Casimir forces in a T-operator approach

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(Received 4 September 2007; revised manuscript received 24 April 2008; published 8 July 2008)

We explore the scattering approach to Casimir forces. Our main tool is the description of Casimir energy in terms of transition operators. The approach is valid for scalar fields as well as for electromagnetic fields. We provide several equivalent derivations of the formula presented by Kenneth and Klich [Phys. Rev. Lett. **97**, 160401 (2006)]. We study the convergence properties of the formula and how to utilize it together with scattering data to compute the force. Next, we discuss the form of the formula in special cases such as the simplified form obtained when a single object is placed next to a mirror. We illustrate the approach by describing the force between scatterers in one dimension and three dimensions, where we obtain the interaction energy between two spherical bodies at all distances. We also consider the cases of scalar Casimir effect between spherical bodies with different radii as well as different dielectric functions.

DOI: 10.1103/PhysRevB.78.014103 PACS number(s): 12.20.−m, 03.65.−w, 03.70.+k

I. INTRODUCTION

The Casimir force[1] is one of the fundamental predictions of quantum physics. It explores the interplay between a quantum field and external "classical" objects such as boundary conditions, background dielectric bodies, or space-time metric. While the classical objects modify the behavior of the field due to their presence, the field, in turn, acts on the objects, typically by exerting forces. Much work has been devoted to understanding the effect, as it appears in varied branches of physics: from condensed matter (interaction between surfaces in fluids) to gravitation and cosmology.

The precise measurement of the effect by Lamoreaux[2] signaled a different age of Casimir force measurements and led to a revived interest in the theory behind the effect. In recent years, the force between various objects (such as two plates, plate and a sphere, corrugated plate and sphere, etc.[2–4]) was measured. Moreover, the dependence on various properties of the materials used, such as corrections due to finite conductivity and temperature,[5,6] as well as on geometry has been investigated. There is excellent agreement between the experiments and the theoretical predictions, which is being constantly improved. For the introduction to the subject as well as reviews of progress, see, e.g., Refs. 7–10. Different variants (both material and geometric) of the force have been proposed, discussed, and motivated by pure theoretical interest as well as by potential eventual application in nanomechanical structures.[11,12]

The original method used by Casimir, that of mode summation, has led to a large body of work on the effect in simple geometries, where the modes may be exactly computed. For more general cases, one has to use other available approaches such as the Green's function approach or the path-integral approach. Significant progress in utilizing these techniques numerically has been reported lately.[13,14]

In the one-dimensional (1D) case, scattering approach to Casimir physics has proved very useful. Indeed, many of the calculations of Casimir interaction between bodies are based on scattering theory, as the photon spectrum in an open geometry is continuous and its description requires scattering.

In this paper, we explore a scattering approach to Casimir effect in higher dimensions. The approach is based on the analysis of a determinant formula for Casimir interactions obtained in Ref. 15 and may be viewed as a generalization of previous formulas, especially related to scattering, such as the Lifshitz formula[16] and the results of Balian and Duplantier.[17] Within this approach, the Casimir energy is encoded in a determinant of the operator $1-T_AG_0T_BG_0$, where T_A, T_B are Lippmann–Schwinger T operators associated with bodies A and B, and G_0 is the photons Green's function; we shall therefore refer to the formula as the *TGTG* formula.

In Ref. 15, it was shown how general results regarding the direction of the force between bodies related by reflection can be obtained from the *TGTG* formula. For example, the sign problem of interaction between two hemispheres was resolved. This result was subsequently extended to a large class of interacting fields possessing the "reflection positivity" property[19] (see also Ref. 20 where use is made of reflection positivity arguments to infer attraction between vortices and antivortices in a frustrated *XY* model). In Ref. 21, an alternative derivation of the formula was presented.

The paper is organized as follows. In Sec. II, we start with a derivation of the determinant formula as well as supply alternative derivations in terms of Green's functions and the T operator of a pair of perturbations. Section III illustrates how one obtains the appropriate formula in the vector [electromagnetic (EM)] case. Sections IV and V cover simplified cases: the special case of a body placed next to a perfect mirror, and the dilute limit, which deals with very weak dielectrics by expanding round $\epsilon=1$.

We then proceed to show how the formula is to be applied in actual calculations. We explain how the formula is to be used together with partial wave expansions of the scattered states (Secs. VI and VII). In one dimension where only two modes (left and right movers) exist at each ω, this leads to a known closed form formula for the Casimir energy in terms of the reflection coefficient (see, e.g., Refs. 22 and 23).

In Sec. VIII, we use a spherical wave expansion to obtain explicit expansion for the Casimir interaction between compact bodies. We demonstrate this by computing the force between two spheres at all distances, thereby generalizing the approach of Ref. 24 to spheres beyond Dirichlet boundary conditions and going beyond the proximity force approximation. We also consider cases of spheres with unequal radii, as well as spheres with arbitrary dielectric function. In Sec. IX, results are extended to the electromagnetic case. While this paper was finalized, we have learned that related results were reported in Ref. 21 for the Casimir interaction between spheres with equal radii, as well as an alternative derivation of the determinant formula. Our results agree perfectly with those of Refs. 21 and 24.

A number of appendices describe some technical details of the calculations. Most notably, in Appendix B, we give additional details about the mathematical validity of the formula, which were not included in Ref. 15. These details help establish rigorously the validity of the present approach to calculations of Casimir forces. In particular, we show that the formula is given in terms of $\log\det(1+A)$, where $\mathrm{Tr}|A|<\infty$, and so mathematically well defined. (This appendix is written in a "mathematical physics" style and may be skipped by readers not interested in these issues.)

II. *TGTG* FORMULA: CASIMIR INTERACTION AS A REGULAR DETERMINANT

In this section, we explain how the part of the free energy of a Gaussian theory that depends on distance between bodies, and as such is responsible for the Casimir force, may be expressed in terms of a regular determinant and discuss some of its properties. Here, some of the material covered appeared in literature, however, as far as we know, the final formula was never written in this general form; furthermore, its mathematical properties were not rigorously addressed previously. We note, however, that an elaborate and rigorous analysis of a related problem involving impenetrable disks was carried out in Ref. 25.

We start by presenting the derivation of the *TGTG* formula (11) in the path-integral approach.[22,26,27] We first treat the case of a scalar field and explain later how the result is extended to the EM field. Alternative derivations of Eq. (11) are elaborated in the following subsections.

The action of a real massless scalar field in the presence of dielectrics can be written as

$$S[\phi]=\frac{1}{2}\int d^d\mathbf{r}\int\frac{d\omega}{2\pi}\phi^*_\omega[\nabla^2+\omega^2\epsilon(\mathbf{x},\omega)]\phi_\omega, \tag{1}$$

where $\phi^*_\omega=\phi_{-\omega}$ and $\epsilon(\omega,\mathbf{x})=1+\chi(\mathbf{x},\omega)$ is the dielectric function (we use units $\hbar=c=1$). This action is the simplest action that yields the scalar analog of the Maxwell equation

$$\nabla\times\nabla\times\vec{A}-\frac{\omega^2}{c^2}\epsilon(\omega,x)\vec{A}=0 \tag{2}$$

for the vector potential in the radiation gauge. Alternatively, this action can be derived by coupling a scalar field to an auxiliary field living on the regions of space where $\epsilon\neq 1$, and then integrating out these fields as done, e.g., in Ref. 27.

Formally, the free energy of the system is obtained from the partition function $\mathcal{Z}$ given by

$$\mathcal{Z}=\int\mathcal{D}\phi e^{iS[\phi]}. \tag{3}$$

Performing the Gaussian integration, one finds that the change in energy due to introduction of χ in the system is

$$E_C=E_\chi-E_{\chi=0}=-i\int_0^\infty\frac{d\omega}{2\pi}\log\det{}_\Lambda[1+\omega^2\chi(\mathbf{x},\omega)(\nabla^2+\omega^2+i0)^{-1}]. \tag{4}$$

At this point, we encounter one of the main features of Casimir physics—the need to properly isolate the physically relevant part of the energy out of a formally ill-defined expression. A determinant [such as in Eq. (4)] is mathematically well defined only if it has the form $\det(1+A)$, where A is a "trace class" operator, i.e., $\Sigma_i|\lambda_i|<\infty$, with λ_i eigenvalues of A (for properties, see Appendix C and Refs. 18 and 28). If A is not a trace class operator, one may obtain different or infinite results for the determinant, depending on the order in which the eigenvalues of $1+A$ are multiplied. The expression above is not of the required form. To see this, note that A in our case is given by

$$\omega^2\chi(\mathbf{x},\omega)(\nabla^2+\omega^2+i0)^{-1}. \tag{5}$$

This is an operator of the form $g(x)f(\nabla)$. If such an operator is trace class, then its trace is known to be given by the Birman–Solomyak result,[28]

$$\mathrm{Tr}[g(x)f(i\nabla)]=\int d^3x g(x)\int d^3k f(k), \tag{6}$$

in our case, we have $\int d^3x\chi(x)<\infty$, however, $\int d^3k(-k^2+\omega^2+i0)^{-1}$ diverges and indicates that the operator involved does not have a well-defined trace.[29]

As such, expression (4) only has meaning when specifying physical cutoffs. Removing physical cutoffs will leave us with an ill-defined expression and so we keep in mind cutoffs at high momenta in the notation $\det_\Lambda$.

At high frequencies, $\chi(\omega,\mathbf{x})\to 0$ provides a physical frequency cutoff. For $\mathrm{Re}\,\omega,\mathrm{Im}\,\omega>0$, both $\chi(\omega)$ and $(\nabla^2+\omega^2+i0)^{-1}$ are analytic, which justify the Wick rotation of the integration to the imaginary axis $i\omega$, ending up with

$$E_C=\int_0^\infty\frac{d\omega}{2\pi}\log\det{}_\Lambda[1+\omega^2\chi(\mathbf{x},i\omega)G_0(\mathbf{x},\mathbf{x}')], \tag{7}$$

where $G_0(\mathbf{x},\mathbf{x}')=\langle\mathbf{x}|\frac{1}{-\nabla^2+\omega^2}|\mathbf{x}'\rangle$. Restricting the operator $(1+\omega^2\chi G_0)$ to the support of χ (more precisely to $L^2[\mathrm{supp}(\chi)]$) clearly does not affect its determinant. Note that Eq. (7) is still ill defined if one removes the cutoff, as can be immediately seen from the argument based on Eq. (6).

We now consider the case, depicted in Fig. 1, of two bodies A,B immersed in vacuum. χ is assumed nonzero only inside the volumes of the two dielectrics A,B and we therefore consider in the following $(1+\omega^2\chi G_0)$ as an operator on $H_A\oplus H_B\to H_A\oplus H_B$, where $H_A=L^2(A)$ and $H_B=L^2(B)$.[30] It is then convenient to write

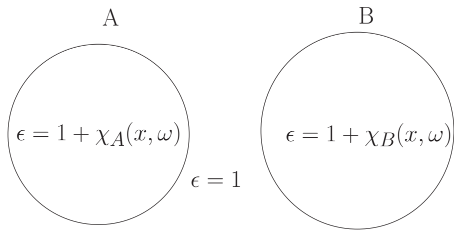

FIG. 1. Bodies *A* and *B*.

$$(1+\omega^2\chi G_0)|_{H_A\oplus H_B} = \begin{pmatrix} 1_A + \omega^2\chi_A G_{0AA} & \omega^2\chi_A G_{0AB} \\ \omega^2\chi_B G_{0BA} & 1_B + \omega^2\chi_B G_{0BB} \end{pmatrix}, \tag{8}$$

where $G_{0\alpha\beta}$ is G_0 restricted to $H_\alpha \to H_\beta$ (equivalently, $G_{0\alpha\beta} = P_\alpha G_0 P_\beta$, where $P_A = 1\oplus 0$ and $P_B = 0\oplus 1$ are projections on H_A, H_B respectively). It turns out that the part of the energy that depends on mutual position of the bodies, and as such is responsible for the force, is a well-defined quantity, which is independent of the cutoffs. To see this, we subtract contributions that do not depend on relative positions of the bodies A,B,

$$E_C = E_C(A\cup B) - E_C(A) - E_C(B). \tag{9}$$

As in Ref. 27, this amounts to subtracting the diagonal contributions to the determinant, which are not sensitive to the distance between the bodies (i.e., only contributes to their self-energies). This yields

$$\begin{aligned} E_C &= \int_0^\infty \frac{d\omega}{2\pi}\left\{\log \det{}_\Lambda \begin{bmatrix} 1+\omega^2\chi_A G_{0AA} & \omega^2\chi_A G_{0AB} \\ \omega^2\chi_B G_{0BA} & 1+\omega^2\chi_B G_{0BB}\end{bmatrix}\right. \\ &\quad \left. - \log\det{}_\Lambda \begin{bmatrix} 1+\omega^2\chi_A G_{0AA} & 0 \\ 0 & 1+\omega^2\chi_B G_{0BB}\end{bmatrix}\right\} \\ &= \int_0^\infty \frac{d\omega}{2\pi}\left[\log\det{}_\Lambda \begin{pmatrix} 1 & T_A G_{0AB} \\ T_B G_{0BA} & 1\end{pmatrix}\right], \end{aligned} \tag{10}$$

where $T_\alpha = \frac{\omega^2}{1+\omega^2\chi_\alpha G_{0\alpha\alpha}}\chi_\alpha$. Finally, using the relation

$$\det\begin{pmatrix} 1 & X \\ Y & 1\end{pmatrix} = \det(1 - YX),$$

which holds for block matrices, we have

$$E_C(a) = \int_0^\infty \frac{d\omega}{2\pi}\log\det(1 - T_A G_{0AB} T_B G_{0BA}). \tag{11}$$

Henceforth, we refer to Eq. (11) as the *TGTG* formula throughout the paper. Up to the Wick rotation, the operators T_α are exactly the T operators appearing in the Lippman–Schwinger equation, as will be discussed in Sec. II B. The Wick rotation $T(\omega)\to T(i\omega)$ has the effect of turning T_α into Hermitian operators as well as of avoiding potential singularities (which may occur at real frequencies).

In Eq. (11), we disposed of the cutoff Λ as the expression is well defined in the continuum limit. In practical terms, this means that replacing the infinite dimensional matrix of $1 - T_A G_{0AB} T_B G_{0BA}$ by its upperleft $n\times n$ block with n large enough and calculating the resulting ordinary determinant gives an arbitrarily good approximation to a (finite) quantity, which we call $\det(1 - T_A G_{0AB} T_B G_{0BA})$. This point is discussed in detail in Appendix B, where we prove some mathematical properties of the operators involved. The details are not essential for understanding the applications of the formula, so a reader not interested in mathematical rigor may skip them.

A. Dirichlet and Neumann boundary conditions

In many cases, and indeed in the original presentation by Casimir, one is interested in sharp boundary conditions, such as Dirichlet or Neumann. Sharp boundary conditions result in singular energy density at the surface, as field modes are required to vanish for all momentum scales. Typically, the local energy density diverges as the inverse fourth power of the distance from the boundary.[31]

It is important to point out that the above considerations also describe the conducting case with minor changes. Following Ref. 27, assume that conducting boundary conditions are given over a surface Σ, which is parametrized by internal coordinate u and by the embedding in $\mathbb{R}^3$ given by $\mathbf{x}(u)$. One may describe a simple metal by taking $\chi(i\omega) = \frac{\omega_p^2}{4\pi\omega^2}$ on Σ and letting Σ to have a thickness of a few skin depths $l/\omega_p, l \sim \mathcal{O}(1)$, where ω_p is the plasma frequency (proportional to the effective electron density in the metal). In the limit of large ω_p, one retains the same expression as Eq. (11), with the following substitutions:

$$\begin{aligned} E_C(a) = -\frac{1}{4\pi}\int_0^\infty d\omega\Bigg[\log\det\Bigg(1 \\ - \mathcal{M}_{BA}\frac{1}{1+\mathcal{M}_A}\mathcal{M}_{AB}\frac{1}{1+\mathcal{M}_B}\Bigg)\Bigg], \end{aligned} \tag{12}$$

where in the Dirichlet case, $\mathcal{M}$ is given by

$$M^{(D)}(u,u';\omega) = l\omega_p\sqrt{g(u)}G_0[\mathbf{x}(u),\mathbf{x}(u')]\sqrt{g(u')} \tag{13}$$

and acting on the surfaces Σ. Similarly, Neumann boundary conditions may be treated in the path-integral method by taking[32]

$$M^{(N)}(u,u';\omega) = \sqrt{g(u)}\sqrt{g(u')}\partial_{n(u)}\partial_{n(u')}G_0[\mathbf{x}(u),\mathbf{x}(u')] \tag{14}$$

in Eq. (12). We remark that rigorous discussion of the formula in the Neumann case requires further analysis that we did not pursue in this paper [see remarks after Eq. (41)].

B. Derivation using Green's functions and *T* operators

To make contact with Green's function approach, we supply in this section an alternative derivation of the *TGTG* formula. Most of the derivation is standard and may be skipped by readers interested only in new results. However, we point out that our approach where the T operator of the combined scatterers is utilized seems new. Here, we first use the Green's function in order to express the density of states (DOS) of a differential operator with background and then perform the mode summation by integrating over energies.

We briefly remind the reader some of the required material. The standard discussion of this is usually done in the context of nonrelativistic quantum mechanics. The retarded and advanced $G^{\pm}$ are then defined by

$$(E \pm is - \mathcal{H})G^{\pm}(E) = I. \tag{15}$$

This equation should be understood as an operator identity. If $\mathcal{H}$ is a differential operator, for example, $\mathcal{H}=-\Delta$, then it is the operator form of the differential equation,

$$(E \pm is + \Delta)G(x,x') = \delta(x-x'). \tag{16}$$

Using the representation $\langle n|G^{\pm}(E)|n'\rangle = \lim_{s\to 0}\frac{\delta_{nn'}}{E\pm is-E_n}$, one finds that the DOS is given by

$$\frac{1}{\pi}\text{Im Tr } G^{\pm}(E) = \mp \sum_n \delta(E-E_n) = \mp \rho(E). \tag{17}$$

Since $\partial_E \log[E\pm is-E_n]=\frac{1}{E\pm is-E_n}$, one can rewrite this as

$$\rho(E) = \pm \frac{1}{\pi}\text{Im } \partial_E \text{ Tr log } G^{\pm}(E). \tag{18}$$

We are more interested in the relativistic version of this. (Indeed, the Casimir force vanishes in the nonrelativistic limit, as the exchange of very massive virtual particles is suppressed.) In the relativistic context, the Feynman propagator G is defined by a similar formula to that of G^{+},

$$H(\omega^2 + is)G = I. \tag{19}$$

For example, action (1) corresponds to $H=-\Delta-\omega^2\epsilon$. In free space $\epsilon=1$, we obtain the same equation as Eq. (16) apart from the substitution $E\to\omega^2$. (There is also a not very interesting conventional overall minus sign, which is the reason some signs in the following equations are different from what the reader may remember.) In the presence of nontrivial background (e.g., dielectric), the ω dependence of H can take a quite arbitrary form, which slightly complicates the derivation of the DOS. One may take advantage of the relation

$$\text{Im}\frac{F'(x\pm is)}{F(x\pm is)} = \mp \pi \sum_n \delta(x-x_n),$$

where $F(x)$ is any real function having simple zeroes at the points $\{x_n\}$. Indeed, away from the zeroes $\{x_n\}$, the fact that F is real guarantees vanishing of the left hand side, while near the zero x_n, we have $\text{Im}\frac{F'(x\pm is)}{F(x\pm is)}=\text{Im}\frac{F'(x_n)}{(x\pm is-x_n)F'(x_n)}=\mp\frac{s}{(x-x_n)^2+s^2}\to\mp\pi\delta(x-x_n)$. Generalizing the relation from real functions $F(x)$ to Hermitian operators $H(\omega^2)$ (Ref. 33) allows writing

$$\text{Im } \partial_\omega \text{ Tr log } G(\omega) = -\text{ Im Tr } H'(\omega)G(\omega) = \pi\rho(\omega), \tag{20}$$

which is the obvious analog of Eq. (18). (Note, however, that similar generalization of Eq. (17) would usually be false.) In Eq. (20), we implicitly assumed $\omega>0$ to avoid an extra $\text{sgn}(\omega)$ factor.

Now, assume that G_0 is known for H_0 and we add a perturbation V, i.e.,

$$[H_0(\omega^2+is) + V(\omega^2+is)]G = I. \tag{21}$$

The change in DOS due to introduction of the potential V is formally

$$\Delta\rho = \frac{1}{\pi}\text{Im } \partial_\omega \text{ Tr log } GG_0^{-1}. \tag{22}$$

We will be interested in the change in energy due to change in the distance a between two separated potentials V_A and V_B, which make up $V=V_A+V_B$.

Thus,

$$\begin{aligned}\partial_a\Delta\rho(\omega) &= \frac{1}{\pi}\text{Im } \partial_\omega\partial_a \text{ Tr log}(GG_0^{-1}) \\ &= \frac{1}{\pi}\text{Im } \partial_\omega\partial_a \text{ Tr log}(I+G_0V)^{-1}.\end{aligned} \tag{23}$$

Defining the T matrix by

$$T = V(I+G_0V)^{-1}, \tag{24}$$

we may also write

$$\partial_a\Delta\rho(\omega) = \frac{1}{\pi}\text{Im } \partial_\omega\partial_a \text{ Tr log}(I-G_0T). \tag{25}$$

Alternatively, formally writing $\partial_a \det(V_A+V_B)=0$ since V_A, V_B act in different subspaces, one can write that

$$\partial_a\Delta\rho(\omega) = \frac{1}{\pi}\text{Im } \partial_\omega\partial_a \text{ Tr log } T. \tag{26}$$

This last formal expression, however, should be handled with care, and so we avoid using it.

The T matrix satisfies

$$G(\omega) = G_0(\omega) - G_0(\omega)T(\omega)G_0(\omega) \tag{27}$$

(here, $\omega>0$ is actually $\omega+is$) and frequently appears in scattering theory. Also note $T=V-VGV$.

The operator T appears in the Lippmann–Schwinger equation as follows. Given a solution ϕ of the free equation, without a potential $H_0(\omega)\phi=0$, one constructs a solution ψ of the eigenvalue equation $(H_0+V)\psi=0$ having the same incoming part $\psi_{\text{in}}=\phi_{\text{in}}$. Formally, this is done by looking for a solution of

$$\psi = \phi - G_0V\psi,$$

which is the Lippmann–Schwinger equation. It follows that $\psi=(I+G_0V)^{-1}\phi=(I-G_0T)\phi$, thus we may build a new solution ψ from a solution ϕ of the free equation. For example, choosing ϕ to be a plane wave solution, one obtains

$$\psi_k = e^{ikx} - \int dk' G_0(k)\langle k|T|k'\rangle e^{ik'x}. \tag{28}$$

Note that our relativistic normalization convention implies that T is related to the scattering matrix via $S=1-2\pi i\delta(\omega^2 - H_0)T$.

We now address the case of the two potentials V_A, V_B. We assume for simplicity that cutoffs are in place and so work with the T operators as matrices. We compute the joint transition matrix for both perturbations $T_{A\cup B}$ and show that the part independent of "self-energy" is exactly Eq. (11).

By using formula (27) as $G_i = G_0 - G_0 T_i G_0$ (with $i=A,B$), together with the definition of T [Eq. (24)] and straightforward algebraic manipulations, we obtain

$$\frac{1}{1+G_0(V_A+V_B)} = (1-G_0T_A)\frac{1}{1-G_0T_BG_0T_A}(1-G_0T_B), \tag{29}$$

and so the joint T operator of a pair of perturbations may be factored as

$$\begin{aligned} T_{A\cup B} &= (V_A+V_B)\frac{1}{1+G_0(V_A+V_B)} \\ &= (V_A+V_B)(1-G_0T_A) \\ &\quad\times \frac{1}{1-G_0T_BG_0T_A}(1-G_0T_B). \end{aligned} \tag{30}$$

The important feature of this expression is the observation that the only part of the expression which directly mixes between A and B is the factor $1-G_0T_BG_0T_A$. Indeed, plugging Eq. (29) in Eq. (23), we see that the contribution of frequency ω to the force is now given by

$$\begin{aligned} \partial_a \Delta\rho(\omega) &= \frac{1}{\pi}\mathrm{Im}\ \partial_\omega\partial_a\ \mathrm{Tr}\ \log[I+G_0(V_A+V_B)]^{-1} \\ &= \frac{1}{\pi}\mathrm{Im}\ \partial_\omega\partial_a[\log\det(1-G_0T_A) + \log\det(1-G_0T_B) \\ &\quad - \log\det(1-G_0T_AG_0T_B)] \\ &= -\frac{1}{\pi}\mathrm{Im}\ \partial_\omega\partial_a \log\det(1-G_0T_AG_0T_B), \end{aligned} \tag{31}$$

leading again to our expression for the energy [Eq. (11)]. Alternatively, one may simply verify the correctness of Eq. (11) by noting that

$$\begin{aligned} 1-G_0T_AG_0T_B &= 1 - G_0V_A\frac{1}{1+G_0V_A}G_0V_B\frac{1}{1+G_0V_B} \\ &= \frac{1}{1+G_0V_A}[(1+G_0V_A)(1+G_0V_B) \\ &\quad - G_0V_AG_0V_B]\frac{1}{1+G_0V_B} \\ &= \frac{1}{1+G_0V_A}[1+G_0(V_A+V_B)]\frac{1}{1+G_0V_B} \end{aligned} \tag{32}$$

and using Eq. (23).

III. ELECTROMAGNETIC CASE

Here, we follow the approach of Ref. 34. The statistical properties of the electromagnetic field in a medium are described by the appropriate photonic Green's function. The electromagnetic fields are derived from the electromagnetic potentials A^α, where $\alpha=0,..,3$. (It is convenient to work in the gauge $A^0=0$.) The retarded Green's function $\mathcal{D}_{ik}$ is defined by

$$\mathcal{D}_{ik}(X_1,X_2) = \begin{cases} \langle A_i(X_1)A_k(X_2) - A_k(X_2)A_i(X_1)\rangle, & t_1 < t_2 \\ 0, & \text{otherwise}, \end{cases} \tag{33}$$

where X_1, X_2 are four-vectors $(X_1^0, \ldots, X_1^3)$ and $k,i=1,\ldots,3$. The angular brackets denote averaging with respect to the Gibbs distribution.

The interaction of the electromagnetic field with a classical current $\mathbf{J}$ set in the medium is given by

$$V = -\frac{1}{c}\int \mathbf{J}\cdot\mathbf{A}.$$

Kubo's formula allows us to treat this interaction within linear response. By Kubo's formula, the mean value $\overline{\mathbf{A}}_i$ in the presence of a current $\mathbf{J}$ satisfies

$$\overline{\mathbf{A}}_i(\mathbf{r})_\omega = -\frac{1}{\hbar c}\int \mathcal{D}^R_{ik}(\omega;\mathbf{r},\mathbf{r}')\mathbf{J}_k(\mathbf{r}')_\omega d^3\mathbf{r}', \tag{34}$$

where

$$\mathcal{D}^R_{ik}(\omega;\mathbf{r},\mathbf{r}') = \int_0^\infty e^{i\omega t}\mathcal{D}^R_{ik}(t;\mathbf{r},\mathbf{r}')dt. \tag{35}$$

The function $\mathcal{D}$ is sometimes referred to as the generalized susceptibility of the system.[34]

From Maxwell's equations, it follows that in a medium with a given permittivity tensor ϵ_{ij}, permeability tensor μ_{ij}, and current $\mathbf{J}$, the vector potential A_i satisfies

$$\left(\nabla\times(\mu^{-1}\nabla\times) - \frac{\omega^2}{c^2}\epsilon\right)\overline{\mathbf{A}} = \frac{4\pi}{c}\mathbf{J}_\omega. \tag{36}$$

Substituting Eq. (34) in Eq. (36), we see that $\mathcal{D}$ is a Green's function for the equation,

$$\nabla\times\mu^{-1}\nabla\times\mathcal{D} - \frac{\omega^2}{c^2}\epsilon\mathcal{D} = -4\pi\hbar I\delta(\mathbf{r}-\mathbf{r}'), \tag{37}$$

where I is the three-dimensional unit matrix. In the following, we shall work in units where $c=\hbar=1$.

The Green's function $\mathcal{D}$ is then used to obtain the well-known expression (80.8) of Lifshitz and Pitaevskii[34] for the change in free energy due to variation of the dielectric function ϵ at a temperature T,

$$\delta F = \delta F_0 + \frac{1}{2} T \sum_{n=-\infty}^{\infty} \omega_n^2 \, \mathrm{Tr}(\mathcal{D}\delta\epsilon). \quad (38)$$

Here, F_0 is the free energy due to material properties not related to long wavelength photon field, and $\omega_n = 2\pi nT$ are the Matsubara frequencies. $\mathcal{D}$ is the temperature Green's function of the long wave photon field given by $\mathcal{D}(\vec{x},\vec{x}',i\omega)_{ij} = \langle \vec{x} | \frac{1}{\nabla\times\nabla\times+\omega^2\epsilon(r,i|\omega|)} | \vec{x}' \rangle_{ij}$.

Equation (38) may be written as $\delta F = \delta F_0 + \delta F_C$, where

$$F_C = \frac{T}{2} \sum_{n=-\infty}^{\infty} \{\log \det{}_\Lambda [\nabla \times \nabla \times + \omega_n^2 \epsilon(x,i\omega_n)] - \log \det{}_\Lambda (\nabla \times \nabla \times + \omega_n^2)\}$$
$$= \frac{1}{2} T \sum_{n=-\infty}^{\infty} \log \det{}_\Lambda [1 + \omega_n^2 \chi(x,i\omega_n) \mathcal{D}_0(i\omega_n)]. \quad (39)$$

Here, $\mathcal{D}_0(\vec{x},\vec{x}',i\omega_n)_{ij} = \langle \vec{x} | \frac{1}{\nabla\times\nabla\times+\omega_n^2} | \vec{x}' \rangle_{ij}$. Note that F_C is exactly the same as Eq. (7), with the scalar propagator G_0 replaced by the vector propagator $\mathcal{D}_0$. For later reference, we write here the explicit expression for $\mathcal{D}_0$:

$$\mathcal{D}_{0ij}(k,i\omega) = \frac{1}{k^2+\omega^2} \left(\delta_{ij} + \frac{k_i k_j}{\omega^2} \right). \quad (40)$$

Thus, starting with this expression, one repeats Eqs. (9) and (10) to get Eq. (11), replacing G_0 by $\mathcal{D}_0$ everywhere (including in the definition of the T operators). The analysis of the determinant now proceeds exactly as in the scalar case.

Alternatively, the EM case may similarly be derived starting from the functional determinant corresponding to an EM action analogous to Eq. (1). In the axial gauge, this action takes the form

$$S = \frac{1}{2} \int d^3\mathbf{r} \int \frac{d\omega}{2\pi} \vec{\mathcal{A}}_\omega^* [-\nabla \times \nabla \times + \omega^2 \epsilon(\mathbf{x},\omega)] \vec{\mathcal{A}}_\omega. \quad (41)$$

A permeable body may similarly be described within our approach by replacing the dielectric interaction term $\vec{\mathcal{A}}\omega^2\chi(x)\vec{\mathcal{A}}$ in the Lagrangian by a magnetic term: $\vec{\mathcal{A}}\nabla\times(1-\frac{1}{\mu})\nabla\times\vec{\mathcal{A}}$. One may then go on through our derivation using the (differential) operator $\nabla\times(1-\frac{1}{\mu(x)})\nabla\times\cdots$ instead of $-\omega^2\chi(x)$ everywhere. One major difference between the two cases is worth noting: whereas the dielectric term is always described (after Wick rotation) by a positive operator, the operator in the magnetic term turns out to be always negative. This fact can be related to the known Casimir electric-magnetic repulsion. Moreover, the ideal $\mu\to\infty$ limit is seen to correspond to a Lagrangian in which the term $(\nabla\times\mathcal{A})^2$ is missing (inside the body), which makes a highly irregular Lagrangian. Analogy with a scalar field satisfying Neumann boundary conditions suggests that this situation may be described by dropping the $(\nabla\phi)^2$ term inside the Neumann body. There are also other arguments in favor of that approach;[35] however, we did not bring these arguments to a completely rigorous form.

IV. DIELECTRIC IN FRONT OF A MIRROR

A somewhat simplified, but useful in practice, version of the formula is obtained in the case of a body placed close to a mirror. Consider the body A to the left of a Dirichlet mirror B located at $x_n = a/2$. It is well known (using the image method) that the effect of the Dirichlet mirror is to replace the free propagator G_0 by

$$G_B(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') - G_0[\mathbf{x},J(\mathbf{x}')], \quad (42)$$

where $J(\mathbf{x}_\parallel,x_\perp) = (\mathbf{x}_\parallel, a-x_\perp)$ denotes reflection through the mirror plane. This may be written as $G_B - G_0 = -G_0\mathcal{J}$, where $\mathcal{J}$ is the operator defined by $\mathcal{J}\psi(\mathbf{x}) = \psi[J(\mathbf{x})]$. Noting standard relation (27) $G_B = G_0 - G_0 T_B G_0$ between the Green's function in the presence of scatterer B to its T matrix, one concludes that $G_0 T_B G_0 = G_0\mathcal{J}$ which when substituted in Eq. (11) gives

$$E_C(a) = \int_0^\infty \frac{d\omega}{2\pi} \log \det(1 - G_0 \mathcal{J} T_A). \quad (43)$$

An alternative (though closely related) approach is to note that by complete analogy to Eq. (7), the energy it costs to place a body A near a mirror B is

$$E_C = \int_0^\infty \frac{d\omega}{2\pi} \log \det{}_\Lambda [1 + \omega^2 \chi_A(\mathbf{x},i\omega) G_B(\mathbf{x},\mathbf{x}')].$$

Subtracting the energy $E_C = \int_0^\infty \frac{d\omega}{2\pi} \log \det_\Lambda [1 + \omega^2 \chi_A(\mathbf{x},i\omega) G_0(\mathbf{x},\mathbf{x}')]$, it cost to place A in vacuum then gives the Casimir interaction energy. Using the relation

$$(1 + G_B V_A)/(1 + G_0 V_A) = 1 + (G_B - G_0) T_A = 1 - G_0 \mathcal{J} T_A \quad (44)$$

leads again to Eq. (43).

Yet, another way of obtaining the same result is by substituting $\chi_B = \lambda \delta(x_n - a/2)$ in the definition of T_B and doing the algebra. One then finds

$$G_0 T_B G_0 = \int \frac{d^2k_\perp}{(2\pi)^2} e^{ik_\perp (x-x')_\perp} \frac{\lambda\omega^2}{2q(\lambda\omega^2 + 2q)} \times e^{-q|x_n| - q|x_n'|} \Big|_{q=\sqrt{\omega^2+k_\perp^2}}, \quad (45)$$

which in the limit $\lambda\to\infty$ reduces, as expected, to the expression $G_0\mathcal{J}$ obtained through the image method.

We now address the case of a Neumann mirror. Note that the Green's function in the presence of a Neumann mirror is $G = G_0 + G_0\mathcal{J}$. By repeating the arguments above, we find that the Casimir interaction between an object A and a Neumann mirror is given by a similar formula to Eq. (43), which involves the determinant $\det(1 + G_0\mathcal{J}T_A)$. We remark that while the Dirichlet mirror may be considered as the limit $\lambda\to\infty$ of a dielectric having, e.g., $\chi_B = \lambda\delta(x_n - a/2)$ [or in more realistic model $\chi_B = \lambda\theta(x_n - a/2)$], it is hard to find a simple analog $\chi_B(x)$ that would lead in a similar limit to a Neumann mirror. (See, however, remark at the end of Sec. III.)

A similar treatment is applicable in the more physically relevant EM case. The boundary conditions $E_\parallel = 0$ may be enforced by requiring the vector potential to satisfy

$\mathcal{J}A=-A$, where $\mathcal{J}$ is defined to act on vectors as $\mathcal{J}A(x)=\{A_\parallel[J(x)],-A_\perp[J(x)]\}$. (Here, $A_\parallel,A_\perp$ denote the components of A parallel and normal to the mirror surface. The temporal component is considered as a parallel component although, in practice, we usually choose a gauge where it vanishes.)

The EM Casimir interaction between a dielectric and a mirror is then given by a formula similar to Eq. (43) with $G_0,\mathcal{J}$ replaced by the EM propagator $\mathcal{D}_0$ and the vectorial $\mathcal{J}$ defined above. It is interesting to also consider an ideal permeable mirror (having $\mu\to\infty,\epsilon=1$). This corresponds to the boundary condition $B_\parallel=0$ that may be enforced by requiring the vector potential to satisfy $\mathcal{J}A=+A$. Thus, the Casimir interaction of body A with such a mirror will be given by an expression involving the determinant $\det(1+T_A\mathcal{D}_0\mathcal{J})$.

V. DILUTE LIMIT

In the following sections, we consider strategies of using the *TGTG* formula in actual calculations. A particularly simple case is when χ is small, which is commonly referred to as the "dilute" case (and sometimes as "low contrast"). Here, we briefly sketch how to best use the formula in this limit. From Theorem B6 and Lidski's theorem (Appendix C) it follows that we may expand the $\log\det(1-\ldots)$ expression (11) in powers,

$$E_C=-\int\frac{d\omega}{2\pi}\sum\frac{1}{m}\mathrm{Tr}(T_AG_0T_BG_0)^m. \tag{46}$$

In the dilute limit $\chi_\alpha<1$, so one may also substitute the expansion

$$T_\alpha=-\sum_{n=0}^{\infty}(-\omega^2\chi_\alpha G_0)^n\omega^2\chi_\alpha \tag{47}$$

in Eq. (46) and compute the involved integrals to desired order. This expansion is the continuous equivalent to summation of two body forces and is equal to the Born series appearing, for example, in Ref. 34.

VI. SCATTERING APPROACH

As remarked above, the operator $T_AG_0T_BG_0$ appearing in our formula is closely related to scattering data. The purpose of this section is to clarify this relation and make it more explicit. In order to keep better touch with conventions used in scattering theory, we usually avoid in the following sections using Wick rotation and thus we work in Lorentzian rather than Euclidean space with real rather than imaginary frequency and with the Feynman rather than the Euclidean propagator.

As mentioned above, the arguments of G_0 in Eq. (11) never coincide, implying that when $G_0(x_a,x_b)$ is considered as a function of x_b alone, it is a solution of the (homogeneous) free wave equation. Thus, one may expand $G_0(x_a,x_b)$ in the form $\Sigma\mathcal{C}_{\alpha\beta}\phi^*_\alpha(x_a)\phi_\beta(x_b)$, where $\{\phi_\alpha(x_a)\},\{\phi_\beta(x_b)\}$ are some sets of free wave solutions of energy ω. There is, of course, great freedom in choosing the sets $\{\phi_\alpha(x_a)\},\{\phi_\beta(x_b)\}$. In practice, one would choose these in a way that makes subsequent calculations easier. As mentioned earlier, we consider $T_AG_0T_BG_0$ as acting only on the volume of object A; therefore, these considerations also apply to the propagator on the right of this expression.

The Lippmann–Schwinger operator $T(\omega)$ is related to the S matrix by[36]

$$S=1-2\pi i\delta(\omega^2-\omega'^2)T_\omega. \tag{48}$$

Therefore, $T(\omega)$ has the property that its matrix element $\langle\alpha|T|\beta\rangle$ between a pair of free states α,β having energy ω is equal to the corresponding matrix element of the transition matrix. Since the operator T_B in $T_AG_0T_BG_0$ is sandwiched between a pair of free Feynman propagators corresponding to energy ω, we may identify it with the corresponding transition matrix. Due to the cyclicity of the determinant $\det(1-T_AG_0T_BG_0)$, the same is true of T_A.

Substituting the expansion $G_0(x_a,x_b)=\Sigma\mathcal{C}_{\alpha\beta}\phi^*_\alpha(x_a)\phi_\beta(x_b)$, we arrive at

$$T_AG_0T_BG_0=\sum_{\alpha\alpha'\beta\beta'}T_A|\alpha\rangle\mathcal{C}_{\alpha\beta}\langle\beta|T_B|\beta'\rangle\mathcal{C}_{\alpha'\beta'}\langle\alpha'|.$$

The Casimir interaction will then be given explicitly by

$$E=\int_0^\infty\frac{d\omega}{2\pi}\log\det[1-K(i\omega)]. \tag{49}$$

Here, $K_{\alpha''\alpha'}=(T_A)_{\alpha''\alpha}\mathcal{C}_{\alpha\beta}(T_B)_{\beta\beta'}\mathcal{C}_{\alpha'\beta'}$.

VII. PARTIAL WAVES EXPANSION

In the following section, we consider strategies of using representation (49) by restricting the K matrix to a finite subspace, which gives the dominant contribution to the force. Indeed, in many cases of interest, only a few partial waves are significantly scattered; the best example for this is when objects are far apart and from a large distance, they look pointlike. At this limit, one expects significant contribution only from s-wave scattering. In the more general case, K may be approximated by a finite dimensional matrix corresponding to several partial waves. In order to see how this works, in practice, we consider below a few simple cases.

A. One-dimensional systems

A particularly simple case occurs when the system is one dimensional. Consider, e.g., a scalar field in 1D. All states of energy ω are then spanned by two modes: left and right movers $|L\rangle,|R\rangle=\frac{1}{\sqrt{2\pi}}e^{\pm i\omega x}$. Hence, in this case, the determinant Eq. (11) can be easily evaluated. To see how this is done, we write the Feynman propagator explicitly as

$$G_0=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{e^{ikx}}{\omega^2-k^2+i0}=-\frac{i}{2\omega}e^{i\omega|x|}. \tag{50}$$

We consider a pair of scatterers A,B such that A is on the left of B. This immediately implies that we have $x_a<x_b$ and therefore

$$G_{0BA}(x_b,x_a)=-\frac{i}{2\omega}e^{i\omega(x_b-x_a)}=\frac{-2i\pi}{2\omega}|R\rangle\langle R|. \tag{51}$$

Similarly, we also have $G_{0AB}=\frac{-2i\pi}{2\omega}|L\rangle\langle L|$. Using this, we see that the operator K in Eq. (49) turns into the c-number,

$$K = \left(\frac{-2i\pi}{2\omega}\right)^2 \langle R|T_A|L\rangle\langle L|T_B|R\rangle = \tilde{r}_A(\omega) r_B(\omega). \quad (52)$$

Here, r_B ($\tilde{r}_A$) is the reflection coefficient for a wave hitting scatterer B from the left (A from the right) to be reflected back. Note that the normalization of T implied by Eq. (48) is responsible for the canceling of the factor $\frac{-2i\pi}{2\omega}$. (Had we used relativistic normalization for $|L,R\rangle$, the factor 2ω would not have appeared.) Thus, we conclude

$$\det(1 - T_A G_0 T_B G_0) = 1 - \tilde{r}_A(\omega) r_B(\omega).$$

The tilde on r_A serves to remind us that it is the reflection coefficient from the right side of A.

We remark that $\tilde{r}_A(\omega) r_B(\omega)$ implicitly depends on the distance between A,B through the (phase) dependence of r_A, r_B on the locations of the scatterers. To make this explicit, note that moving a scatterer a distance a affects the reflection coefficients as $r \to e^{-2ia\omega} r, \tilde{r} \to e^{2ia\omega}\tilde{r}$.

Moving the scatterers a distance a apart therefore results in

$$\det(1 - T_A G_0 T_B G_0) \to 1 - e^{2ia\omega}\tilde{r}_A(\omega) r_B(\omega).$$

Substituting in Eq. (49), we obtain the familiar formula for 1D Casimir interaction between scatterers.[22,23,37]

B. Multicomponent field in one dimension

The considerations used above for a single scalar field in one dimension extend to a situation where $\phi = (\phi_1, \phi_2, \ldots, \phi_n)$ is an n component field. In this case, the reflection coefficients $r_{A,B}$ turn into $n \times n$ matrices and one finds $\det(1 - T_A G_0 T_B G_0) = \det[1 - \tilde{r}_A(\omega) r_B(\omega)]$ where the determinant on the right is of a usual $n \times n$ matrix.

C. Plane wave expansion

In physical three dimensional space, there are many different possible ways to expand the propagator $G_0(x_a, x_b) = \Sigma C_{\alpha\beta}\phi^*_\alpha(x_a)\phi_\beta(x_b)$ in terms of free wave solutions $\{\phi_\alpha(x_a)\}$, $\{\phi_\beta(x_b)\}$. In Sec. VIII, we describe the expansion in spherical waves (which is probably the most useful expansion), and we demonstrate its use for calculating the Casimir force between compact object. However, for the sake of simplicity, we first describe here a plane wave expansion that is the immediate generalization of Eq. (51). A simple heuristic way to arrive at this generalization is to formally think of the field ϕ in three dimensions as one-dimensional field having infinitely many components labeled by its transverse momenta. Indeed, such point of view has been successfully used in describing transport in quasi-1D conductors in mesoscopic physics, whereby each transverse component corresponds to a scattering channel (see, for example, Ref. 38). This suggests splitting $\vec{k}$ into it's z-component k_z and its transverse components $k_\parallel = (k_x, k_y)$. The three-dimensional propagator may then be written as

$$G_0 = -\int \frac{d^2k_\parallel}{(2\pi)^2} \frac{ie^{i|z|k_z} e^{ik_\parallel x_\parallel}}{2k_z}\Bigg|_{k_z = \sqrt{\omega^2 - k_\parallel^2 + i0}}.$$

Here, $\sqrt{\omega^2 - k_\parallel^2 + i0}$ may be either real and positive (for $\omega^2 > k_\parallel^2$) or pure imaginary (for $\omega^2 < k_\parallel^2$) in which case the $i0$ prescription implies that it must be chosen on the positive imaginary axis. Assuming that A is located to the left of B along the z axis, it follows that

$$T_A G_0 T_B G_0 = \int \frac{dk_x dk_y dq_x dq_y}{(2\pi)^4} T_A|(q_x, q_y, -q_z)\rangle \frac{1}{2q_z}\langle(q_x, q_y, -q_z)| \times T_B|(k_x, k_y, k_z)\rangle \frac{1}{2k_z}\langle(k_x, k_y, k_z)|, \quad (53)$$

where $q_z = \sqrt{\omega^2 - q_x^2 - q_y^2 + i0}$ and $k_z = \sqrt{\omega^2 - k_x^2 - k_y^2 + i0}$.

When considering only the terms satisfying $\omega^2 > q_x^2 + q_y^2, k_x^2 + k_y^2$, Eq. (53) indeed looks like a straightforward generalization of the one-dimensional result. However, as this expression shows, to get the correct result, one must also include the contribution of evanescent waves ($q_\parallel^2 > \omega^2$). Upon Wick rotation, however, the distinction between ordinary and evanescent waves disappears. It may also be noted that (since in general $q_z \neq k_z$) the variation of the $\langle(q_x, q_y, -q_z)|T_B|(k_x, k_y, k_z)\rangle$ matrix elements upon moving B along the z axis is considerably more complicated than in the one-dimensional case.

The above representation may be helpful in problems where the scatterers A,B have exact or approximate planar geometry (e.g., corrugated plates). Although the theorem guaranteeing finite trace does not apply for infinite plates, one may show that dividing by the plate area leads to finite result. We remark that actual calculation of the determinant requires discretizing $k_\parallel$, which corresponds to assuming large but finite plates. Alternatively, one may use Eq. (46) with continuous $k_\parallel$.

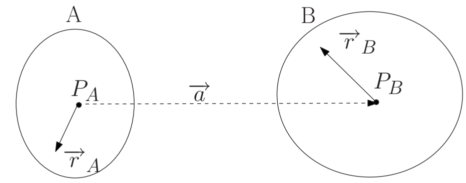

FIG. 2. Coordinate system used for the partial wave approach.

VIII. SPHERICAL WAVE EXPANSION

When describing interaction between two compact bodies, often it is convenient to represent the transition matrices T in a spherical wave basis. To do so, we choose two points P_A, P_B inside bodies A,B, respectively. We parametrize the points of body A by the radius vector $\vec{r} = r_A$ measured from the point P_A and the points of B by the radius vector $\vec{r}' = \vec{r}_B$ measured from the point P_B. The vector connecting P_A and P_B will be denoted by $\vec{a}$ (Fig. 2). In the scalar case, the free spherical waves centered at P_A, P_B are given by

$$|(lm)_{A,B}\rangle = \sqrt{\frac{2\omega^2}{\pi}} j_l(\omega r_{A,B}) Y_{lm}(\hat{r}_{A,B}), \quad (54)$$

with the normalization $\langle\omega' l' m' | \omega l m\rangle = \delta_{ll'}\delta_{mm'}\delta(\omega - \omega')$.

To use Eq. (49), the scalar three-dimensional Green's function $G_0 = -\frac{e^{i\omega r}}{4\pi r}$ is expanded in terms of the spherical harmonic functions centered around P_A and those centered around P_B.

$$G_\omega = \sum_{lm;l'm'} |(lm)_B\rangle \mathcal{C}_{lm;l'm'} \langle (l'm')_A|, \tag{55}$$

where (see Appendix A for a proof of the following equations)

$$\mathcal{C}_{lm;l'm'}(\omega) = -\frac{i\pi}{2\omega} \sum_{l'',m''} C\begin{pmatrix} l & l' & l'' \\ m & m' & m'' \end{pmatrix} \times i^{l''+l'-l} h_{l''}^{(1)}(\omega a) Y_{l''m''}(\hat{a}), \tag{56}$$

Y_{lm} are the spherical harmonics, j_l, h_l are the spherical Bessel and Hankel functions, and the coefficients

$$C\begin{pmatrix} l & l' & l'' \\ m & m' & m'' \end{pmatrix}$$

have known expressions in terms of the $3j$ symbol or as an integral of spherical functions,

$$C\begin{pmatrix} l & l' & l'' \\ m & m' & m'' \end{pmatrix} = 4\pi \int d\Omega Y_{lm} Y^*_{l'm'} Y^*_{l''m''} = (-1)^m \sqrt{4\pi(2l+1)(2l'+1)(2l''+1)} \times \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & l'' \\ m & -m' & -m'' \end{pmatrix}. \tag{57}$$

In actual computations, it is often more convenient to use the Wick-rotated expression. This may be expressed as $\mathcal{C}_{lm;l'm'}(i\omega) = -\frac{\pi}{2\omega} i^{l'-l} g_{lm;l'm'}$, where the coefficients,

$$g_{lm;l'm'} = \sum_{l'',m''} C\begin{pmatrix} l & l' & l'' \\ m & m' & m'' \end{pmatrix} \sqrt{\frac{2}{\pi\omega a}} K_{l''+1/2}(\omega a) Y_{l''m''}(\hat{a}), \tag{58}$$

are real. Here $K_{l''+1/2}$ is a modified Bessel function of the second kind. Equations (56) and (58) may be somewhat simplified by choosing the z axis along $\hat{a}$.

The above expansion of G_ω allows expressing $T_A G_0 T_B G_0$ in terms of matrix elements $\langle l'm'|T|lm\rangle$ of the transition matrices of the two scatterers. The Casimir interaction may then be written as in Eq. (49) where

$$K_{lm;l'm'} = (-1)^{l_1+l_2} (T_A)_{lm;l_1m_1} \mathcal{C}_{l_1m_1;l_2m_2} (T_B)_{l_2m_2;l_3m_3} \mathcal{C}_{l_3m_3;l'm'}. \tag{59}$$

Here, $\mathcal{C}_{lm;l'm'}$ are given by Eq. (56) or (58), summation over l_1, m_1, l_2, m_2, l_3, m_3 is implied, and we note that the extra sign resulted from $\mathcal{C}_{lm;l'm'}(-\hat{a}) \equiv (-1)^{l+l'} \mathcal{C}_{lm;l'm'}(\hat{a}) = \mathcal{C}_{l'm';lm}(\hat{a})$.

If we assume that only waves having $l \le l_0$ are significantly scattered, then K will turn into a finite $(l_0+1)^2 \times (l_0+1)^2$ matrix [since the dimension of the subspace $l \le l_0$ is $\Sigma_{l=0}^{l_0}(2l+1) = (l_0+1)^2$]. We stress that this argument *does not* require us to assume spherical symmetry of the scatterers.

When A, B are very far apart, the interaction between them is governed by waves of very low frequency and therefore also low l. At this limit, the leading contribution comes from the s-wave scattering transition matrix element $\langle l=0|T_{A,B}|l=0\rangle \simeq 2\omega^2 \lambda_{A,B}/\pi$, where λ is the scattering length.

The matrix K then reduces to the scalar $K = -\omega^2 \lambda_A \lambda_B [h_0^{(1)}(\omega a)]^2 = 4\pi \frac{\lambda_A \lambda_B}{a^2} e^{2ia\omega}$. Doing the integral of Eq. (49), one arrives at

$$E_C = -\frac{\lambda_A \lambda_B}{a^3}.$$

This limit corresponds to the scalar version of the well-known Casimir–Polder interaction. Our formalism, however, allows calculating corrections to it up to any desirable finite order in $\frac{1}{a}$. For example, for two Dirichlet spheres of radii R_1, R_2 at distance a between their centers, the expansion gives

$$E = -\frac{R_1R_2}{4\pi a^3} - \frac{R_1R_2(R_1+R_2)}{8\pi a^4} - \frac{R_1R_2(34R_1^2 + 9R_1R_2 + 34R_2^2)}{48\pi a^5} - \frac{R_1R_2(R_1+R_2)(2R_1^2 + 21R_1R_2 + 2R_2^2)}{36\pi a^6} + \cdots. \tag{60}$$

A. Spherical scatterers

Significant simplification is possible whenever A, B have spherical symmetry. First, the T matrices are diagonal in angular momentum basis and so may be expressed as

$$\langle l'm'|T_{A,B}|lm\rangle = \delta_{ll'} \delta_{mm'} \frac{2i\omega}{2\pi} (e^{2i\delta_l^{A,B}(\omega)} - 1),$$

where the normalization factor $\frac{2i\omega}{2\pi}$ follows from Eq. (48). A second consequence is that rotation around $\hat{a}$ (which from now on we take as coinciding with the $\hat{z}$ axis) is a symmetry of the whole system. The determinant therefore factors as a product of terms corresponding to different values of the azimuthal number m. The energy turns into a sum of the corresponding terms,

$$E = \sum_m \int \frac{d\omega}{2\pi} \log \det[1 - K^{(m)}(i\omega)].$$

The matrices $\{K_{ll'}^{(m)}\}_{ll'=|m|}^{\infty}$ defined for each $m \in \mathbb{Z}$ (actually $K^{(-m)} = K^{(m)}$) are infinite dimensional but may be approximated in numerical calculations by finite matrices corresponding to $l, l' \le$ some l_0. The operator $K^{(m)}$ may be written explicitly as

$$K_{ll'}^{(m)} = \sum_j g_{lj}^{(m)} t_j^{(A)} g_{jl'}^{(m)} t_{l'}^{(B)},$$

where we used the notation

$$t_j = \frac{1}{2}(-1)^j (e^{2i\delta_j} - 1),$$

$$g^{(m)}_{l_1,l_2}(i\omega) = (-1)^{m+1}\sqrt{(2l_1+1)(2l_2+1)}\sum_l (2l+1) \times \sqrt{\frac{2}{\pi a\omega}}K_{l+1/2}(a\omega)\begin{pmatrix} l_2 & l_1 & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & l_1 & l \\ m & -m & 0 \end{pmatrix}. \quad (61)$$

Note that both $g^{(m)}_{l_1,l_2}(i\omega)$ and $t_j(i\omega)$ are real.

B. Dirichlet spheres

The simplest example for which the above may be applied is the interaction of two hard (Dirichlet) spheres. The T-matrix elements are well known in this case and are given by $t_j(\omega)=(-1)^{j+1}\frac{j_j(\omega R)}{h_j^{(1)}(\omega R)}$, which translates to

$$t_j(i\omega) = \frac{\pi}{2}\frac{I_{j+1/2}(\omega R)}{K_{j+1/2}(\omega R)} \quad (62)$$

on the imaginary frequency line. (Here, R is the sphere's radius and $I_{j+1/2}$ is a modified Bessel function of the first kind.)

In the special case where the two spheres have equal radii $R_1=R_2$, an extra simplification occurs. One can then write $K=\tilde{K}^2, \tilde{K}_{ll'}=g_{ll'}t_{l'}$, which implies $\log\det(1-K)=\log\det(1+\tilde{K})+\log\det(1-\tilde{K})$. The numerical calculation of the two determinants $\det(1\pm\tilde{K})$ is then somewhat easier than direct calculation of $\det(1-K)$. Moreover, comparison to Sec. IV shows that the two determinants $\det(1\pm\tilde{K})$ [actually with $\tilde{K}_{ll'}=(-1)^m g_{ll'}t_{l'}$] correspond to the Casimir interaction energies $E_{D,N}$ of a single hard sphere and a Dirichlet/Neumann mirror at a distance $a/2$ away. The symmetric two hard sphere system then has the energy $E_S=E_D+E_N$. (One may also understand this in terms of decomposition into even and odd modes.)

We have done the calculation including partial waves of $l\leq l_0$ for different values of l_0 and considered the l_0 dependence of the results as a test for convergence. Most calculations included modes of up to $l_0=10$, but for small values of sphere separation a, we used larger l_0 even up to $l_0=72$ for $a/R=2.1$. Since we expected the error to behave roughly as $E_c-E(l_0)\sim O(e^{-cl_0})$, we tried to fit the results with this assumed asymptotics. The numbers suggest that both in the sphere-sphere and in the sphere-plate cases, we have $c\sim 2\log(1+d/R)$, where d is the distance between the two objects [i.e., $d=a-2R$ for E_S and $d=(a-2R)/2$ for E_D,E_N]. The table below shows the value of the constant c for identical spheres as a function of their distance as well as the value of l_0 at which the error dropped to within 1% of the exact result. It should be remarked that the estimate for c is a bit crude since our numerics is consistent with c being a slowly growing function of l_0 (which might be due to subleading asymptotics). By matching our results with the assumed asymptotics, one can obtain a corrected estimate for E_C. The comparison of this estimate with results obtained by increasing l_0 gave good agreement.

a/R	c	$L(1\%)$
2	0	∞
2.1	0.18	31
2.2	0.34	16
2.35	0.57	9
2.5	0.78	7
2.75	1.06	5
3	1.33	3 – 4
3.5	1.78	2 – 3
4	2.14	2
5	2.75	1
7	3.44	1

(63)

The following table and Fig. 3 show the results for the Casimir energy itself (measured in units of $\frac{\hbar c}{R}$). E_D denotes the energy of Dirichlet-mirror+(Dirichlet) sphere system, E_N denotes the energy of Neumann mirror+(Dirichlet) sphere system, and E_S denotes the energy of the symmetric two hard sphere configuration (having $E_S=E_D+E_N$). The result for E_D are in perfect agreement with a similar calculation done in Ref. 24.

a/R	E_D	E_N	E_S
2.1	−8.75	7.66	−1.0939
2.2	−2.2129	1.9382	−0.27477
2.35	−0.739	0.6488	−0.090 282
2.5	−0.3688	0.3245	−0.044 300
2.75	−0.1679	0.1483	−0.019 589
3	−0.09703	0.08613	−0.010 893
3.5	−0.044 981	0.040 303	−0.004 677
4	−0.026 197	0.023 676	−0.002 520
5	−0.012 304	0.011 285	−0.001 019
7	−0.004 777	0.004 472	−0.000 304
10	−0.001 998	0.001 904	−0.000 093
13	−0.001 102	0.001 061	−0.000 040
16	−0.000 700	0.000 679	−0.000 021

(64)

It may be remarked that E_D,E_N correspond to sphere-mirror distance, which is half the sphere-sphere distance in the corresponding calculation of E_S. This fact is responsible among other things to slower convergence in calculation of E_D,E_N and hence to a smaller number of calculated significant digits compared to E_S.

We would like to mention two points regarding the actual implementation of the numerical calculation. (Our earlier numerical attempts failed because we were not fully aware of these points.)

The expressions of $g_{ll'}(i\omega),t_l(i\omega)$ may attain at small ω's very large or small values, respectively, in such a way that only their product remains finite. At large ω's, similar phenomena occur with $t_l(i\omega)$ large and $g_{ll'}(i\omega)$ small. Thus, to avoid computer overflow, it is much better to "renormalize"

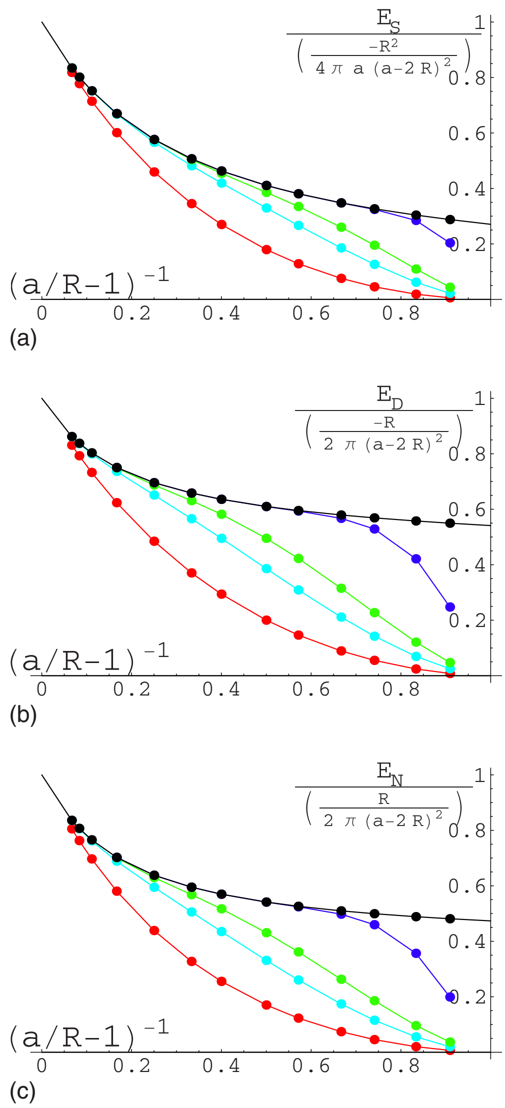

FIG. 3. (Color online) The calculated Casimir energy of the (a) two Dirichlet spheres of radius R at distance a between their centers. [(b) and (c)] A Dirichlet sphere of radius R whose center is at a distance $a/2$ from a Dirichlet/Neumann mirror. The graphs show E/E_0 as a function of $(a/R-1)^{-1}$, where E_0 is the large distance asymptotic expression of it. Specifically, (a) $E_0^S=-\frac{R^2}{4\pi(a-2R)^2 a}$ and [(b) and (c)] $E_0^{D,N}=\mp\frac{R}{2\pi(a-2R)^2}$. At short distances, E/E_0 approach the PFA prediction, (a) $\frac{\pi^4}{360}\sim 0.27$, (b) $\frac{\pi^4}{180}\sim 0.54$, and (c) $\frac{7\pi^4}{1440}\sim 0.47$. The black curve shows the calculated exact result for $l_0\to\infty$. We extrapolated it to $a=2R$ and $a=\infty$ using the known asymptotics. The colored graphs show how the computed energy increases as a result of including partial waves of $l\le l_0$ where $l_0=0$ (red), $l_0=1$ (sky blue), $l_0=2$ (green), and $l_0=10$ (blue).

these two quantities redefining $\tilde{g}_{ll'}=z_l z_{l'} g_{ll'}$, $\tilde{t}_l=t_l/z_l^2$, with $z_l\sim(R\omega)^{l+1/2}e^{R\omega}$.

A second important point is that one should make sure that the computer program doing the calculation does not use the expansion of $I_{l+1/2}(x)$ in terms of elementary functions.

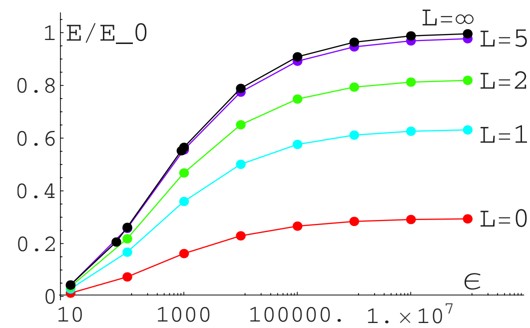

FIG. 4. (Color online) The calculated Casimir energy of two (scalar) Dielectric spheres of radii $R_2=2R_1$ at centers distance $a=4R_1$ depicted as a function of their dielectric constant $\epsilon_1=\epsilon_2$. The energy E was normalized by the Dirichlet spheres result E_0 so that at $\epsilon\to\infty$, we obtain $E/E_0=1$.

In MATHEMATICA (which we used), this expansion is an automatic default whenever the index of the Bessel function is half integer. However, this expansion is known to be numerically unstable (except for very small l) and using it would lead to errors.

The general formula works well for $R_1\neq R_2$. For example, taking $R_1=R_0$, $R_2=2R_0$ and measuring E in units of $\frac{\hbar c}{R_0}$, we found the interaction between a sphere of radius R_0 and a sphere of radius $2R_0$.

a/R_0	E
3.1	−1.4554
3.2	−0.367 535
3.3	−0.164 591
3.4	−0.093 105 7
3.5	−0.059 829 5
3.67	−0.033 452 5
3.83	−0.021 821
4	−0.015 015 11
5	−0.003 623 65
6	−0.001 519 659 48
8	−0.000 479 701 26
10	−0.000 215 369 763 16
14	−0.000 069 638 024 1
18	−0.000 031 036 935 06
22	−0.000 016 492 132 2

(65)

C. Dielectric spheres

The formula also works well for finite dielectric constant. For example, the numerical results for $R_1=R_0$; $R_2=2R_0$; $a=4R_0$ as a function of $\epsilon_1=\epsilon_2$ are given by the following table and Fig. 4.

$$\begin{array}{ll} \epsilon & E \\ \hline 64 & -0.003\,092 \\ 100 & -0.003\,927 \\ 900 & -0.008\,29 \\ 10^3 & -0.008\,483 \\ 10^4 & -0.011\,84 \\ 10^5 & -0.013\,64 \\ 10^6 & -0.014\,47 \\ 10^7 & -0.014\,83 \\ 10^8 & -0.014\,95 \\ \infty & -0.015\,015 \end{array} \qquad (66)$$

The calculation may easily be repeated for any given $R_1, R_2, \epsilon_1, \epsilon_2, a$.

IX. ELECTROMAGNETIC FIELD

To extend the ideas of Sec. VIII from the scalar to the EM case, one needs to present the EM propagator in a form analogous to Eqs. (55)–(57). The required representation of the EM propagator (derived in Appendix A) is

$$\overleftrightarrow{\mathcal{D}}_0 = |(jm\alpha)_B\rangle \mathcal{C}_{jm\alpha;j'm'\alpha'}\langle (j'm'\alpha')_A|, \qquad (67)$$

where α,α' can take the two values 0,1 corresponding to the TE (magnetic multipole) or TM (electric multipole) modes, respectively. The $\mathcal{C}$ coefficients are given by

$$\mathcal{C}_{jm\alpha;j'm'\alpha'} = -\frac{2i\pi^2}{\omega}\sum_{l''m''} i^{l''+j'-j+\alpha-\alpha'} h^{(1)}_{l''}(\omega a) Y_{l''m''}(\hat{a}) \times \int d\Omega Y^*_{l''m''}(\vec{Y}^{(\alpha)}_{jm}\cdot \vec{Y}^{(\alpha')*}_{j'm'}), \qquad (68)$$

where $\vec{Y}^{(\alpha)}_{jm}$ may be defined in terms of vectorial spherical harmonics as

$$\vec{Y}^{(0)}_{jm} = \vec{Y}_{jjm}, \qquad (69)$$

$$\vec{Y}^{(1)}_{jm} = \sqrt{\frac{j+1}{2j+1}}\vec{Y}_{j,j-1,m} + \sqrt{\frac{j}{2j+1}}\vec{Y}_{j,j+1,m}. \qquad (70)$$

These functions satisfy $i\vec{Y}^{(1)}_{jm}=\hat{r}\times\vec{Y}^{(0)}_{jm}, i\vec{Y}^{(0)}_{jm}=\hat{r}\times\vec{Y}^{(1)}_{jm}$.

After Wick rotating, we obtain $\mathcal{C}_{jm\alpha;j'm'\alpha'}(i\omega) = i^{j'-j+\alpha-\alpha'}\frac{\pi}{2\omega}g_{jm\alpha;j'm'\alpha'}$, where the coefficients

$$g_{jm\alpha;j'm'\alpha'}(i\omega) = \sqrt{\frac{32\pi}{\omega a}} \times \sum_{l''m''} K_{l''+1/2}(\omega a) Y_{l''m''}(\hat{a}) \times \int d\Omega Y_{l''m''}(\vec{Y}^{(\alpha)*}_{jm}\cdot\vec{Y}^{(\alpha')}_{j'm'}) \qquad (71)$$

are real.

The integrals $\int d\Omega Y_{j_3m_3}(\vec{Y}^{(\alpha)*}_{j_1m_1}\cdot\vec{Y}^{(\alpha')}_{j_2m_2})$ appearing in Eqs. (68) and (71) can be expressed explicitly in terms of $3j$ symbols as follows. For $\alpha=\alpha'$, it is given by

$$\frac{j_1(j_1+1)+j_2(j_2+1)-j_3(j_3+1)}{2\sqrt{j_1(j_1+1)j_2(j_2+1)}} \times \sqrt{\frac{(2j_1+1)(2j_2+1)(2j_3+1)}{4\pi}} \times \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & m_2 & m_3 \end{pmatrix}, \qquad (72)$$

which vanishes unless $j_1+j_2+j_3\equiv 0 \bmod 2$. For $\alpha\neq\alpha'$, the integral is nonzero only provided $j_1+j_2+j_3\equiv 1 \bmod 2$, in which case it is given by

$$(-1)^{m_1}\sqrt{\frac{(2j_1+1)(2j_2+1)(2j_3+1)}{4\pi}} \times \begin{pmatrix} j_1 & j_2 & j_3 \\ 1 & -1 & 0 \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & m_2 & m_3 \end{pmatrix}. \qquad (73)$$

Equation (72) may be derived from Eq. (57) by using the identity $\sqrt{j(j+1)}\vec{Y}^{(0)}_{jm}=\vec{L}Y_{jm}$ (where $\vec{L}$ is the angular momentum operator) and integration by parts. Relation (73) was found with the help of Eq. (18) of Ref. 39.

A. Spherical scatterers

Assuming spherically symmetric scatterers, one may define phase shifts $\delta^j_{\mathrm{TE}}(\omega), \delta^j_{\mathrm{TM}}(\omega)$ (by parity, these two channels do not mix). Similarly to the scalar case, we use the notation $t_{j\alpha}=\frac{1}{2}(-1)^{j+\alpha}(e^{2i\delta^{(\alpha)}_j(i\omega)}-1)$.

Choosing the z axis along $\hat{a}$, the operator $K=TGTG$ splits to independent blocks $K^{(m)}$ corresponding to the values of the azimuthal number m. In a given block, the g-matrix elements become

$$g^{(m)}_{j\alpha;j'\alpha'} = \sum_l \sqrt{\frac{8}{\omega a}(2l+1)}K_{l+1/2}(\omega a)\int d\Omega Y_{l,0}(\vec{Y}^{(\alpha)*}_{jm}\cdot\vec{Y}^{(\alpha')}_{j'm}). \qquad (74)$$

The matrix $K^{(m)}(i\omega)$ is then written explicitly as

$$K^{(m)}_{j\alpha;j''\alpha''}(i\omega) = t^{(A)}_{j\alpha}g^{(m)}_{j\alpha;j'\alpha'}t^{(B)}_{j'\alpha'}g^{(m)}_{j'\alpha';j''\alpha''}.$$

In the particular case of a perfectly conducting sphere of radius R, one has

$$t^j_{\mathrm{TE}}(i\omega) = \frac{\pi}{2}\frac{I_{j+1/2}(\omega R)}{K_{j+1/2}(\omega R)}, \qquad (75)$$

$$t^j_{\mathrm{TM}}(i\omega) = -\left.\frac{\pi}{2}\frac{\frac{d}{dx}[\sqrt{x}I_{j+1/2}(x)]}{\frac{d}{dx}[\sqrt{x}K_{j+1/2}(x)]}\right|_{x=\omega R}. \qquad (76)$$

Using this, we numerically calculated the electromagnetic Casimir energy for a pair of conducting spheres at distance a between their centers. As in the scalar case, writing $K=\tilde{K}^2$ and considering $\det(1\pm\tilde{K})$ separately allowed us to also find the interaction energies E_e, E_m of a sphere near a conducting

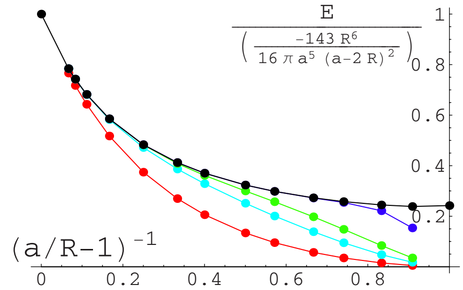

FIG. 5. (Color online) EM Casimir energy of two conducting spheres of radius R at distance a between their centers. The graphs show E/E_0 as a function of $(a/R-1)^{-1}$, where E_0 is the large distance asymptotic expression of it. $E_0^S=-\frac{143R^6}{16\pi(a-2R)^2a^5}$. The black curve shows the calculated exact result for $j_0\to\infty$. We extrapolated it to $a=2R$ and $a=\infty$ using the known asymptotics. The colored graphs show the result of including partial waves of $j\leq j_0$ where $j_0=1$ (red), $j_0=2$ (sky blue), $j_0=4$ (green), and $j_0=10$ (blue).

and/or infinitely permeable mirror placed $a/2$ from its center. The two sphere energy is then the sum $E_s=E_e+E_m$. Most of the calculations were done by including modes having $j\leq 10$; however, for the shortest distances $a=2.35,2.2,2.1$, where convergence is slower, we extended the retained modes up to $j=20,40,60$, respectively. The results are shown in the following table (written in units where $R=1$) and Fig. 5.

a	E_e	E_m	E_s
2.1	−16.15	14.5	−1.662
2.2	−3.82	3.48	−0.337 635
2.35	−1.157	1.073	-8.356×10^{-2}
2.5	−0.53	0.50	-3.18×10^{-2}
2.75	−0.211	0.201	-9.595×10^{-3}
3	−0.1074	0.1036	-3.787×10^{-3}
3.5	-3.97×10^{-2}	3.88×10^{-2}	-8.917×10^{-4}
4	-1.89×10^{-2}	1.86×10^{-2}	-2.864×10^{-4}
5	-6.24×10^{-3}	6.19×10^{-3}	-4.887×10^{-5}
7	-1.38×10^{-3}	1.37×10^{-3}	-3.965×10^{-6}
10	-3.06×10^{-4}	3.06×10^{-4}	-3.032×10^{-7}
13	-1.04×10^{-4}	1.04×10^{-4}	-4.703×10^{-8}
16	-4.47×10^{-5}	4.47×10^{-5}	-1.085×10^{-8}

(77)

The numerical results seem to converge as $j_0\to\infty$ at roughly an exponential rate. The following graph (Fig. 6) shows how the speed of convergence depends on the distance between the bodies. It is interesting to note that the results obtained in Sec. VIII for the scalar case give almost the same graph. Also, one can easily check that the results for E_s are basically the same as the ones obtained in Ref. 21, taking into account that we chose to normalize the energy in comparison to the large distance asymptotic expression for the energy.

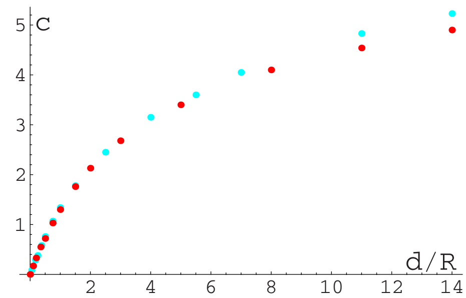

FIG. 6. (Color online) Including partial waves of $j\leq j_0$ results in error behaving roughly as e^{-cj_0}. The graph shows the constant c as a function of the separation distance d. The blue dots correspond to our results for two conducting spheres (where $d=a-2R$) and the red dots to conducting sphere + conducting plate (where $d=a/2-R$). At small distances, both cases give $c\sim1.7d/R$.

APPENDIX A: PROOF OF THE GREEN'S FUNCTION EXPANSIONS [EQS. (55) AND (67)]

1. Scalar case

Suppose $\vec{R}=\vec{a}+\vec{r}'$ then obviously $e^{i\vec{k}\cdot\vec{R}}=e^{i\vec{k}\cdot\vec{a}}e^{i\vec{k}\cdot\vec{r}'}$. Inserting the well-known expansion,

$$e^{i\vec{k}\cdot\vec{r}}=4\pi\sum i^lY_{lm}^*(\hat{k})Y_{lm}(\hat{r})j_l(kr),$$

we get

$$\sum i^lY_{lm}^*(\hat{k})Y_{lm}(\hat{R})j_l(kR)=4\pi\Big[\sum i^{l''}Y_{l''m''}^*(\hat{k})Y_{l''m''}(\hat{a})j_{l''}(ka)\Big]\times\Big[\sum i^{l'}Y_{l'm'}^*(\hat{k})Y_{l'm'}(\hat{r}')j_{l'}(kr')\Big].$$

Multiplying both sides by $Y_{lm}(\hat{k})$ and integrating $\int d\Omega_k$, we find

$$j_l(kR)Y_{lm}(\hat{R})=4\pi\sum_{l'm'l''m''}\left(\int d\Omega Y_{lm}Y_{l'm'}^*Y_{l''m''}^*\right)i^{l''+l'-l}\times j_{l''}(ka)Y_{l''m''}(\hat{a})j_{l'}(kr')Y_{l'm'}(\hat{r}'). \quad (A1)$$

Concentrating on the case $R,a>r'$, it makes sense to separate the ingoing and outgoing parts in the last equation. This amounts to replacing the Bessel functions $j_l(kR),j_l(ka)$ by Hankel functions $h_l(kR),h_l(ka)$ of the first or second type corresponding to outgoing or ingoing waves. Since this argument may seem as hand waving, we will return and elaborate on it more at the end of the proof. Equating the outgoing parts, we have

$$h_l^{(1)}(kR)Y_{lm}(\hat{R})=4\pi\sum_{l'm'l''m''}\left(\int d\Omega Y_{lm}Y_{l'm'}^*Y_{l''m''}^*\right)i^{l''+l'-l}\times h_{l''}^{(1)}(ka)Y_{l''m''}(\hat{a})j_{l'}(kr')Y_{l'm'}(\hat{r}'). \quad (A2)$$

It is well known that for $R>r$, the free propagator may be expanded as

$$-\frac{1}{4\pi}\frac{1}{|\vec{R}-\vec{r}|}e^{ik|\vec{R}-\vec{r}|}=-ik\sum j_l(kr)h_l^{(1)}(kR)Y_{lm}^*(\hat{r})Y_{lm}(\hat{R}).$$

Substituting here Eq. (A2), we finally get

$$G(\vec{r},\vec{a}+\vec{r}\,') = -4\pi i\omega \sum i^{l''+l'-l}\left(\int d\Omega Y_{lm}Y^*_{l'm'}Y^*_{l''m''}\right)j_l(\omega r) \times j_{l'}(\omega r')h^{(1)}_{l''}(\omega a)Y^*_{lm}(\hat{r})Y_{l'm'}(\hat{r}')Y_{l''m''}(\hat{a}), \tag{A3}$$

which is exactly Eq. (55).

Let us now return to the derivation of Eq. (A2) from Eq. (A1). We first note that the function $h^{(1)}_{l_0}(kR)Y_{l_0m_0}(\hat{R})$ with $\vec{R}=\vec{a}+\vec{r}$ being a solution of the free wave equation may be expanded around $\vec{r}=0$ in the form

$$h^{(1)}_{l_0}(kR)Y_{l_0m_0}(\hat{R}) = \sum [c^{(1)}_{lm}h^{(1)}_l(kr) + \tilde{c}^{(1)}_{lm}h^{(2)}_l(kr)]Y_{lm}(\hat{r})$$

for some ($\vec{a}$ dependent) constants $c^{(1)}_{lm},\tilde{c}^{(1)}_{lm}$. To be more precise, $h^{(1)}_{l_0}(kR)Y_{l_0m_0}(\hat{R})$ is a solution only for $\vec{r}\neq-\vec{a}$ (i.e., $\vec{R}\neq 0$); therefore, one has two separate expansions: one for $r<a$ and another for $r>a$. We concentrate on the latter.

Since $h^{(1)}_{l_0}(kR)Y_{l_0m_0}(\hat{R})$ is a purely outgoing wave, it is clear that the expansion in terms of $\vec{r}$ must also contain only outgoing waves, i.e., $\tilde{c}^{(1)}_{lm}\equiv 0$. This claim is based on "physical intuition." A more rigorous mathematical argument may be constructed by considering first pure imaginary $k=iq$, with $q>0$. One then notes that $h^{(1)}_{l_0}(iqR)$ is exponentially decreasing as $R\to\infty$ which imply that the same must hold for the right hand side. Since the Y_{lm}'s are linearly independent, this requires all the $\tilde{c}^{(1)}_{lm}$'s to vanish.

A similar expansion obviously exists also for $h^{(2)}$:

$$h^{(2)}_{l_0}(kR)Y_{l_0m_0}(\hat{R}) = \sum c^{(2)}_{lm}h^{(2)}_l(kr)Y_{lm}(\hat{r}).$$

Summing the two expansions, we have

$$j_{l_0}(kR)Y_{l_0m_0}(\hat{R}) \equiv \frac{1}{2}[h^{(1)}_{l_0}(kR)+h^{(2)}_{l_0}(kR)]Y_{l_0m_0}(\hat{R}) = \frac{1}{2}\sum [c^{(1)}_{lm}h^{(1)}_l(kr) + c^{(2)}_{lm}h^{(2)}_l(kr)]Y_{lm}(\hat{r}).$$

However, such an expansion is clearly unique. Therefore, it must be the same as the expansion in Eq. (A1). Comparing the two [and using $j_l\equiv\frac{1}{2}(h^{(1)}+h^{(2)})$], we deduce

$$c^{(1)}_{lm} = c^{(2)}_{lm} = 4\pi\sum_{l''m''} i^{l''+l-l_0}\left(\int d\Omega Y_{l_0m_0}Y^*_{lm}Y^*_{l''m''}\right) \times j_{l''}(ka)Y_{l''m''}(\hat{a}),$$

which proves Eq. (A2).

2. Electromagnetic case

To derive the EM expansion [Eq. (67)], we similarly start by using the identity

$$e^{i\vec{k}\cdot\vec{r}}\times\overleftrightarrow{\mathbf{1}} = 4\pi\sum i^l j_l(kr)\vec{Y}^*_{jlm}(\hat{k})\otimes\vec{Y}_{jlm}(\hat{r}). \tag{A4}$$

Repeating the same steps as for the scalar, we then find that

$$\overleftrightarrow{G}_0 = -\frac{e^{i\omega r}}{4\pi r}\times\overleftrightarrow{\mathbf{1}}$$

may be expanded as

$$\overleftrightarrow{G}_\omega = |(jlm)_B\rangle\mathcal{C}_{jlm;j'l'm'}\langle(j'l'm')_A|, \tag{A5}$$

where

$$|(jlm)_{A,B}\rangle = \sqrt{\frac{2\omega^2}{\pi}}j_l(\omega r_{A,B})\vec{Y}_{jlm}(\hat{r}_{A,B}) \tag{A6}$$

are the free vectorial spherical wave functions centered at P_A,P_B. The $\mathcal{C}$ coefficients may be written as

$$\mathcal{C}_{jlm;j'l'm'} = -\frac{i\pi}{2\omega}\sum_{l'',m''}\tilde{C}_{jj'}\begin{pmatrix} l & l' & l'' \\ m & m' & m''\end{pmatrix} \times i^{l''+l'-l}h^{(1)}_{l''}(\omega a)Y_{l''m''}(\hat{a}). \tag{A7}$$

Here, $\vec{Y}_{jlm}$ are the vectorial spherical harmonics, Y_{lm} are the usual scalar spherical harmonics, and j_l,h_l are the spherical Bessel and Hankel functions. The coefficients

$$\tilde{C}_{jj'}\begin{pmatrix} l & l' & l'' \\ m & m' & m''\end{pmatrix}$$

are found to be expressed as the following integral of spherical functions:

$$\tilde{C}_{jj'}\begin{pmatrix} l & l' & l'' \\ m & m' & m''\end{pmatrix} = 4\pi\int d\Omega(\vec{Y}_{jlm}\cdot\vec{Y}^*_{j'l'm'})Y^*_{l''m''}. \tag{A8}$$

The radiation gauge propagator $\mathcal{D}_0$ is given by the transverse part of $\overleftrightarrow{G}_0$. In Eq. (A6), each j,m correspond to three different spherical function $|jlm\rangle$ (having $l=j-1,j,j+1$). These may be decomposed in terms of the TE and TM modes and a nonphysical longitudinal mode.

$$|\mathrm{TE}\rangle = |jjm\rangle,$$

$$|\mathrm{TM}\rangle = \sqrt{\frac{j+1}{2j+1}}|j,j-1,m\rangle - \sqrt{\frac{j}{2j+1}}|j,j+1,m\rangle,$$

$$|L\rangle = \sqrt{\frac{j}{2j+1}}|j,j-1,m\rangle + \sqrt{\frac{j+1}{2j+1}}|j,j+1,m\rangle.$$

To obtain the required expansion of the radiation gauge propagator $\mathcal{D}_0$, we need to rewrite Eq. (A5) in terms of these three modes and drop the parts containing the longitudinal mode. This can be done quite straightforwardly leading to results (67)–(70).

APPENDIX B: ANALYTICAL PROPERTIES OF THE $T_AG_0T_BG_0$ OPERATOR

Having established the form [Eq. (11)] for the energy, we turn here to discuss the properties of this expression. The main aim of this appendix is to rigorously show that the object log $\det(1-T_A G_{0AB} T_B G_{0BA})$ is well defined and finite. The main mathematical notions and theorems, which we use here, are briefly reviewed in Appendix C.

As already remarked in Sec. I, it is well known that $\det(1-M)$ is well defined whenever M is a trace class (t.c.) operator (definition C4). We would like to show that for a large class of situations (including a pair of disjoint finite bodies A,B, separated by a finite distance), the operator $T_A G_{0AB} T_B G_{0BA}: H_A \to H_A$ is trace class in the continuum limit, and so prove that indeed expression (11) is finite and well defined.

Indeed, by theorem C5, the mere fact that $G_0(x,y)$ is a smooth function for $x \neq y$ is sufficient to guarantee that for any pair of compact volumes $A,B \in \mathbb{R}^3$ at finite mutual distance, the operator G_{0AB} is trace class. To deduce that $T_A G_{0AB} T_B G_{0BA}$ is trace class [and by similar argument also $1-G_0 \mathcal{J} T_A$ appearing in Eq. (43)], it is then enough (proposition C6) to make sure that $T_{A,B}(i\omega)$ are bounded (definition C2).

In the context of dielectric interaction, it is particularly easy to show that $T(i\omega)$ is bounded. In physical systems at equilibrium, it follows from causality properties of the dielectric function[34] that $\chi(i\omega,x) \geq 0$. We then have the following.

Lemma B1. For $\chi(i\omega,x) > 0$, the T operators are positive and bounded.

Proof: Since $G_0,\chi > 0$ (definition C3), one may write $T = \sqrt{\chi}\frac{\omega^2}{1+\omega^2\sqrt{\chi}G_0\sqrt{\chi}}\sqrt{\chi}$ from which it is seen that $T > 0$ and that in the operator norm $\|T\| \leq \omega^2 \|\chi\|$. ■

In fact, this also holds for nonlocal χ as long as $f(x) \mapsto \int_A \chi(i\omega,x,x') f(x') dx'$ is a bounded positive operator $H_A \to H_A$. In the context of more general type of interactions which may not be positive, one needs to use some assumption on the stability of the system to guarantee that $T(i\omega)$ is bounded. Here, we do not elaborate on this.

An alternative approach to proving the trace class property of $T_A G_{0AB} T_B G_{0BA}$ is based on the notion of a Hilbert–Schmidt operator (definition C7 also denoted HS). Here, the frequently used strategy in operator analysis is to use the following fact: if $U \in \mathrm{HS}$ and $V \in \mathrm{HS}$, then $UV \in$ t.c. The advantage of this approach is that it is very easy to check if an operator is Hilbert–Schmidt. Since the Hilbert–Schmidt norm is $\|A\|_{\mathrm{HS}}^2 = \mathrm{Tr}(A^\dagger A)$, one may evaluate it directly [e.g., by computing $\int |A(x,x')|^2$].

Theorem B2. For any two bodies A,B such that $\int_{A\times B} dxdy |G_0(x,y)|^2 < \infty$, $T_A G_{0AB} T_B G_{0BA}$ is trace class.

Proof: First, we show that $T_A G_{0AB}$ and $T_B G_{0BA}$ are Hilbert–Schmidt operators. This can be verified in the following way. We have just seen that T_A, T_B are bounded operators. Now, note that G_{0AB} is Hilbert–Schmidt, since

$$\|G_{0AB}\|_{\mathrm{HS}}^2 = \int_{A\times B} dxdy |G_{0AB}(x,y)|^2, \tag{B1}$$

which is finite under the condition above. Now, the inequality $\|T_A G_{0AB}\|_{\mathrm{HS}} \leq \|T_A\| \|G_{0AB}\|_{\mathrm{HS}}$ implies that $T_A G_{0AB}$ is Hilbert–Schmidt. Finally, using $U,V \in \mathrm{HS} \Rightarrow UV \in$ t.c., we see that $T_A G_{0AB} T_B G_{0BA} \in$ t.c. ■

Corollary B3. For any finite bodies A,B, such that distance$(A,B) > 0$, and any Green's function that is finite away from the diagonal, $T_A G_0 T_B G_0 \in$ t.c.

Example B4. For the scalar field discussed above, $G_0(x,y) = \frac{e^{-\omega|x-y|}}{4\pi|x-y|}$, the condition is satisfied. In the same way, it is satisfied for the electromagnetic field (one has to take into account also matrix indices, but these discrete indices do not change finiteness of the integrals).

Remark B5. The ω integration in Eq. (11) is convergent. To see this note that G_0 decays exponentially with ω therefore, $\|G_0\|_{\mathrm{HS}}$ decays exponentially, also the $\|T\|$'s do not grow more than quadratically in ω.

In the EM case, one may also worry due to the factor $\frac{1}{\omega^2}$ appearing in $\mathcal{D}_{0ij}(x,y) = (\delta_{i,j} - \frac{1}{\omega^2}\nabla_i^{(x)}\nabla_j^{(y)}) G_0(x,y)$ about convergence for $\omega \sim 0$. This factor, however, get cancelled since $\|T\| \leq \omega^2 \|\chi\|$, as shown in Lemma B1.

One may also show that G_{0AB} are t.c. themselves by using HS properties. The bodies are assumed not to touch, thus we can choose a C_0^∞ (compactly supported and infinitely smooth) function f_A, such that $P_A f_A = P_A$ and $P_B f_A = 0$, where P_A, P_B are the projections on $L^2(A), L^2(B)$ [i.e., $f_A(x) = 1$ for $x \in A$, and it then smoothly goes to 0, before reaching body B].

Writing

$$G_{0AB} = L_1 L_2,$$

$$L_1 = P_A \frac{1}{(p^2+\omega^2)^\alpha}, \quad L_2 = (p^2+\omega^2)^\alpha f_A G_0 P_B, \tag{B2}$$

we see that if $4\alpha > d$,

$$\|L_1\|_{\mathrm{HS}}^2 = \mathrm{Tr}\left(P_A \frac{1}{(p^2+\omega^2)^\alpha}\right)\left(P_A \frac{1}{(p^2+\omega^2)^\alpha}\right)^\dagger = \mathrm{Vol}(A) \int d^d p \left| \frac{1}{(p^2+\omega^2)^{2\alpha}} \right| < \infty \tag{B3}$$

and so L_1 is Hilbert–Schmidt. Next, we check that $L_2 \in \mathrm{HS}$. To see this last point, note that

$$\langle x | L_2 | x' \rangle = \langle x | (p^2+\omega^2)^\alpha f_A G_0 P_B | x' \rangle = (-\Delta_x + \omega^2)^\alpha f_A(x) G_0(x-x') P_B(x'). \tag{B4}$$

Since $G_0(x-x')$ is smooth away from $x=x'$, where the expression is anyway zero because $f_A P_B = 0$, and since $\langle x|L_2|x'\rangle$ has compact support (for integer α), we see that $\|L_2\|_{\mathrm{HS}}^2 = \int dxdx' |L_2|^2 < \infty$. Thus, G_{0AB} can be written as a product of two HS operators and as such is trace class.

Finally, we have that

Theorem B6. (Eigenvalues of *TGTG*). For $\chi > 0$, *all* eigenvalues λ of the (compact) operator $T_A G_{0AB} T_B G_{0BA}$ appearing in Eq. (11) satisfy $1 > \lambda \geq 0$.

Proof: We will repeatedly use that for bounded operators X,Y, the nonzero eigenvalues of XY and YX are the same. Note first that $G_0, \chi \geq 0$ (as operators) implies

$$\mathrm{spec}(\chi G_0) \setminus \{0\} = \mathrm{spec}(\sqrt{G_0}\chi\sqrt{G_0}) \setminus \{0\} \subset [0,\infty). \tag{B5}$$

Writing $T_\alpha G_0 = 1 - \frac{1}{1+\omega^2 \chi_\alpha G_0}$ as an operator on $L^2(\mathbb{R}^3)$, it is then clear that its spectrum lies in $[0,1)$. The same conclusion then applies to the operator $\sqrt{G_0} T_\alpha \sqrt{G_0}$, but since it is Hermitian, one concludes also $\|\sqrt{G_0}T_\alpha\sqrt{G_0}\|<1$ from which it follows $\|\sqrt{G_0}T_A G_0 T_B\sqrt{G_0}\|<1$ and hence $\lambda<1$. Similarly, $\sqrt{G_0}T_\alpha\sqrt{G_0}\geq 0$ imply $\lambda\geq 0$. ■

APPENDIX C: SOME PROPERTIES OF (INFINITE DIMENSIONAL) OPERATORS

Here, we recall some mathematical notions that we have used in describing the trace class properties of Eq. (11).

Definition C1. For an operator $B:H\to H$, the operator norm of $\|B\|$ is defined as $\|B\|=\sup_{\psi\in H,\psi\neq 0}\frac{|\langle\psi|B|\psi\rangle|}{\langle\psi|\psi\rangle}$.

Definition C2. An operator B is bounded if $\|B\|<\infty$.

Definition C3. An operator $A:H\to H$ is called a "positive operator" (denoted $A>0$) if $\langle\psi|A|\psi\rangle\geq 0$ for every $\psi\in H$.

This implies that A is Hermitian and its spectrum nonnegative. If $A:H\to H$ is a positive operator, then there exist a unique positive operator $B:H\to H$ satisfying $A=B^2$. B is called the "square root" of A and denoted $\sqrt{A}$.

Definition C4. An operator $A:H_1\to H_2$ is called trace class (and denoted $A\in$ t.c. or $A\in\mathcal{J}_1$) if $\Sigma\|A\psi_n\|<\infty$, where $\{\psi_n\}_{n=1}^{\infty}$ is some orthonormal basis of H_1. It can be shown that this condition does not depend on the choice of the orthonormal basis. (Note that the definition makes sense even when $H_1\neq H_2$.)

If $A:H\to H$ is trace class, then for any orthonormal basis $\{\psi_n\}_{n=1}^{\infty}$ of H, the sum $\Sigma\langle\psi_n|A|\psi_n\rangle$ converges to the same (finite) value which is denoted tr(A) and called the trace of A. One then also has $\mathrm{tr}(A)=\Sigma\lambda_n$, where $\{\lambda_n\}$ are the eigenvalues of A (Lidski's theorem).

If $A:H\to H$ is trace class, then the determinant $\det(1+A)$ may also be rigorously defined and one has $\det(1+A)=\Pi(1+\lambda_n)$.

The following theorem may be proved using the well-known fact that the Fourier coefficients of a smooth $K(x,y)$ decay faster than any power. (Note that these coefficients also serve as the matrix elements with respect to the Fourier basis of the operator defined by K.)

Theorem C5. Consider an operator $A:L^2(D_1)\to L^2(D_2)$, where D_1,D_2 are some domains in $\mathbb{R}^n$ which is given explicitly as an integral $A\psi(x)=\int_{D_1}K(x,y)\psi(y)dy$. A sufficient condition for A to be the trace class is that D_1,D_2 are compact and $K(x,y)$ is smooth in a neighborhood of $D_1\times D_2$.

Proposition C6. If A is trace class and B bounded, then AB and BA are also trace class and $\mathrm{Tr}(|AB|),\mathrm{Tr}(|BA|)\leq\|B\|\mathrm{Tr}(|A|)$.

Definition C7. M is a Hilbert–Schmidt operator (denoted $M\in$ HS or $M\in J_2$) if $\|M\|_{\mathrm{HS}}^2\equiv\mathrm{Tr}\,M^\dagger M<\infty$.

In particular, we mention that the product of the two Hilbert–Schmidt operators always gives a trace class operator.

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