seen that the potential can be thought of as being the superposition of the potential of an electric atom and that of a magnetic atom. For the cases where the atom under consideration is embedded in a host medium, where the field experienced by the atom differs from the macroscopic one, the local-field corrections to the single-atom vdW potential are presented using the real-cavity model. The corrections come into effect via frequency-dependent factors, which depend on the magnetoelectric properties of the medium at the location of the atom. The resulting expression has been applied for an atom in the presence of a planar, magnetoelectric, multilayer media and then for a homogeneous, medium-sized magnetoelectric sphere. It is found that, in both examples, the electric and magnetic parts of the vdW potential can be transformed into one another by duality transformations. The

sphere example has been considered also for the limiting cases of a large sphere and a small sphere. In particular, in the limiting case of a small sphere the formula of the interaction potential between two atoms in free space, both having electric and magnetic polarizabilities, is reobtained by replacing the sphere polarizabilities with those of a single atom. In a many-atom case as long as the interatomic potentials are disregarded comparing to the atom-body potentials, e.g., in a dilute gas near a magnetoelectric media, the vdW potential of a many-atom system can be obtained by a summation over the single-atom vdW potentials. As the interatomic distances are reduced, the interatomic potentials can not be discarded.

The two-atom vdW interaction potential has been derived employing fourth-order perturbation theory. It is seen that the interaction potential, can be considered as the superposition of the interaction potentials for the four different possible scenarios, in which each atom has either electric or magnetic polarizability. The local-field corrections to the formulae for the cases where one or both atoms are embedded in host media have been presented, again using the real-cavity model. By applying the theory to the case where the two atoms are embedded in a bulk magnetoelectric medium, it is inferred that (i) in general, unless the local-field corrections are taken into account the resulting expressions for the potential do not respect the electromagnetic duality properties, (ii) the real-cavity model is an appropriate tool for obtaining the local-field corrections, and (iii) a medium-induced enhancement or reduction in the interaction potential is possible depending on the electric and magnetic strength of the polarizabilities of both atoms and the medium. In particular, in the retarded limit the interaction is always screened by the medium.

The formula found for the two-atom vdW interaction potential has also been applied to calculate the interaction potential between two electric atoms in the presence of a planar magnetoelectric multilayer, and then to two atoms with both electric and magnetic polarizabilities in the presence of a magnetoelectric homogeneous sphere. As simpler cases for the former application, the interaction potential in the presence of a perfectly reflecting plate and in the presence of a thick magnetoelectric layer (half-space) are calculated with special emphasis on the limiting cases of retarded and nonretarded, and particular arrangements of the atoms with respect to the bodies. Developing the applications to more complex geometries may facilitate controlling the dispersion forces via manipulating the surrounding environment. Repulsive components of the forces would open interesting possibilities of reducing or even eliminating the potentially disturbing effects of attractive forces.

In computing the interaction potential in the presence of a sphere, for the sake of trans-

parency, we broke the calculation down into two cases of equal-type atoms and opposed-type atoms, with respect to their electric or magnetic polarizabilities, and we could thus shorten the calculation by showing that the potential expressions do respect the duality transformations. As in the case of single-atom potential, we have also considered the two limiting cases of a large sphere and a small sphere for the two-atom interaction potential. In particular, making use of the result for a small sphere, we have generalized an existing formula for the non-additive interaction potential between three electric atoms to atoms owning, simultaneously, both electric and magnetic polarizabilities.

To illustrate the effect of the bodies on the vdW interaction potential, the examples of two atoms in the presence of a half-space and the one for two atoms in the presence of a sphere are followed by numerical results, where the atoms are at equal distances from the body, or aligned on a straight line perpendicular to the surface of the body. The numerical calculations show that — compared to the case of the atoms being in free space — the vdW interaction can be enhanced as well as reduced, depending on the electromagnetic properties of the body, the position of the atoms with respect to the body, and the position of the atoms relative to each other. Finally, the body-induced enhancement or reduction of the vdW interatomic potential (shown by the numerical results) in the nonretarded limit are interpreted, qualitatively, exploiting the method of image-charges.

The theory can be extended in various aspects. The medium-assisted single- and two-atom vdW potentials, for atoms being in arbitrary energy eigenstates, are already given in the literature for electric atoms (for the two-atom case see, e.g., Refs. [108, 109]). It is almost a trivial step to include paramagnetic atoms in the perturbative calculations. When dealing with excited atoms, a possible time-dependence of the vdW forces may need to be taken into account. This is particularly the case where some atomic transition frequencies are neighboring some resonant frequencies of the material environment. In such cases the perturbation theory may become invalid because of the strong atom-field coupling. One possible solution would be a non-perturbative aproach similar to the one given for a single electric atom in Ref. [42]. By using a more general formalism for macroscopic QED in linear media [87], the theory can be extended to the cases of anisotropic or non-local responding media. The influence of finite temperatures could be included by replacing the ground-state expectation value of the medium-assisted field with its thermal expectation value at the beginning of the perturbative calculations.

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List of publications and presentations

Publications

[HS1] *Body-assisted van der Waals interaction between two atoms*, H. Safari, S. Y. Buhmann, D.-G. Welsch, and D. T. Ho, Phys. Rev. A **74**, 042101 (2006).

[HS2] *Microscopic origin of Casimir-Polder forces*, S. Y. Buhmann, H. Safari, D.-G. Welsch, and D. T. Ho, Open Sys. Inf. Dyn. **13**, 427 (2006).

[HS3] *Two-atom van der Waals interaction between polarizable/magnetizable atoms near magnetoelectric bodies*, S. Y. Buhmann, H. Safari, D. T. Ho, and D.-G. Welsch, Opt. Spectrosc. **103**, 374 (2007).

[HS4] *Interatomic van der Waals potential in the presence of a magnetoelectric sphere*, H. Safari, D.-G. Welsch, D. T. Ho, and S. Y. Buhmann, Phys. Rev. A **77**, 053824 (2008).

[HS5] *van der Waals potentials of paramagnetic atoms*, H. Safari, D.-G. Welsch, S. Y. Buhmann, and S. Scheel, Phys. Rev. A **78**, 062901 (2008).

[HS6] *Dispersion forces and duality*, S. Y. Buhmann, S. Scheel, H. Safari, and D.-G. Welsch, e-print: arXiv:0811.429871.

Presentation

Body-assisted van der Waals interaction between two atoms, talk (DPG-Tagung, Düsseldorf, 2007)

Appendix A

Heisenberg's equations of motion

The Maxwell equations (2.76) and (2.77) are established in Ref. [42] by making use of Heisenberg equation of motion (2.37) for induction and displacement fields, but for the case where only a single atom interacts with medium-assisted electromagnetic field and the spin-filed interaction is absent. Since the induction field commutes with $\hat{\mathbf{r}}_\alpha$, $\hat{\mathbf{p}}_\alpha$, $\hat{\mathbf{s}}_\alpha$, $\hat{\mathbf{A}}$, and $\hat{\mathbf{P}}_A$, the presence of the atoms and particles spin do not affect the commutation relation $[\hat{\mathbf{B}}(\mathbf{r}), \hat{H}]$ with $\hat{H}$ being given by Eq. (2.67) and it reduces to $[\hat{\mathbf{B}}(\mathbf{r}), \hat{H}_F]$. Hence, Eq. (2.76) remains unchanged with respect to Ref. [42].

In order to prove Eqs. (2.77) and (2.78) it is useful to decompose the Hamiltonian (2.67) into two parts as

$$\hat{H} = \hat{H}_0 + \hat{H}_s \tag{A.1}$$

with $\hat{H}_0$ representing the first four terms in Eq. (2.67) and $\hat{H}_s$ being the Pauli interaction term

$$\hat{H}_s = -\sum_A \sum_{\alpha \in A} \gamma_\alpha \, \hat{\mathbf{s}}_\alpha \cdot \hat{\mathbf{B}}(\mathbf{r}_\alpha). \tag{A.2}$$

Thus the Heisenberg equation of motion for displacement vector becomes

$$\dot{\hat{\boldsymbol{\mathcal{D}}}}(\mathbf{r}) = \frac{1}{i\hbar}[\hat{\boldsymbol{\mathcal{D}}}(\mathbf{r}), \hat{H}_0] + \frac{1}{i\hbar}[\hat{\boldsymbol{\mathcal{D}}}(\mathbf{r}), \hat{H}_s]. \tag{A.3}$$

The firs and second terms on the right-hand side of this equation are responsible for the generalization of the counterpart equation in Ref. [42] to many-atom case and spin-present case, respectively. The generalization to many-atom case can be performed in a procedure completely analogous to the single-atom case in Ref. [42] and leads to

$$\frac{1}{i\hbar}[\hat{\boldsymbol{\mathcal{D}}}(\mathbf{r}), \hat{H}_0] = \boldsymbol{\nabla} \times \hat{\boldsymbol{\mathcal{H}}}(\mathbf{r}) - \sum_A \sum_{\alpha \in A} \frac{q_\alpha}{2} \big[\dot{\hat{\mathbf{r}}}_\alpha \delta(\mathbf{r} - \hat{\mathbf{r}}_\alpha) + \delta(\mathbf{r} - \hat{\mathbf{r}}_\alpha)\dot{\hat{\mathbf{r}}}_\alpha\big]. \tag{A.4}$$

Recalling Eqs. (A.2) and (2.71) together with Eq. (2.58) and noting that $\hat{\mathbf{r}}_\alpha$ commutes with both $\hat{\mathbf{s}}_\alpha$ and $\hat{\mathbf{B}}(\hat{\mathbf{r}}_\alpha)$ we will find

$$[\hat{\boldsymbol{\mathcal{D}}}(\mathbf{r}), \hat{H}_s] = [\hat{\mathbf{D}}(\mathbf{r}), \hat{H}_s]. \tag{A.5}$$

Combining Eqs. (A.5), (A.2), and (2.45) we obtain

$$\begin{aligned}\frac{1}{i\hbar}[\hat{\boldsymbol{\mathcal{D}}}(\mathbf{r}), \hat{H}_s] &= \sum_A \sum_{\alpha \in A} \frac{\gamma_\alpha}{i\hbar}[\hat{\mathbf{D}}(\mathbf{r}), \hat{\mathbf{A}}(\mathbf{r}_\alpha)] \times \overleftarrow{\boldsymbol{\nabla}}_\alpha \cdot \hat{\mathbf{s}}_\alpha = \sum_A \sum_{\alpha \in A} \gamma_\alpha \, \hat{\mathbf{s}}_\alpha \cdot \boldsymbol{\nabla} \times \boldsymbol{\delta}^\perp(\mathbf{r} - \mathbf{r}_\alpha) \\ &= \sum_A \sum_{\alpha \in A} \gamma_\alpha \, \hat{\mathbf{s}}_\alpha \cdot \boldsymbol{\nabla} \times [\delta(\mathbf{r} - \mathbf{r}_\alpha)\boldsymbol{I}] = \sum_A \sum_{\alpha \in A} \gamma_\alpha \, \hat{\mathbf{s}}_\alpha \times \boldsymbol{\nabla}\delta(\mathbf{r} - \mathbf{r}_\alpha),\end{aligned} \tag{A.6}$$

where in the second equality the commutation relation between the displacement field and vector potential is used [42]

$$[\hat{\mathbf{D}}(\mathbf{r}), \hat{\mathbf{A}}(\mathbf{r}')] = i\hbar\boldsymbol{\delta}^{\perp}(\mathbf{r}-\mathbf{r}'). \tag{A.7}$$

Finally, combining Eqs. (A.3), (A.4), and (A.6) leads to the equation of motion (2.77) with $\hat{\mathbf{j}}_A(\mathbf{r})$ given by Eq. (2.73).

For concluding the equation of motion (2.78), again we make use of the decomposition (A.1) and apply the Heisenberg equation on $\dot{\hat{\mathbf{r}}}_\alpha$

$$\ddot{\hat{\mathbf{r}}}_\alpha = \frac{1}{i\hbar}\left[\dot{\hat{\mathbf{r}}}_\alpha, \hat{H}_0\right] + \frac{1}{i\hbar}\left[\dot{\hat{\mathbf{r}}}_\alpha, \hat{H}_s\right]. \tag{A.8}$$

Although the first term on the right-hand side of Eq. (A.8) is given in Ref. [42] for a single-atom case as

$$\frac{1}{i\hbar}\left[\dot{\hat{\mathbf{r}}}_\alpha, \hat{H}_0\right] = \frac{q_\alpha}{m_\alpha}\hat{\boldsymbol{\mathcal{E}}}(\hat{\mathbf{r}}_\alpha) + \frac{q_\alpha}{2m_\alpha}\left[\dot{\hat{\mathbf{r}}}_\alpha \times \hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\alpha) - \hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\alpha)\times\dot{\hat{\mathbf{r}}}_\alpha\right], \tag{A.9}$$

it can be found easily that in the many-atom case it does not show any explicit change, such that the total electric field $\hat{\boldsymbol{\mathcal{E}}}$ contains the contributions from all atoms. Using Eqs. (2.74) and (A.2) we will find

$$\begin{aligned}\frac{1}{i\hbar}\left[\dot{\hat{\mathbf{r}}}_\alpha, \hat{H}_s\right] &= -\frac{1}{i\hbar m_\alpha}\sum_A\sum_{\beta\in A}\gamma_\beta\left[\hat{\mathbf{p}}_\alpha\,, \hat{\mathbf{s}}_\beta\cdot\hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\beta)\right] = \frac{1}{m_\alpha}\sum_A\sum_{\beta\in A}\gamma_\beta\boldsymbol{\nabla}_\alpha\left[\hat{\mathbf{s}}_\beta\cdot\hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\beta)\right] \\ &= \frac{\gamma_\alpha}{m_\alpha}\boldsymbol{\nabla}_\alpha\left[\hat{\mathbf{s}}_\alpha\cdot\hat{\boldsymbol{\mathcal{B}}}(\hat{\mathbf{r}}_\alpha)\right].\end{aligned} \tag{A.10}$$

By combining Eqs. (A.8)–(A.10) we arrive at the equation of motion (2.78).

Appendix B

Scattering Green tensor in the presence of a sphere

For two arbitrarily chosen points $\mathbf{r}_1=(r_1,\theta_1,\phi_1)$ and $\mathbf{r}_2=(r_2,\theta_2,\phi_2)$, upon recalling Eqs. (3.47) and (3.48), for performing the summations over m and p in the scattering part of the Green tensor given by Eq. (3.46) we can write

$$\sum_{m=0}^{n}\sum_{p=\pm1}\frac{(n-m)!}{(n+m)!}(2-\delta_{0m})\mathbf{M}^{(1)}_{nm,p}(\mathbf{r}_1,\omega/c)\mathbf{M}^{(1)}_{nm,p}(\mathbf{r}_2,\omega/c)$$
$$=Q_n\Big\{\frac{\mathbf{e}_{\theta_1}\mathbf{e}_{\theta_2}}{\sin\theta_1\sin\theta_2}S_1-\frac{\mathbf{e}_{\theta_1}\mathbf{e}_{\phi_2}}{\sin\theta_1}S_2+\frac{\mathbf{e}_{\phi_1}\mathbf{e}_{\theta_2}}{\sin\theta_2}S_3+\mathbf{e}_{\phi_1}\mathbf{e}_{\phi_2}S_4\Big\}, \quad \text{(B.1)}$$

$$\sum_{m=0}^{n}\sum_{p=\pm1}\frac{(n-m)!}{(n+m)!}(2-\delta_{0m})\mathbf{N}^{(1)}_{nm,p}(\mathbf{r}_1,\omega/c)\mathbf{N}^{(1)}_{nm,p}(\mathbf{r}_2,\omega/c)=\frac{c^2}{\omega^2 r_1 r_2}\Big\{n^2(n+1)^2Q_n\mathbf{e}_{r_1}\mathbf{e}_{r_2}S_5$$
$$+n(n+1)Q_n^B\mathbf{e}_{r_1}\mathbf{e}_{\theta_2}S_6-\frac{n(n+1)}{\sin\theta_2}Q_n^B\mathbf{e}_{r_1}\mathbf{e}_{\phi_2}S_7+n(n+1)Q_n^A\mathbf{e}_{\theta_1}\mathbf{e}_{r_2}S_8+L_n\mathbf{e}_{\theta_1}\mathbf{e}_{\theta_2}S_4$$
$$-\frac{L_n}{\sin\theta_2}\mathbf{e}_{\theta_1}\mathbf{e}_{\phi_2}S_3+\frac{n(n+1)}{\sin\theta_1}Q_n^A\mathbf{e}_{\phi_1}\mathbf{e}_{r_2}S_7+\frac{L_n}{\sin\theta_1}\mathbf{e}_{\phi_1}\mathbf{e}_{\theta_2}S_2+\frac{L_n}{\sin\theta_1\sin\theta_2}\mathbf{e}_{\phi_1}\mathbf{e}_{\phi_2}S_1\Big\}, \quad \text{(B.2)}$$

where Q_n, Q_n^A, Q_n^B, and L_n are given by Eqs. (4.122)–(4.125) (with r_1, r_2 and $-i\omega$ instead of r_A, r_B and u, respectively), and S_1–S_8 are defined as

$$S_1=\sum_{m=0}^{n}C_{mn}m^2P_n^m(\cos\theta_1)P_n^m(\cos\theta_2)\cos(m\bar{\phi}), \quad \text{(B.3)}$$

$$S_2=\sum_{m=0}^{n}C_{mn}mP_n^m(\cos\theta_1)\frac{\mathrm{d}P_n^m(\cos\theta_2)}{\mathrm{d}\theta_2}\sin(m\bar{\phi}), \quad \text{(B.4)}$$

$$S_3=\sum_{m=0}^{n}C_{mn}m\frac{\mathrm{d}P_n^m(\cos\theta_1)}{\mathrm{d}\theta_1}P_n^m(\cos\theta_2)\sin(m\bar{\phi}), \quad \text{(B.5)}$$

$$S_4=\sum_{m=0}^{n}C_{mn}\frac{\mathrm{d}P_n^m(\cos\theta_1)}{\mathrm{d}\theta_1}\frac{\mathrm{d}P_n^m(\cos\theta_2)}{\mathrm{d}\theta_2}\cos(m\bar{\phi}), \quad \text{(B.6)}$$

$$S_5=\sum_{m=0}^{n}C_{mn}P_n^m(\cos\theta_1)P_n^m(\cos\theta_2)\cos(m\bar{\phi}), \quad \text{(B.7)}$$

$$S_6=\sum_{m=0}^{n}C_{mn}P_n^m(\cos\theta_1)\frac{\mathrm{d}P_n^m(\cos\theta_2)}{\mathrm{d}\theta_2}\cos(m\bar{\phi}), \quad \text{(B.8)}$$

$$S_7 = \sum_{m=0}^{n} C_{mn} m P_n^m(\cos\theta_1) P_n^m(\cos\theta_2) \sin(m\bar{\phi}), \tag{B.9}$$

$$S_8 = \sum_{m=0}^{n} C_{mn} \frac{\mathrm{d}P_n^m(\cos\theta_1)}{\mathrm{d}\theta_1} P_n^m(\cos\theta_2) \cos(m\bar{\phi}) \tag{B.10}$$

($\bar{\phi} \equiv \phi_2 - \phi_1$) with

$$C_{mn} = \frac{(n-m)!}{(n+m)!}(2 - \delta_{0m}). \tag{B.11}$$

To perform the summations S_1–S_8 we make use of the addition theorem for spherical harmonics, which reads

$$\sum_{m=0}^{n} C_{mn} \cos(m\lambda) P_n^m(\cos\theta_1) P_n^m(\cos\theta_2), = P_n(\psi) \tag{B.12}$$

where

$$\psi = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos\lambda. \tag{B.13}$$

The summation in the left hand side of Eq. (B.12) coincides with S_5, where λ is replaced by $\bar{\phi}$. The rest, introduced in Eqs. (B.3)–(B.6) and (B.8)–(B.10), can be found by proper differentiations of S_5, for example

$$S_1 = -\frac{\mathrm{d}^2 S_5}{\mathrm{d}\bar{\phi}^2} = \sin\theta_1 \sin\theta_2 [\cos\bar{\phi}\, P_n'(\psi) - \sin\theta_1 \sin\theta_2 \sin^2\bar{\phi}\, P_n''(\psi)]. \tag{B.14}$$

B.1 Derivation of Eqs. (3.53), (4.121), and (4.152)

Now by setting $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, to $\mathbf{r}_A$ and $\mathbf{r}_B$ given by Eq. (4.120), the nonzero summations in Eqs. (B.3)–(B.10) are found to be

$$S_1 = -\sin\theta_A \sin\theta_B P_n'(\gamma), \quad S_4 = -F_n(\gamma), \quad S_5 = P_n(\gamma), \quad S_6 = S_8 = -\sin\Theta P_n'(\gamma) \tag{B.15}$$

with γ being defined below Eq. (4.121). Using Eqs. (B.1) and (B.2) together with Eq. (B.15) in Eq. (3.46) leads to Eq. (4.121).

In the calculation of the single-atom potential where $\mathbf{r}_1 = \mathbf{r}_2 = (r, \theta, \phi)$, we will find

$$S_1 = \frac{1}{2} n(n+1) \sin^2\theta, \quad S_2 = S_3 = S_6 = S_7 = S_8 = 0, \quad S_4 = \frac{1}{2} n(n+1), \quad S_5 = 1. \tag{B.16}$$

Substituting Eqs. (B.1) and (B.2) with S_1–S_8 given by Eq. (B.16) into Eq. (3.46) leads to Eq. (3.53).

The tensor $\boldsymbol{K}^{(1)}(\mathbf{r}_B, \mathbf{r}_A, \omega)$, which is required for calculating $V_{em}^{(b)}$ can be obtained from Eq. (4.26) by replacing $\boldsymbol{G}$ in the right-hand side with $\boldsymbol{G}^{(1)}$ given by Eq. (3.46), i.e.,

$$\boldsymbol{K}^{(1)}(\mathbf{r}_B, \mathbf{r}_A, \omega) = \frac{i\omega^2}{4\pi c^2} \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \sum_{m=0}^{n} \frac{(n-m)!}{(n+m)!}(2-\delta_{0m})$$
$$\times \sum_{p=\pm 1} \left[B_n^M(\omega) \mathbf{N}_{nm,p}(\mathbf{r}_B, \omega/c) \mathbf{M}_{nm,p}(\mathbf{r}_A, \omega/c) + B_n^M(\omega) \mathbf{N}_{nm,p}(\mathbf{r}_B, \omega/c) \mathbf{M}_{nm,p}(\mathbf{r}_A, \omega/c) \right], \tag{B.17}$$

where relations (3.49) and (3.50) have been used. The summations over m and p can be performed in the same way as outlined above for deriving Eq. (4.121) that leads to

$$\sum_{m=0}^{n} \sum_{p=\pm 1} C_{mn} \mathbf{N}_{nm,p}(\mathbf{r}_B, k) \mathbf{M}_{nm,p}(\mathbf{r}_A, k) = \frac{c}{r_B \omega} \Big\{ n(n+1) Q_n \sin\Theta \, P_n'(\gamma) \mathbf{e}_{r_B} \mathbf{e}_{\phi_A}$$
$$+ Q_n^B F_n(\gamma) \mathbf{e}_{\theta_B} \mathbf{e}_{\phi_A} - Q_n^B P_n'(\gamma) \mathbf{e}_{\phi_B} \mathbf{e}_{\theta_A} \Big\}, \tag{B.18}$$

$$\sum_{m=0}^{n} \sum_{p=\pm 1} C_{mn} \mathbf{M}_{nm,p}(\mathbf{r}_B, k) \mathbf{N}_{nm,p}(\mathbf{r}_A, k) = \frac{c}{r_A \omega} \Big\{ - Q_n^A P_n'(\gamma) \mathbf{e}_{\theta_B} \mathbf{e}_{\phi_A}$$
$$+ n(n+1) Q_n \sin\Theta \, P_n'(\gamma) \mathbf{e}_{\phi_B} \mathbf{e}_{r_A} + Q_n^A F_n(\gamma) \mathbf{e}_{\phi_B} \mathbf{e}_{\theta_A} \Big\}, \tag{B.19}$$

where $\mathbf{r}_A$ and $\mathbf{r}_B$ are given by Eqs. (4.120). Equation (4.152) is the result of the substitution of Eqs. (B.18) and (B.19) in Eq. (B.17)

B.2 The limiting cases of large and small sphere

When in the case of a large sphere the conditions (4.131) and (4.132) are satisfied, then the leading contributions to the sums in Eqs. (4.121) and (4.152) come from terms with $n \gg 1$ (also see Ref. [82]) for which, the spherical Bessel and Hankel functions approximate to [101]

$$j_n(z) = \frac{z^n}{(2n+1)!!} \left[1 - \frac{z^2}{4n+6} + \frac{z^4}{(16n+24)(2n+5)} \right] \tag{B.20}$$

and

$$h_n^{(1)}(z) = -i \frac{(2n-1)!!}{z^{n+1}} \left[1 + \frac{z^2}{4n-2} + \frac{z^4}{(16n-8)(2n-3)} \right], \tag{B.21}$$

respectively. Hence, Eqs. (3.51) and (3.52) approximate to

$$B_n^M(iu) = \frac{(-1)^{n+1} (Ru/c)^{2n+1}}{[(2n+1)!!]^2} \left(a_1 n + a_0 + a_{-1} n^{-1} \right) \tag{B.22}$$

and

$$B_n^N(iu) = \frac{(-1)^{n+1} (Ru/c)^{2n+1}}{[(2n+1)!!]^2} \left(b_1 n + b_0 + b_{-1} n^{-1} \right), \tag{B.23}$$

respectively, where

$$a_1 = 2\frac{\mu-1}{\mu+1}, \tag{B.24}$$

$$a_0 = [1+3\mu+(1+\mu)R^2u^2/c^2]\frac{\mu-1}{(\mu+1)^2} \tag{B.25}$$

$$a_{-1} = \frac{1}{4(\mu+1)^3}\big\{4\mu(\mu-1)^2-4\mu(\mu+1)(2\varepsilon\mu-\mu-1)R^2u^2/c^2+(\mu-\varepsilon\mu+1)(\mu^2-1)R^4u^4/c^4\big\} \tag{B.26}$$

$[\varepsilon=\varepsilon(iu),\ \mu=\mu(iu)]$, and b_1, b_0, and b_{-1} can be found from a_1, a_0, and a_{-1}, respectively, by interchanging of μ and ε. Equations (4.122)–(4.125) then approximate to

$$Q_n = \Big(\frac{-1}{ab}\Big)^n[(2n-1)!!]^2\bigg[1-\frac{1}{4}(a^2+b^2)n^{-1}+\frac{1}{32}(a^2+b^2)(a^2+b^2-4)n^{-2}\bigg], \tag{B.27}$$

$$Q_n^A = \Big(\frac{-1}{ab}\Big)^n[(2n-1)!!]^2\bigg[-n+\frac{1}{4}(a^2+b^2)-\frac{1}{32}(b^4-4b^2+a^4+2a^2b^2+12a^2)n^{-1}\bigg], \tag{B.28}$$

$$L_n = \Big(\frac{-1}{ab}\Big)^n[(2n-1)!!]^2\bigg[n^2-\frac{1}{4}(a^2+b^2)n+\frac{1}{32}(a^2+b^2)(a^2+b^2-12)\bigg] \tag{B.29}$$

($a=r_Au/c$; $b=r_Bu/c$; Q_n^B can be found from Q_n^A by interchanging of a and b). In order to illustrate the application of the approximation scheme to the Green tensors (4.121) and (4.152), let us consider the element $G_{rr}^{(1)}(\mathbf{r}_A,\mathbf{r}_B,iu)$ for example, which using Eqs. (B.23) and (B.27) yields the form

$$G_{rr}^{(1)}(\mathbf{r}_A,\mathbf{r_B},iu) = \frac{-c^2}{4\pi u^2R^3}\bigg\{\frac{\varepsilon-1}{\varepsilon+1}\,s_2+\frac{(2\varepsilon+1)(\varepsilon-1)}{(\varepsilon+1)^2}\,s_1+\frac{1}{8(\varepsilon+1)^3}\big[8\varepsilon^2(\varepsilon-1) - 4(1+\varepsilon)(\varepsilon^2+2\mu\varepsilon^2-2\varepsilon-1)R^2u^2/c^2-\varepsilon(\varepsilon^2-1)\mu R^4u^4/c^4\big]s_0\bigg\}, \tag{B.30}$$

$[t=R^2/(r_Ar_B)]$ where

$$s_k = \sum_{n=1}^{\infty} n^k t^n P_n(\gamma). \tag{B.31}$$

Using the identity [101]

$$\sum_{n=1}^{\infty} t^n P_n(\gamma) = \frac{1}{\sqrt{1-2t\gamma+t^2}}-1 \tag{B.32}$$

and performing suitable differentiations with respect to t, we will obtain

$$s_0 = \frac{1}{\sqrt{1-2t\gamma+t^2}}-1, \tag{B.33}$$

$$s_1 = \frac{\gamma-t}{[1-2t\gamma+t^2]^{3/2}}\,, \tag{B.34}$$

$$s_2 = \frac{\gamma t+(\gamma^2-2)t^2-\gamma t^3+t^4}{[1-2t\gamma+t^2]^{5/2}}\,. \tag{B.35}$$

Recalling the conditions (4.131) and (4.132), we can further simplify the result. Up to second order in the small parameters $\delta_{A'}/R$, we have

$$t^k = 1 - k\frac{\delta_A + \delta_B}{R} + \frac{k(k+1)}{2}\frac{\delta_A^2 + \delta_B^2}{R^2} + k^2\frac{\delta_A\delta_B}{R^2}, \tag{B.36}$$

implying that

$$1 - 2t\gamma + t^2 \simeq \Theta^2 + \frac{(\delta_A + \delta_B)^2}{R^2} = \frac{l_+^2}{R^2}. \tag{B.37}$$

Using Eqs. (B.33)–(B.37) in Eq. (B.30), we find that within this order,

$$G_{rr}^{(1)}(\mathbf{r}_A, \mathbf{r_B}, iu) = \frac{c^2}{4\pi u^2}\Bigg\{\frac{X^2 - 2\delta_+^2}{l_+^5}\frac{\varepsilon - 1}{\varepsilon + 1} - \frac{\delta_+}{Rl_+^3}\frac{(2\varepsilon+1)(\varepsilon-1)}{(\varepsilon+1)^2} - \frac{1}{8(\varepsilon+1)^3}\big[8\varepsilon^2(\varepsilon-1) - 4(1+\varepsilon)(\varepsilon^2 + 2\mu\varepsilon^2 - 2\varepsilon - 1)R^2u^2/c^2 - \varepsilon(\varepsilon^2-1)\mu R^4u^4/c^4\big]\frac{1}{R^2 l_+}\Bigg\}, \tag{B.38}$$

with X, $\delta_\pm$ and l_+ being defined below Eq. (4.133). Recalling that X, l_+, $\delta_+ \ll R$, it can be seen that unless $|\varepsilon - 1| \ll 1$, the third term in the curly brackets in Eq. (B.38) can be approximately ignored and hence, in this term ε may be set to 1, that leads to

$$G_{rr}^{(1)}(\mathbf{r}_A, \mathbf{r_B}, iu) = \frac{c^2}{4\pi u^2}\Bigg\{\frac{X^2 - 2\delta_+^2}{l_+^5}\frac{\varepsilon - 1}{\varepsilon + 1} - \frac{\delta_+}{Rl_+^3}\frac{(2\varepsilon+1)(\varepsilon-1)}{(\varepsilon+1)^2} + \frac{u^2}{4c^2 l_+}(\mu - 1)\Bigg\}. \tag{B.39}$$

The free-space counterpart of this tensor element can be simply found from Eq. (4.127), with the conditions (4.131) and (4.132) applied, as

$$G_{rr}^{(0)}(\mathbf{r}_A, \mathbf{r}_B, iu) = \frac{c^2(X^2 - 2Z^2)}{4\pi u^2 l^5}\,. \tag{B.40}$$

The other Green tensor elements in Eqs. (4.121) and (4.127) can be evaluated in a quite similar way. Substituting the resulting expression for $\boldsymbol{G}^{(0)}$ and $\boldsymbol{G}^{(1)}$ in Eqs. (4.66) and (4.67) and summing them in accordance with Eq. (4.65), we eventually arrive at Eq. (4.133). A similar calculation leads to Eq. (4.155) for electric-magnetic part of the interaction potential.

In the limiting case of a small sphere where the condition (4.136) holds, the leading contributions to the frequency integrals in Eqs. (4.129) and (4.130) come from the region where $u \ll c/R$, or equivalently $|z_0|$, $|z_1| \ll 1$ (also see Ref. [82]). In this region we may approximate the spherical Bessel and Hankel functions appearing in Eqs. (3.51) and (3.52) by their next-to-leading order expansions in z [101], i.e.,

$$j_n(z) = \frac{z^n}{(2n+1)!!}\left(1 - \frac{z^2}{4n+6}\right) \tag{B.41}$$

and

$$h_n^{(1)}(z) = -i\frac{(2n-1)!!}{z^{n+1}}\left(1 - \frac{z^2}{2-4n}\right), \tag{B.42}$$

so that Eqs. (3.51) and (3.52), respectively, approximate to

$$B_n^M = \frac{(2n+1)i}{[(2n+1)!!]^2(n\mu+n+1)}\left[(n+1)(\mu-1)\left(\frac{iRu}{c}\right)^{2n+1} + O\left(\frac{iRu}{c}\right)^{2n+3}\right] \tag{B.43}$$

and

$$B_n^N = \frac{(2n+1)i}{[(2n+1)!!]^2(n\varepsilon+n+1)}\left[(n+1)(\varepsilon-1)\left(\frac{iRu}{c}\right)^{2n+1} + O\left(\frac{iRu}{c}\right)^{2n+3}\right], \tag{B.44}$$

revealing that $V_{ee}^{(2)}$ is small in comparison to $V_{ee}^{(1)}$ [compare Eqs. (4.129) and (4.130)] and can be neglected, so that, in leading order of Ru/c, $V^{(b)} = V^{(1)}$. Further, it can be seen that in the sums in Eq. (4.129) the terms with $n = 1$ is the leading one, for which

$$Q_n = -\frac{(1+a)(1+b)}{a^2b^2}\, e^{-a-b}, \tag{B.45}$$

$$Q_1^A = \frac{f(a)(1+b)}{a^2b^2}\, e^{-a-b}, \tag{B.46}$$

$$Q_1^B = \frac{(1+a)f(b)}{a^2b^2}\, e^{-a-b}, \tag{B.47}$$

$$L_1 = -\frac{f(a)f(b)}{a^2b^2}\, e^{-a-b}, \tag{B.48}$$

$$F_1(\gamma) = P_1(\gamma) = \gamma, \tag{B.49}$$

$$B_1^M(iu) = \frac{2}{3}\frac{\mu(iu)-1}{\mu(iu)+2}\left(\frac{Ru}{c}\right)^3, \tag{B.50}$$

$$B_1^N(iu) = \frac{2}{3}\frac{\varepsilon(iu)-1}{\varepsilon(iu)+2}\left(\frac{Ru}{c}\right)^3. \tag{B.51}$$

Substituting Eqs. (B.45)–(B.51) in Eq. (4.129), we arrive at Eq. (4.137). Equation (4.157) is derived by calculation similar to the one outlined above for obtaining Eq. (4.137).

Appendix C

Sum over the energy denominators

From the energy denominators given in Tab. (4.1), it is strightforward to obtain

$$\frac{1}{D_{1b}}+\frac{1}{D_2}\pm\frac{1}{D_3}+\frac{1}{D_{6b}}+\frac{1}{D_7}\pm\frac{1}{D_8}=\frac{1}{\omega_A^k+\omega_B^l}\left[\left(\frac{1}{\omega_A^k+\omega}+\frac{1}{\omega_B^l+\omega}\right)\left(\frac{1}{\omega+\omega'}\mp\frac{1}{\omega-\omega'}\right)\right.$$
$$\left.+\left(\frac{1}{\omega_A^k+\omega'}+\frac{1}{\omega_B^l+\omega'}\right)\left(\frac{1}{\omega+\omega'}\pm\frac{1}{\omega-\omega'}\right)\right]. \quad \text{(C.1)}$$

Since the denominators appear in combinations of the form of Eq. (4.12) and (4.21), where they are multiplied with terms (the two factors in square brackets) which are always the same and symmetric with respect to ω and ω', we may interchange $\omega \leftrightarrow \omega'$ in the second term and recombine it with the first one to obtain

$$\frac{1}{D_{1b}}+\frac{1}{D_2}\pm\frac{1}{D_3}+\frac{1}{D_{6b}}+\frac{1}{D_7}\pm\frac{1}{D_8}\rightarrow\frac{2}{\omega_A^k+\omega_B^l}\left(\frac{1}{\omega_A^k+\omega}+\frac{1}{\omega_B^l+\omega}\right)\left(\frac{1}{\omega+\omega'}\pm\frac{1}{\omega-\omega'}\right), \quad \text{(C.2)}$$

where the symbol $\rightarrow$ denotes equality under the double frequency integral. Similarly we have

$$\frac{1}{D_{1a}}\pm\frac{1}{D_4}\pm\frac{1}{D_5}=\frac{1}{(\omega_A^k+\omega')(\omega_B^l+\omega')}\left(\frac{1}{\omega+\omega'}\pm\frac{1}{\omega-\omega'}\right)\mp\frac{1}{(\omega_B^l+\omega')(\omega_A^k+\omega)(\omega-\omega')}, \quad \text{(C.3)}$$

$$\frac{1}{D_{6a}}\pm\frac{1}{D_9}\pm\frac{1}{D_{10}}=\frac{1}{(\omega_A^n+\omega')(\omega_B^m+\omega')}\left(\frac{1}{\omega+\omega'}\pm\frac{1}{\omega-\omega'}\right)\mp\frac{1}{(\omega_A^k+\omega')(\omega_B^l+\omega)(\omega-\omega')}. \quad \text{(C.4)}$$

The second terms in Eqs. (C.3) and (C.4) cancel each other after an interchange of $\omega \leftrightarrow \omega'$ to yield

$$\frac{1}{D_{1a}}\pm\frac{1}{D_4}\pm\frac{1}{D_5}+\frac{1}{D_{6a}}\pm\frac{1}{D_9}\pm\frac{1}{D_{10}}\rightarrow\frac{2}{(\omega_A^k+\omega)(\omega_B^l+\omega)}\left(\frac{1}{\omega+\omega'}\mp\frac{1}{\omega-\omega'}\right). \quad \text{(C.5)}$$

Summation of the right-hand sides of Eqs. (C.2) and (C.5) immediately results (4.13) and (4.23).

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Zusammenfassung

In dieser Arbeit wurde das van-der-Waals-Potential eines Atoms im Grundzustand sowie die van-der-Waals-Wechselwirkung zweier Grundzustandsatome in Anwesenheit beliebiger linear reagierender magnetoelektrischer Körper im Rahmen der makroskopischen Quantenelektrodynamik untersucht. Den Schwerpunkt der Arbeit stellt die Erweiterung der schon bekannten Theorie für elektrisch polarisierbare Atome auf den Fall polarisierbarer und magnetisierbarer Grundzustandsatome dar. Ausgehend von den makroskopischen Maxwellgleichungen für das körpergestützte elektromagnetische Feld wurde zunächst das bekannte Quantisierungsschema für das mediengestützte elektromagnetische Feld unter Annahme eines spinlosen Atoms auf den Fall mehrerer Atome erweitert, wobei Atomkern und Elektronen Spin besitzen um die paramagnetische Atom-Feld-Wechselwirkung zu berücksichtigen. Man erhält einen spinabhängigen Term in der Formel für das magnetische Dipolmoment der Atome. Es wird gezeigt, dass der bei der Quantisierung eingeführte Hamiltonian in konsistenter Weise auf die korrekten zeitabhängigen Maxwellgleichungen und die Newtonschen Bewegungsgleichungen für die geladenen Teilchen führt. Der Hamiltonian wird in die multipolar gekoppelte Form transformiert, wobei eine Langwellennäherung benutzt wird und mögliche diamagnetische Eigenschaften der Atome vernachlässigt werden. Der Anteil des Hamiltonians, der die Wechselwirkung zwischen Atom und mediengestütztem Feld beschreibt, lässt sich als Summe der Wechselwirkungen der (transformierten) elektrischen und magnetischen Dipole mit den (transformierten) elektrischen und (magnetischen) Feldern schreiben. Dabei wird angenommen, dass die Schwerpunktsbewegung der Atome hinreichend langsam ist.

Das van-der-Waals-Potential eines Atoms im Grundzustand, das sowohl elektrisch als auch magnetisch polarisierbar ist und sich in der Nähe eines beliebigen Systems magnetoelektrischer Materie befindet, wurde durch Störungstheorie in zweiter Ordnung berechnet. Die gefundene Formel zeigt, dass das Potential als eine Überlagerung des Potentials eines elektrischen Atoms und desjenigen eines magnetischen Atoms dargestellt werden kann. Besonders betrachtet wurde das van-der-Waals-Potential eines Grundzustandsatoms, das in ein magnetoelektrisches Medium eingebettet ist, so dass Lokalfeldkorrekturen nötig werden, da sich das mikroskopische (lokale) Feld am Ort des Atoms vom makroskopischen unterscheidet. Die Lokalfeldkorrektur wurde im Rahmen des Real-Cavity-Modells durchgeführt und schlägt sich in zwei frequenzabhängigen Faktoren nieder, die von den magnetoelektrischen Eigenschaften des Mediums am Standort des Atoms abhängen. Der resultierende Ausdruck

für das van-der-Waals-Potential wurde für zwei Beispiele spezialisiert. Zum einen wurde das van-der-Waals-Potential eines Atoms in einem planaren magnetoelektrischen Vielschichtsystem analytisch untersucht und numerisch weiter ausgewertet. Zum anderen wurde die allgemeine Formel auf den Fall einer makrokopischen homogenen magnetoelektrischen Kugel angewandt. Es hat sich herausgestellt, dass in beiden Beispielen die elektrischen und magnetischen Teile des van-der-Waals-Potentials durch Anwendung geeigneter Dualitätstransformationen ineinander transformiert werden können. Das Beispiel der Kugel wurde für die Grenzfälle einer sehr großen und einer sehr kleiner Kugel näher untersucht. Das Ergebnis im Fall der sehr kleinen Kugel fällt mit dem Resultat für die van-der-Waals-Wechselwirkung zwischen zwei Atomen im freien Raum zusammen, wenn die elektrische und die magnetische Polarisierbarkeit der Kugel mit den betreffenden Größen eines Atoms gleichgesetzt werden. Die gewonnenen Resultate können zudem zur Beschreibung der Wechselwirkung mehrerer Atome mit einem magnetoelektrischen Körper verwendet werden, solange die interatomaren Potentiale gegenüber der Atom-Körper-Wechselwirkung vernachlässigt werden können. Dies ist zum Beispiel in einem verdünnten Gas mit großen Abständen zwischen den einzelnen Gasatomen der Fall. Die van-der-Waals-Wechselwirkung eines solchen Systems mehrerer Atome mit dem makrokopischen Körper ergibt sich dann einfach als Summe der Potentiale der einzelnen Atome.

Durch Anwendung von Störungstheorie vierter Ordnung wurde das van-der-Waals Potential zwischen zwei polarisierbaren und magnetisierbaren Atomen im Grundzustand in Anwesenheit einer beliebigen Anordnung magnetoelektrischer Körper hergeleitet. Das gefundene Potential kann als Superposition der Potentiale der vier möglichen Szenarien betrachtet werden: beide Atome sind nur elektrisch polarisierbar, beide Atome sind nur magnetisch polarisierbar, oder eines ist nur elektrisch, das andere nur magnetisch polarisierbar beziehungsweise umgekehrt. Um die Einbettung eines oder beider Atome in ein Medium zuzulassen, wurden die nötigen Lokalfeldkorrekturen mit angegeben. Die Untersuchung der Wechselwirkung zweier Atome in einem unendlich ausgedehnten homogenen magnetoelektrischen Medium zeigt insbesondere, dass (i) die geforderte Dualitätsbeziehung zwischen elektrischen und magnetischen Termen nur dann erhalten bleibt, wenn Lokalfeldkorrekturen einbezogen werden, dass (ii) das Real-Cavity Modell ein geeignetes Werkzeug zur Durchführung der Lokalfeldkorrektur ist, und dass (iii) das van-der-Waals Potential durch die Einbettung der Atome in ein Medium größer oder kleiner werden kann. Die Änderung hängt von der Stärke der elektrischen und magnetischen Polarisierbarkeit der Atome und

des Mediums ab. Insbesondere im retardierten Fall wird die van-der-Waals-Wechselwirkung zwischen den Atomen reduziert, was mit einer Abschirmung durch das Medium begründet werden kann.

Als Anwendung der gefundenen Formel für das Zweiatompotential wurde die Wechselwirkung zweier elektrischer Atome in der Nähe eines planaren magnetoelektrischen Vielschichtsystems berechnet. Als Spezialfälle wurden eine perfekt reflektierende Platte und eine dicke magnetoelektrische Schicht (Halbraum) betrachtet. Besonderes Augenmerk liegt dabei auf den retardierten und nicht-retardierten Limites sowie auf besonderen Anordnungen der Atome im Verhältnis zum magnetoelektrischen Körper. Die Anwendung der Theorie auf komplexere Geometrien könnte dazu genutzt werden Dispersionskräfte auf Atome zu kontrollieren, indem das umliegende Medium manipuliert wird. Insbesondere die Erzeugung abstoßender Kräfte wäre von Interesse, da hierdurch potentiell störende Effekte anziehender Kräfte reduziert oder eliminiert werden könnten.

Als weiteres Beispiel wurden zwei polarisierbare und magnetisierbare Atome in der Nähe einer makroskopischen magnetoelektrischen homogenen Kugel untersucht. Aus Transparenzgründen wurde die Berechnung zunächst für die Spezialfälle zweier Atome mit gleichen bzw. entgegengesetzten Polarisationseigenschaften eingeschränkt (beide Atome nur elektrisch oder magnetisch polarisierbar bzw. eines nur elektrisch und eines nur magnetisch). Durch Dualitätstransformationen konnte wieder auf allgemeinere Fälle geschlossen werden. Wie schon für das Ein-Atom-Potential wurden wiederum die Grenzfälle einer sehr großen und einer sehr kleinen Kugel untersucht. Durch die Anwendung des Resultats für die kleine Kugel konnte die nicht-additive Wechselwirkung dreier elektrischer und magnetischer Atome bestimmt werden. Numerisch berechnet wurden die Fälle, bei denen sich die Atome in gleicher Entfernung vom Körper befinden oder auf einer geraden Linie senkrecht zur Oberfläche des Körpers angeordnet sind. Die numerischen Berechnungen belegen, dass – gegenüber Atomen im freien Raum – die van-der Waals-Wechselwirkungen sowohl verstärkt als auch reduziert werden können, in Abhängigkeit von den elektromagnetischen Eigenschaften des Körpers, der Position der Atome relativ zum Körper und der Lage der Atome zueinander. Das Verhalten des (numerisch berechneten) van-der-Waals-Potentials zwischen zwei Atomen mit gleichen Polarisationseigenschaften im Medium kann qualitativ mit Hilfe der Spiegelladungsmethode für kleine Atom-Atom- und Atom-Körper-Abstände interpretiert werden (nicht-retardierter Grenzfall).

Die Theorie kann in verschiedener Hinsicht erweitert werden: Die Ein- und Zweiatom-

potentiale, bei denen sich die Atome in beliebigen Energieeigenzuständen befinden, sind in der Literatur bisher nur für elektrische Atome angegeben worden (für das Zweiatompotential siehe zum Beispiel die Arbeiten [108, 109]). Es ist ein nahezu trivialer Schritt, paramagnetische Atome in die störungstheoretischen Berechnungen mit einzubeziehen. Bei der Untersuchung angeregter Atome muss eine dann mögliche explizite Zeitabhängigkeit der van-der-Waalskräfte eventuell in Rechnung gestellt werden. Dies ist besonders dann der Fall, wenn atomare Übergangsfrequenzen und Mediumresonanzfrequenzen nah beieinander liegen. In solchen Fällen kann die störungstheoretische Behandlung wegen starker Atom-Feld-Kopplung ihre Gültigkeit verlieren. Eine mögliche Lösung könnte in einem nicht-störungstheoretischen Zugang ähnlich dem, der in [42] für den Fall eines einzelnen, elektrisch polarisierbaren Atoms entwickelt wurde, bestehen. Indem man einen allgemeineren Formalismus für die makroskopische Quantenelektrodynamik in linearen Medien [87] benutzt, kann die Theorie so erweitert werden, dass auch anisotrope oder nicht-lokal reagierende Medien behandelt werden können. Der Einfluss einer endlichen Temperatur kann berücksichtigt werden, indem man zu Beginn der störungstheoretischen Berechnungen Grundzustandserwartungswerte des mediengestützten Feldes durch thermische Erwartungswerte ersetzt.

Ehrenwörtliche Erklärung

Ich erkläre hiermit ehrenwörtlich, dass ich die vorliegende Aufgabe selbständig, ohne unzulässige Hilfe Dritter und ohne Benutzung anderer als der angegebenen Hilfsmittel und Literatur angefertigt habe. Die aus anderen Quellen direkt oder indirekt übernommenen Daten und Konzepte sind unter Angabe der Quelle gekennzeichnet.

Bei der Auswahl und Auswertung des folgenden Materials haben mir die nachstehend aufgeführten Personen in der jeweils beschriebenen Weise entgeltlich/unentgeltlich geholfen:

1. R. Panepinto, K. Panepinto, M. Cumme and A. Sambale: Deutsche Übersetzung der Zusammenfassung (unentgeltlich)
2. A. Sambale: Deutsche Übersetzung des Thesenpapiers (unentgeltlich)

Weitere Personen waren an der inhaltlich-materiellen Erstellung der vorliegenden Arbeit nicht beteiligt. Insbesondere habe ich hierfür nicht die entgeltliche Hilfe von Vermittlungs- bzw. Beratungsdiensten (Promotionsberater oder andere Personen) in Anspruch genommen. Niemand hat von mir unmittelbar oder mittelbar geldwerte Leistungen für Arbeiten erhalten, die im Zusammenhang mit dem Inhalt der vorgelegten Dissertation stehen.

Die Arbeit wurde bisher weder im In- noch im Ausland in gleicher oder ähnlicher Form einer anderen Prüfungsbehörde vorgelegt.

Die geltende Promotionsordnung der Physikalisch–Astronomischen Fakultät ist mir bekannt.

Ich versichere ehrenwörtlich, dass ich nach bestem Wissen die reine Wahrheit gesagt und nichts verschwiegen habe.

Jena, den 07.01.2009 Hassan Safari