Density-of-states calculations and multiple-scattering theory for photons

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The density of states for a finite or an infinite cluster of scatterers in the case of both electrons and photons can be represented in a general form as the sum over all Krein-Friedel contributions of individual scatterers and a contribution due to the presence of multiple scatterers. The latter is given by the sum over all periodic orbits between different scatterers. General three-dimensional multiple-scattering theory for electromagnetic waves in the presence of scatterers of arbitrary shape is presented. Vector structure constants are calculated and general rules for obtaining them from known scalar structure constants are given. The analog of the Korringa-Kohn-Rostocker equations for photons is explicitly written down.

I. INTRODUCTION

Multiple-scattering theory (MST) is a general method for calculating the spectrum of either ordered or disordered media and can deal with impurities as well.[1] It is also rather physical since all that is needed to calculate the spectrum in the presence of many identical scatterers is basically scattering data (phase shifts) from a single scatterer.[1] Moreover, the MST leads naturally to the Korringa-Kohn-Rostocker (KKR) equations.[2] There are at least two important reasons that motivate the generalization of three-dimensional MST and KKR to the case of electromagnetic waves. One of them is motivated by the search for a *photonic band gap* and related impurity problems in dielectric lattices.[3] Low-lying photonic bands have been calculated in two dimensions by some version of the KKR method,[4] plane-wave method,[5] and by the transfer matrix method.[6] In three dimensions they have been quite efficiently calculated by the plane-wave method and a large gap was shown to exist for the diamondlike lattice.[7] Recently, photonic band gaps have been predicted numerically to exist for a body-centered-cubic O_8 lattice of cholesteric blue phases characterized by tensor dielectric properties.[8] An approximative Kohn-Luttinger method for photons was given.[9] However, to calculate efficiently the density of states (DOS), the impurity spectrum, and decide about the existence of a gap even for the fcc lattice of dielectric spheres[10] one needs more sophisticated methods like KKR.[11] In the latter example the first gap has been suggested to appear between the eighth and the ninth band that is quite in contradiction with the electronic case. The second motivation for the three-dimensionsional MST and KKR is the *quantum chaos* since the KKR method and its variations are known to be numerically the most efficient method to quantize various classically ergodic systems such as quantum billiards.[12,13]

In the next section we start with the Lippmann-Schwinger integral equations and derive the three-dimensional MST for electromagnetic waves. We shall consider a nonconducting medium with the current and charge densities equal to zero. Only the simplest isotropic case is considered, $\mathbf{D}(\mathbf{r}) = \epsilon(\mathbf{r})\mathbf{E}(\mathbf{r})$ and $\mathbf{B}(\mathbf{r}) = \mu(\mathbf{r})\mathbf{H}(\mathbf{r})$ where $\mathbf{D}(\mathbf{r})$ $(\mathbf{B}(\mathbf{r}))$ is the electric (magnetic) induction. We shall confine ourselves to monochromatic waves to avoid the nonlocal time relation between $\mathbf{D}(\mathbf{r})$ and $\mathbf{E}(\mathbf{r})$, or $\mathbf{B}(\mathbf{r})$ and $\mathbf{H}(\mathbf{r})$. We shall also allow for complex permeabilities, i.e., for an absorption. In such medium the stationary macroscopic Maxwell equations are symmetric under[14]

$$\mathbf{E}(\mathbf{r}) \to \mathbf{H}(\mathbf{r}), \quad \mathbf{H}(\mathbf{r}) \to -\mathbf{E}(\mathbf{r}), \quad \epsilon(\mathbf{r}) \to \mu(\mathbf{r}). \quad (1)$$

We shall not fix the host permittivity $\epsilon_0 = 1$ in order to be also able to consider voids. For simplicity magnetic permeability $\mu(\mathbf{r})$ will be set to 1. Then the Maxwell equation for the electric intensity $\mathbf{E}$ can be written as

$$\boldsymbol{\nabla} \times [\boldsymbol{\nabla} \times \mathbf{E}(\mathbf{r})] - (\omega/c)^2 v(\mathbf{r})\mathbf{E}(\mathbf{r}) = (\omega/c)^2 \epsilon_0 \mathbf{E}(\mathbf{r}), \quad (2)$$

where $v(\mathbf{r}) = \epsilon(\mathbf{r}) - \epsilon_0$ is an analog of a potential. For notational simplicity we shall set $c = 1$ from now on. Scatterers are allowed to have arbitrary shape and to be arbitrarily arranged in a host homogeneous dielectric medium Ω with permittivity ϵ_0 up to the usual constraint of MST: it will always be assumed that Ω can be divided into nonoverlapping spheres $V_n^{'s}$ each of which contains one and only one scatterer. The number N of scatterers may be either *finite* or *infinite*. The generalization to general non-muffin-tin potentials (i.e., overlapping spheres) can be performed following Faulkner.[15]

In contrast to electrons, in the case of photons one can almost safely ignore photon-photon interaction and rather full control of the scattering potential $v(\mathbf{r}) = \epsilon(\mathbf{r}) - \epsilon_0$ can be achieved in experiment. As a result the single photon approximation, the photonic band structure, as well as the standard assumptions of the MST turn out to be exact. Therefore, experiments on photons on well-controlled samples are appealing for both, testifying the basic ideas about the semiclassical quantization[16] and to provide the check on the MST itself. The KKR equations

and structure constants are explicitly written down. A relation with the standard electronic structure constants is maintained as much as possible. General rules are formulated as to how the photonic structure constants can be obtained from the electronic ones.

In Sec. III the operator content of the MST is discussed in more detail and the connection with the standard calculations within the context of the Schrödinger Hamiltonian is made. Finally, in Sec. IV methods are presented for the calculation of the density of states (DOS) for an ensemble of scatterers. The results are applicable for both electrons and photons. A more detailed analysis of the Lloyd and Smith on-the-energy-shell formalism[1] from the point of view of the Gutzwiller trace formula[16] is made. Surprisingly enough it is found that similar to the latter case, the DOS can be calculated by summing over all periodic orbits in the "phase space." One speaks about the phase space here in a symbolic sense which arises as the consequence of the on-the-energy-shell formalism. The "periodic orbits," which start and end with the same coordinate, angular momentum, and multipole indices, are made from all possible connections (random walks) between the centers of different scatterers with a possible return.

The Krein-Friedel formula[1,17] is discussed, too. Recently we have shown that when it is supplemented with ζ-function regularization it can be used for some infinite range potentials in the *singular* scattering problem like the Aharonov-Bohm one.[18] Here we shall show that it can be used for the Maxwell equations as well.

II. MULTIPLE-SCATTERING THEORY AND THE KKR EQUATIONS FOR PHOTONS

The Maxwell equation (2) for $\mathbf{E}$ quite resembles the Schrödinger equation.[3] However, the behavior of $\mathbf{E}$ across a discontinuity Σ of ϵ is essentially different. Instead of the continuity of fields and their derivatives one has a discontinuity of $E_n(\mathbf{r})$, the normal component of $\mathbf{E}$, and the continuity of $E_t(\mathbf{r})$, the tangential component of $\mathbf{E}(\mathbf{r})$, on Σ,[14]

$$E_n^+ - E_n^- = \frac{\epsilon_- - \epsilon_+}{\epsilon_+} E_n^- = \frac{v(\mathbf{r})}{\epsilon_0} E_n^-, \qquad E_t^+ = E_t^-. \quad (3)$$

The derivative $\nabla_t E_t$ is continuous, $\partial_n \mathbf{E}_t$ and $\nabla_t E_n$ are discontinuous,[19]

$$(\partial_n \mathbf{E}_t^+ - \partial_n \mathbf{E}_t^-)|_\Sigma = \left(\frac{1}{\epsilon_+} - \frac{1}{\epsilon_-}\right) \nabla_t D_n = \frac{v}{\epsilon_0} \nabla_t E_n^- = (\nabla_t E_n^+ - \nabla_t E_n^-)|_\Sigma, \quad (4)$$

while $\partial_n \mathbf{E}_n(\mathbf{r})$ obeys[19]

$$(\partial_n E_n^+ - \partial_n E_n^-)\big|_\Sigma = -\left(\frac{1}{\epsilon_+^2}(\partial_n \epsilon)_+ - \frac{1}{\epsilon_-^2}(\partial_n \epsilon)_-\right) D_n. \quad (5)$$

Thus, although the normal component $E_n(\mathbf{r})$ of $\mathbf{E}(\mathbf{r})$ is discontinuous, the side limits of $\partial_n E_n(\mathbf{r})$ coincide provided the side limits of the derivatives of $\epsilon(\mathbf{r})$ at Σ are zero, as is the case of the muffin-tin (piecewise constant) potential. The above relation have been shown to be a general consequence of the (nonstationary) Maxwell equations in a dielectric.[19]

That, generically discontinuous behavior of $\mathbf{E}$ and its derivatives, necessitates the introduction of the concept of *outward* and *inward* integral equations.[19] One has to distinguish strictly between them. The inward formalism is basically that of Kohn-Korringa-Rostocker (KKR) (Ref. 2) while the outward formalism is originally due to Morse.[20] In the case of the Schrödinger equation both formalisms coincide.

One way to derive the MST is to use *outward* integral equations under the presence of an incident wave $\mathbf{E}_0(\mathbf{r})$. To keep track with the standard derivation[1] one starts with the Lippmann-Schwinger equation for $\mathbf{E}(\mathbf{r})$,[19]

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) - \omega^2 \sum_n \left\{ \int_{V_n} G_\sigma(\mathbf{r},\mathbf{r}')\, v(\mathbf{r}')\, \mathbf{E}(\mathbf{r}')\, d^3\mathbf{r}' - \int_{V_{n+}} [\nabla' G_\sigma(\mathbf{r},\mathbf{r}')][\nabla' \cdot \mathbf{E}(\mathbf{r}')]\, d^3\mathbf{r}' \right\}, \quad (6)$$

with n labeling scatterers. V_{n+} is a shorthand for the outward limit through measurable sets Σ_ℓ, $\Omega \supset \Sigma_\ell \supset V_n$, $\lim_{\ell\to\infty} \Sigma_\ell \searrow V_n$. Here $G_\sigma(\mathbf{r},\mathbf{r}')$ is the Green function of the Helmholtz equation,

$$(\nabla^2 + \sigma^2) G_\sigma(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \quad (7)$$

σ^2 being $\sigma^2 = \omega^2 \epsilon_0$, and ω is a given frequency of a photon. $G_\sigma(\mathbf{r},\mathbf{r}')$ will be chosen to satisfy the scattering conditions,

$$G_\sigma(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi} \frac{e^{i\sigma|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}. \quad (8)$$

Equation (6) is essentially the same (up to an integration per parts) as Eq. (4) in Ref. 21 written in terms of the tensorial Green function $\mathbf{d}_0(\mathbf{r},\mathbf{r}')$,

$$\mathbf{d}_0(\mathbf{r},\mathbf{r}') = -\left[\omega^2 \mathbf{1} + \frac{1}{\epsilon_0} \nabla \otimes \nabla\right] G_\sigma(\mathbf{r},\mathbf{r}'), \quad (9)$$

where $\mathbf{1}$ and $\nabla \otimes \nabla$ are, respectively, 3×3 identity and $(\partial_i \partial_j)$ matrices. When the volume integrals are rewritten in terms of the surface integrals and provided $\mathbf{r}$ stays inside the spheres one finds[19]

$$\mathbf{E}_0(\mathbf{r}) = \sum_n \oint_{\partial V_{n+}} dS' [\partial_{r'} G_\sigma(\mathbf{r},\mathbf{r}') - G_\sigma(\mathbf{r},\mathbf{r}')\, \partial_{r'}] \mathbf{E}(\mathbf{r}'), \quad (10)$$

which is nothing but the on-shell Lippmann-Schwinger equation (see also Sec. III). It is probably here when we differ from Ref. 21. It is, however, difficult to say definitely since, in Ref. 21, they do not indicate on which side of the boundary their surface integrals are.

The basic idea of MST (and the KKR method as well) is to rewrite the integral equation into an *algebraic* one. This is accomplished by expanding the Green function and electric field in the basis of spherical harmonics. To make the integration in (10) well defined we have to

choose some $\mathbf{r}$ and divide Ω into regions where, respectively, $r > r'$ or $r < r'$. The reason is that the expansion of the Green function $G_\sigma(\mathbf{r},\mathbf{r}')$ into spherical harmonics does depend as to whether $r < r'$ or $r > r'$,

$$G_\sigma(\mathbf{r},\mathbf{r}') = -i\sigma \sum_L [h_l^+(\sigma r) j_l(\sigma r')\Theta(r-r') + j_l(\sigma r) h_l^+(\sigma r')\Theta(r'-r)] \times Y_L(\theta,\phi) Y_L^*(\theta',\phi'). \quad (11)$$

Here $\Theta(x)$ is the usual Heaviside step function, L is actually multi-index $L = lm$, and j_l and $h_l^+ = j_l + in_l$ are, respectively, the spherical Bessel and the spherical Hankel function, n_l being the spherical Neumann function.[1,22] Since

$$\sum_{m=-l}^{l} Y_L(\theta,\phi) Y_L^*(\theta',\phi') = \sum_{m=-l}^{l} Y_L^*(\theta,\phi) Y_L(\theta',\phi') \quad (12)$$

the arguments of spherical harmonics can be interchanged in Eq. (11). In what follows we shall denote by $\mathbf{R}_n$ the center of the nth sphere V_n, and by r_n its radius. Without any restriction $\mathbf{r}$ can be assumed to be such that $\forall n \neq 0$: $|\mathbf{r}-\mathbf{R}_0| < r_0 < |\mathbf{r}-\mathbf{R}_n|$. Due to translational invariance of the free Green function (8) $\mathbf{R}_0$ can be set to origin. Therefore, on the surface of all spheres the expansion (11) with $r' > r$ will be used in (10).

The use of the Lippmann-Schwinger equation requires that the incident wave be *singularity free* in the whole space.[1,23] Therefore, $\mathbf{E}_0(\mathbf{r})$ is assumed to have an expansion of the form

$$|\mathbf{E}_0(\mathbf{r})\rangle = \sum_{AL} C_{0AL}^0 |\mathbf{J}_{AL}(\mathbf{r})\rangle, \quad (13)$$

with C_{0AL}^0 expansion constants and the parameter A labeling electric and magnetic multipoles,

$$|\mathbf{J}_{ML}(\mathbf{r})\rangle = j_l(\sigma r)|\mathbf{Y}_L^{(m)}\rangle, \quad (14)$$

$$|\mathbf{J}_{EL}(\mathbf{r})\rangle = \frac{i}{(2l+1)\sqrt{\epsilon_0}} \left\{ j_{l-1}(\sigma r) \left[\sqrt{l(l+1)}|\mathbf{Y}_L^{(o)}\rangle + (l+1)|\mathbf{Y}_L^{(e)}\rangle \right] + j_{l+1}(\sigma r) \left[\sqrt{l(l+1)}|\mathbf{Y}_L^{(o)}\rangle - l|\mathbf{Y}_L^{(e)}\rangle \right] \right\}. \quad (15)$$

Here $|\mathbf{Y}_L^{(a)}\rangle$ are normalized *magnetic* ($a = m$), *electric* ($a = e$), and *longitudinal* ($a = o$) vector spherical harmonics (see Appendix A). Note that there are neither magnetic nor electric multipoles for $l = 0$. The above form of the electric multipole is "canonical" one since in the case of constant $\epsilon(r)$ and $\mu(r)$ the Maxwell equations determine a relation between scalars $\mathbf{r}\cdot\mathbf{H}$ and $\mathbf{L}\cdot\mathbf{E}$, and $\mathbf{r}\cdot\mathbf{E}$ and $\mathbf{L}\cdot\mathbf{H}$,[22],

$$\mathbf{r}\cdot\mathbf{H} = \frac{1}{\omega\mu}\mathbf{L}\cdot\mathbf{E}, \qquad \mathbf{r}\cdot\mathbf{E} = -\frac{1}{\omega\epsilon}\mathbf{L}\cdot\mathbf{H}. \quad (16)$$

where $\mathbf{L} = -i(\mathbf{r}\times\nabla)$ is the orbital angular momentum operator. In what follows, however, the factor $\sqrt{\epsilon_0}$ in (15) will be rescaled for it will simplify the resulting formulas.

Now, $|\mathbf{E}(\mathbf{r})\rangle$ is expanded near a scatterer centered at $\mathbf{R}_0$ in the basis of final states $|\mathbf{F}_{AL}(\mathbf{r})\rangle$,

$$|\mathbf{E}(\mathbf{r})\rangle = \sum_{AL} C_{0AL} |\mathbf{F}_{AL}(\mathbf{r})\rangle. \quad (17)$$

Due to (10) one needs to expand $|\mathbf{E}(\mathbf{r})\rangle$ only for $\mathbf{r}$ on the boundaries of spheres. For a given nth sphere one has

$$|\mathbf{E}(\mathbf{r})\rangle = \sum_{AL} C_{nAL} |\mathbf{F}_{nAL}(\mathbf{r}-\mathbf{R}_n)\rangle, \quad (18)$$

where

$$|\mathbf{F}_{nAL}(\mathbf{r})\rangle = |\mathbf{J}_{nAL}(\mathbf{r})\rangle - \oint_{\partial V_{n+}} dS' [\partial_{r'} G_\sigma(\mathbf{r},\mathbf{r}') - G_\sigma(\mathbf{r},\mathbf{r}')\,\partial_{r'}] |\mathbf{F}_{nAL}(\mathbf{r}')\rangle. \quad (19)$$

On the outward side of the scatterer then

$$|\mathbf{F}_{nAL}(\mathbf{r})\rangle = |\mathbf{J}_{AL}(\mathbf{r}_n)\rangle - i \sum_{A'L'} t_{A'L',AL}^n |\mathbf{H}_{A'L'}^+(\mathbf{r}_n)\rangle, \quad (20)$$

where $t_{A'L',AL}^n$ is the transition or t matrix of the nth scatterer,[1] and $\mathbf{r}_n = \mathbf{r} - \mathbf{R}_n$ is the radius vector on the boundary of the sphere V_n.

To find a more convenient expansion of $G_\sigma(\mathbf{r},\mathbf{r}')$ on the boundary of a given nth sphere, $n \neq 0$, one can use the expansion of the (scalar) *scattered* wave from the scatterer centered at $\mathbf{R}_0 = 0$ into an *incident* wave about the scatterer centered at $\mathbf{R}_n$,

$$h_l^+(\sigma r) Y_L^*(\mathbf{r}) = \sum_{L''} j_{l''}(\sigma|\mathbf{r}-\mathbf{R}_n|) \times Y_{L''}^*(\mathbf{r}-\mathbf{R}_n)\, g_{L''L}(\mathbf{R}_n), \quad (21)$$

with $g_{L''L}(\mathbf{R}_n)$ being the scalar structure constant[1] the very same as in the case of electrons.

They are given by

$$g_{L'L}(\mathbf{R}) = -(-1)^{l'} i^{l+l'+1} 4\pi\sigma \times \sum_{L_1} C_{L'L}^{L_1} (-i)^{l_1} h_{l_1}^+(\sigma R) Y_{L_1}^*(\mathbf{R}). \quad (22)$$

The numerical constants $C_{LL'}^{L_1}$ here are the *Gaunt numbers*.[1] For a given pair of $\mathbf{r}$ and $\mathbf{r}'$ such that $|\mathbf{r}-\mathbf{R}_0| < |\mathbf{r}-\mathbf{R}_j|$ $\forall j \neq 0$ and $|\mathbf{r}'-\mathbf{R}_1| < |\mathbf{r}'-\mathbf{R}_j|$ $\forall j \neq 1$, the expansion (11) of the Green function $G_\sigma(\mathbf{r},\mathbf{r}')$ can be rewritten as follows:

$$G_\sigma(\mathbf{r},\mathbf{r}') = \sum_{L,L'} g_{L'L}(\mathbf{R}_1-\mathbf{R}_0) j_l(\sigma r) \times Y_L(\mathbf{r}) j_{l'}(\sigma|\mathbf{r}'-\mathbf{R}_1|) Y_{L'}^*(\mathbf{r}'-\mathbf{R}_1). \quad (23)$$

Now (13), (17), (23), and $dS' = r_n^2 d\Omega$, r_n being the radius of the nth sphere, are inserted in (10). After some manipulations one finds

$$\sum_{AL} C^0_{0AL}|\mathbf{J}_{AL}(\mathbf{r})\rangle = i\sigma \sum_{ALL'} j_l(\sigma r) Y_L\, r_0^2\, \langle Y_L|W[h_l^+, \mathbf{F}_{oAL'}]\rangle_0\, C_{0AL'} + i\sigma \sum_{n\neq 0, ALL'L''} j_l(\sigma r) Y_L\, r_n^2\, \langle Y_{L''}|W[j_{l''}, \mathbf{F}_{nAL'}]\rangle_n\, g_{L''L}(\mathbf{R}_n)\, C_{nAL'}. \quad (24)$$

Where $\langle|\,.\,|\rangle_n$ denotes integration over angle variables on the nth sphere, and index n means that the value of spherical functions is taken at r_n. $W(u,w)$ is the Wronskian,

$$W(u,w) = (u\,\partial_r - \partial_r u)\,w = u\,\partial_r w - \partial_r u\, w. \quad (25)$$

By taking the scalar product, after approaching r_0 by r from below, and by using identities from Appendix B one can rewrite (24) as

$$C^0_{0AL} N^l_A = \sum_{jBKA'L'} [\delta_{oj}\delta_{AA'}\delta_{LL'} N^l_A - \bar{G}^{oj}_{AL,BK} t^j_{BK,A'L'}] C_{jA'L'}, \quad (26)$$

where

$$N^l_A = \begin{cases} j_l^2(\sigma r_0), & A = M \\ \frac{1}{(2l+1)}\left[(l+1)j^2_{l-1}(\sigma r_0) + l j^2_{l+1}(\sigma r_0)\right], & A = E. \end{cases} \quad (27)$$

Here, the quantity $\bar{G}^{ij}_{AL,BK}$ has been introduced,

$$\bar{G}^{ij}_{AL,BK} = \bar{G}_{AL,BK}(\mathbf{R}_j - \mathbf{R}_i) = i\sigma r_j^2 \sum_{L'}\sum_{L''} j_{l'}(\sigma r_i) \times \langle \mathbf{J}_{AL}|Y_{L'}\rangle_i \cdot \langle Y_{L''}|W[j_{l''}, \mathbf{H}^+_{BK}]\rangle_j \times g_{L''L'}(\mathbf{R}_j - \mathbf{R}_i). \quad (28)$$

To calculate $\bar{G}^{ij}_{AL,A'L'}$ explicitly we shall use the basic MST identities collected in Appendix B. By defining quantities $\bar{C}^\alpha$ in terms of $3j$ symbols,

$$\bar{C}^\alpha(l,-1,m) = \sqrt{l+1}\, C^\alpha(l-1, m+\alpha, l, m),$$
$$\bar{C}^\alpha(l,1,m) = -\sqrt{l}\, C^\alpha(l+1, m+\alpha, l, m), \quad (29)$$

and

$$\bar{T}^\alpha_{lm} = \frac{1}{\sqrt{l(l+1)}} T^\alpha_{lm} \quad (30)$$

one can write the resulting expressions in the following compact form:

$$\bar{G}^{ij}_{ML,ML'} = j_l^2(\sigma r_i) \sum_{\alpha=-1}^{1} g^{ij}_{l'm'+\alpha;lm+\alpha}\, \bar{T}^\alpha_{l'm'}\, \bar{T}^\alpha_{lm},$$

$$\bar{G}^{ij}_{ML,EL'} = j_l^2(\sigma r_i) \sum_{\substack{p'=-1\\ p'\neq 0}}^{1} \sum_{\alpha=-1}^{1} g^{ij}_{l'+p',m'+\alpha,lm+\alpha} \bar{C}^\alpha(l',p',m')\, \bar{T}^\alpha_{lm},$$

$$\bar{G}^{ij}_{EL,ML'} = \sum_{\substack{p=-1\\ p\neq 0}}^{1} j^2_{l+p}(\sigma r_i) \sum_{\alpha=-1}^{1} g^{ij}_{l',m'+\alpha,l+p,m+\alpha} \bar{T}^\alpha_{l'm'}\, \bar{C}^\alpha(l,p,m),$$

$$\bar{G}^{ij}_{EL,EL'} = \sum_{\substack{p=-1\\ p\neq 0}}^{1} j^2_{l+p}(\sigma r_i) \sum_{\substack{p'=-1\\ p'\neq 0}}^{1} \sum_{\alpha=-1}^{1} g^{ij}_{l'+p',m'+\alpha,l+p,m+\alpha} \bar{C}^\alpha(l',p',m')\, \bar{C}^\alpha(l,p,m). \quad (31)$$

The quantity $\bar{G}^{ij}_{AL,BK}$ is not yet the vector structure constant $G^{ij}_{AL,BK}$ we are looking for. It depends on the muffin-tin radius r_i that enters the argument of Bessel functions. However, one sees immediately, by comparing (26) and (27) with (31), that N^l_M can be rescaled. To rescale N^l_E is more tricky. By using the relations 10.1.19, 10.1.21, 10.1.22 of Ref. 24 one can show that

$$N^l_E(z) = \left(\frac{j_l(z)}{z} + \sigma j_l'(z)\right)^2 + l(l+1)\frac{j_l^2(z)}{z^2}, \quad (32)$$

$$j^2_{l-1}(z) = N^l_E(z) + l\,\frac{j_l(z)}{z}\left(\frac{j_l(z)}{z} + 2\sigma j_l'(z)\right), \quad (33)$$

$$j^2_{l+1}(z) = N^l_E(z) - (l+1)\frac{j_l(z)}{z}\left(\frac{j_l(z)}{z} + 2\sigma j_l'(z)\right), \quad (34)$$

where $z = \sigma r_0$, and prime means the derivative with respect to r. According to (32) $N^l_E(z)$ is the sum of two non-negative terms. By using the relation 9.5.2 of Ref. 24 about the interlace of zeros of j_l and j_l' one can show that, provided $z \neq 0$, always $N^l_E > 0$. Indeed, if the

first term is zero then the second is nonzero and vice versa. The latter two equations give the expression of the relevant Bessel functions that enter (31) in terms of N_E^l. When columns of $\bar{G}^{ij}_{AL,BK}$ with E labels are divided by N_E^l one has to show that the contributions of the second terms in (33) and (34) cancel. By close inspection one finds that they introduce, respectively, the factor l and $-(l+1)$ to (31). By using the definition (22) of the scalar structure constant $g_{L'L}(\mathbf{R})$ and the properties of $3j$ symbols one finds that the contributions indeed cancel. The rescaled structure constants will be written without bar. Physically $G^{ij}_{AL,A'L'}$ describes what amount of a particular multipole field scattered from the ith site contributes to the particular multipole field incident on the jth site. Relations (31) imply the following rules for obtaining $G^{ij}_{AL,A'L'}$ from scalar $g^{ij}_{L'L}{}'^s$:

(1) If $A = M$ then replace L in $g^{ij}_{L'L}$ by $L = l, m+\alpha$ and multiply $g^{ij}_{L'L}$ by $\bar{T}^{\alpha}_{lm+\alpha}$. If $A' = M$ do the same with primed indices.

(2) If $A = E$ then replace L in $g^{ij}_{L'L}$ by $L = l+p, m+\alpha$ and multiply $g^{ij}_{L'L}$ by $\bar{C}^{\alpha}(l,p,m+\alpha)$. If $A' = E$ do the same with primed indices.

(3) Take the sum over $\alpha = -1, 0, 1$, and (if any) over $p, p' = -1, 1$.

The basic photonic MST equations (24) are written then as follows:

$$C^0_{iAL} = \sum_{jA'L'} \Big[\delta_{ij}\delta_{LL'}\delta_{AA'} - \sum_{A''L''} G^{ij}_{AL,A''L''} t^j_{A''L'',A'L'} \Big] C_{jA'L'}. \quad (35)$$

According to the construction G^{ij} the sum over j runs here over all $j \neq i$. Note that $G^{ij}_{AL,A'L'}$ is not Hermitian. This is a consequence of using the t matrix which also is not Hermitian.[1,2] For spherically symmetric scatterers the t matrix is diagonal and for homogeneous spheres it is explicitly known as the Mie solution.[23]

Provided scatterers are identical and arranged in a periodic way one can take the Fourier transform with regard to the Bloch momentum $\mathbf{k}$. The condition of the existence of a solution to (35) for $C^0_{iAL} = 0$,

$$\det \left| \delta_{LL'}\delta_{AA'} - \sum_{A''L''} G_{AL,A''L''}(\mathbf{k})\, t_{A''L'',A'L'} \right| = 0, \quad (36)$$

then gives the photonic KKR equation. It preserves its distinguished feature known in the case of electrons that is the separation of pure *geometrical* and *scattering* properties of a medium. Geometrical properties are encoded in geometrical structure constants characteristic for the lattice under consideration. They are functions of energy σ and the Bloch momentum $\mathbf{k}$. Scattering properties are as usually encoded in phase shifts of a single scatterer.

Our result for the structure constants (31) essentially disagrees with Ref. 21: our expression is much more symmetric while in Ref. 21 there is no summation over p, p' which is necessary here [see (28)] since electric multipoles have nonzero matrix elements with $Y_{L'}$ only for $l' = l \pm 1$ as it is seen from Eq. (B4) of Appendix B. This is probably the result that, in contrast to them, we have kept trace whether inward or outward values of fields are taken on the surface of spheres which is necessary to do for electromagnetic waves.[19] Moreover, there are no $\bar{T}_L$ factors in the Eq. (27) of Ref. 21 while their presence follows directly from (B3) of Appendix B. To visualize the differences one defines matrices with the entries being column vectors, namely, the diagonal matrix τ,

$$\tau_{LL} = (\bar{T}_L^{-1}, \bar{T}_L^0, \bar{T}_L^1), \quad (37)$$

and the off-diagonal matrix $\mathbf{c}$,

$$\mathbf{c}_{lm;l-1,m} = [\bar{C}^{-1}(l,-1,m), \bar{C}^0(l,-1,m), \bar{C}^1(l,-1,m)], \quad (38)$$

$$\mathbf{c}_{lm;l+1,m} = [\bar{C}^{-1}(l,1,m), \bar{C}^0(l,1,m), \bar{C}^1(l,1,m)], \quad (39)$$

all other entries being zero. According to relations (B12) and (B13) of Appendix B these matrices are like real unitary (orthonormal) matrices. In particular,

$$\tau \cdot \tau^\dagger = \mathbf{c} \cdot \mathbf{c}^\dagger = \mathbf{1}, \quad (40)$$

where $\tau^\dagger$ and $\mathbf{c}^\dagger$ are Hermitian conjugate matrices. The word "like" above is necessary because the entries of these matrices are column vectors and not all the rules of matrix algebra, in particular the cyclicity of trace, are valid for them. The transformation from scalar to vector structure constants can then be written in a matrix form as

$$G^{ij} = \begin{pmatrix} \tau & 0 \\ 0 & \mathbf{c} \end{pmatrix} \begin{pmatrix} \tilde{g}^{ij} & \tilde{g}^{ij} \\ \tilde{g}^{ij} & \tilde{g}^{ij} \end{pmatrix}^{\mathrm{tr}} \begin{pmatrix} \tau & 0 \\ 0 & \mathbf{c} \end{pmatrix}^\dagger, \quad (41)$$

where "tr" means the transposition of AL and $A'L'$ indices. Here the matrix $\tilde{g}^{ij}$ has the entries diagonal 3×3 matrices,

$$\tilde{g}^{ij}_{LL'} = \begin{pmatrix} g^{ij}_{lm-1;l'm'-1} & 0 & 0 \\ 0 & g^{ij}_{lm;l'm'} & 0 \\ 0 & 0 & g^{ij}_{lm+1;l'm'+1} \end{pmatrix}. \quad (42)$$

Provided $|m \pm 1| > l$ or $|m' \pm 1| > l'$ the entry in this matrix can be set in principle to be any finite number since in that case it is multiplied by the zero element of either the τ or $\mathbf{c}$ matrix.

III. OPERATOR FORMALISM FOR THE MAXWELL EQUATIONS

In the case of the Schrödinger operator H_0 with some potential Γ it is common to suppress the spatial indices and to consider all the quantities including the Green functions as operators in the Hilbert space. For example the DOS is then given by the formula

$$\rho(E) = -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\, G(E_+) = -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\, \frac{1}{E_+ - H}, \quad (43)$$

where $H = H_0 + \Gamma$ and E_+ stands for the limit $\lim s \to 0_+$ in $E = E + is$.

In the case of the Maxwell equation the problem is a bit more subtle. The Maxwell equation (2) can be written formally as

$$\tilde{H}\,|\mathbf{E}\rangle = -(\mathbf{1}\,\boldsymbol{\nabla}^2 - \boldsymbol{\nabla}\otimes\boldsymbol{\nabla})|\mathbf{E}\rangle = \omega^2\epsilon\,|\mathbf{E}\rangle. \tag{44}$$

Note that as the consequence of $\boldsymbol{\nabla}\tilde{H} \equiv 0$ any solution of (44) automatically satisfies $\boldsymbol{\nabla}\cdot(\epsilon\,|\mathbf{E}\rangle) = \boldsymbol{\nabla}\cdot|\mathbf{D}\rangle = 0$, the "transversality" condition in the case of spatially varying $\epsilon(\mathbf{r})$. Equation (44) resembles an eigenvalue equation, however, the eigenvalue ω^2 is multiplied by the spatially varying function $\epsilon(\mathbf{r})$. If one defines the Green function as

$$\tilde{G}(\omega^2) = \frac{1}{\omega^2\epsilon\,\mathbf{1} + \mathbf{1}\,\boldsymbol{\nabla}^2 - \boldsymbol{\nabla}\otimes\boldsymbol{\nabla}} \tag{45}$$

one would find that $\tilde{G}$ is not diagonal in the basis of eigenstates $|n\rangle$ of the frequency ω_n and $\mathrm{Im}\mathrm{Tr}\,\tilde{G}(\omega^2 + is)$ is not proportional to the level density $\rho(\omega^2)$,

$$-\frac{1}{\pi}\lim_{s\to 0_+}\mathrm{Im}\mathrm{Tr}\,\tilde{G}(\omega^2 + is) = \sum_n \langle n|\,\epsilon^{-1}\,|n\rangle\delta(\omega^2 - \omega_n^2). \tag{46}$$

The right resolvent which gives correctly the DOS via (43) and is diagonal in the "energy representation" is

$$G(\omega^2) = \frac{1}{\omega^2\,\mathbf{1} + \epsilon^{-1}(\mathbf{1}\,\boldsymbol{\nabla}^2 - \boldsymbol{\nabla}\otimes\boldsymbol{\nabla})} = \tilde{G}(\omega^2)\,\epsilon. \tag{47}$$

For our purposes it is convenient to define the parameter E in the case of photons as $E = \sigma^2 = \omega^2\epsilon_0 = \mathbf{k}_1^2$ where $\mathbf{k}$ is the wave vector in a medium with permittivity ϵ_0. As usually, $E = \mathbf{p}^2/2m$ for electrons. The above considerations then imply that the right analog of H (Ref. 25) in the measure dE is

$$H = -\frac{\epsilon_0}{\epsilon}(\mathbf{1}\,\boldsymbol{\nabla}^2 - \boldsymbol{\nabla}\otimes\boldsymbol{\nabla}). \tag{48}$$

The right separation of H as $H = H_0 + \Gamma$ for the Maxwell equation then reads

$$\begin{aligned} H_0 &= -(\mathbf{1}\,\boldsymbol{\nabla}^2 - \boldsymbol{\nabla}\otimes\boldsymbol{\nabla}),\\ H &= \frac{\epsilon_0}{\epsilon}H_0 = \left(1 - \frac{\epsilon}{v}\right)\Gamma,\\ \Gamma &= H - H_0 = \left(\frac{\epsilon_0 - \epsilon}{\epsilon}\right)H_0 = -\frac{v}{\epsilon}H_0 = -\frac{v}{\epsilon_0}H. \end{aligned} \tag{49}$$

Despite the formal similarity of (2) with the Schrödinger equation note the principal difference: the differential operators are generically multiplied by spatially varying functions [see (48) and (49)]. All that is the consequence of (2) where the eigenvalue ω^2 multiplies the potential $v(\mathbf{r})$, and, therefore, this feature persists for any differential equation with energy dependent potential. In the language of the Schrödinger equation the problem of finding the spectrum of (2) reads as follows: look for different Hamiltonians H_ω with the potential $\omega^2\epsilon(\mathbf{r})$ and find all ω such that H_ω has zero in its spectrum. The price we pay for removing the energy dependence is the introduction of potential Γ which is itself a differential operator. However, because of (49), the potential Γ reduces to a purely multiplicative operator on eigenfunctions of both H_0 and H.

Let us now find the free Green function $G_0(z) = (z - H_0)^{-1}$ for electromagnetic waves. We shall show that

$$G_0(z) = \left[\mathbf{1} + \frac{1}{z}\boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\right]\frac{1}{z + \boldsymbol{\nabla}^2} = -\frac{1}{\omega^2}\mathbf{d}_0$$

and

$$\boldsymbol{\nabla}\cdot G_0(z) = \frac{1}{z}\boldsymbol{\nabla}. \tag{50}$$

The Green function $\mathbf{d}_0$ here is the same as defined in (9),

$$\mathbf{d}_0 = -\left[\omega^2\mathbf{1} + \frac{1}{\epsilon_0}\boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\right]\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2}. \tag{51}$$

Obviously, Eq. (50) is equivalent to

$$-H_0\mathbf{d}_0 = (\mathbf{1}\,\boldsymbol{\nabla}^2 - \boldsymbol{\nabla}\otimes\boldsymbol{\nabla})\mathbf{d}_0 = -\omega^2\,\mathbf{1} - \omega^2\epsilon_0\mathbf{d}_0$$

and

$$\boldsymbol{\nabla}\cdot\mathbf{d}_0 = -\frac{1}{\epsilon_0}\boldsymbol{\nabla}\cdot \tag{52}$$

To prove it one uses

$$\boldsymbol{\nabla}^2\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2} = 1 - \sigma^2\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2} \tag{53}$$

to show that the contributions of

$$\boldsymbol{\nabla}^2\left(\boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2}\right) = \boldsymbol{\nabla}\otimes\boldsymbol{\nabla} - \sigma^2\boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2} \tag{54}$$

and

$$-\boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\left(\boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2}\right) = -\boldsymbol{\nabla}\otimes\boldsymbol{\nabla} + \sigma^2\boldsymbol{\nabla}\otimes\boldsymbol{\nabla}\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2} \tag{55}$$

cancel. Since

$$(\mathbf{1}\boldsymbol{\nabla}^2 - \boldsymbol{\nabla}\otimes\boldsymbol{\nabla})\left(\omega^2\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2}\right) = \omega^2\mathbf{1} + \omega^2\epsilon_0\mathbf{d}_0, \tag{56}$$

one easily shows the first of relations (52). As for the second one, note that

$$\boldsymbol{\nabla}\cdot\mathbf{d}_0 = -\boldsymbol{\nabla}\left[\omega^2\mathbf{1} + \frac{1}{\epsilon_0}\boldsymbol{\nabla}^2\right]\frac{1}{\sigma^2 + \boldsymbol{\nabla}^2} = -\frac{1}{\epsilon_0}\boldsymbol{\nabla}. \tag{57}$$

It is worthwhile to see how the Lippmann-Schwinger equation (6) of the preceding section works within the operator formalism. Equation (6) is written now as

$$|\mathbf{E}\rangle = |\mathbf{E}_0\rangle - G_0\omega_n^2 v|\mathbf{E}\rangle, \tag{58}$$

where $v = \epsilon - \epsilon_0$, $|\mathbf{E}_0\rangle$ is the eigenfunction of H_0 corresponding to an eigenenergy $E_n = \omega_n^2\epsilon_0$, and $G_0 = G_0(E_n + i0)$. This equation is seemingly in contradiction with the standard form of the Lippmann-Schwinger equation[1] for electric intensity $|\mathbf{E}\rangle$ with regard to the decomposition (49) of H as $H = H_0 + \Gamma$ which implies it to be

$$|\mathbf{E}\rangle = |\mathbf{E}_0\rangle + G_0\Gamma\,|\mathbf{E}\rangle. \tag{59}$$

Formally, since $H_0G_0(z) = -1 + zG_0(z)$,

$$H_0|\mathbf{E}\rangle = E_n|\mathbf{E}_0\rangle - \Gamma\,|\mathbf{E}\rangle + E_nG_0\Gamma\,|\mathbf{E}\rangle. \tag{60}$$

By iterating this equation with the help of Eq. (59) one generates the Rayleigh-Schrödinger perturbation series.[26] After their summation one obtains then the desired result,

$$\begin{aligned} H\,|\mathbf{E}\rangle &= (H_0 + \Gamma)|\mathbf{E}\rangle = E_n(1 + G_0\Gamma \\ &\quad + G_0\Gamma G_0\Gamma + \ldots)|\mathbf{E}_0\rangle \\ &= E_n\frac{1}{1 - G_0\Gamma}\,|\mathbf{E}_0\rangle = E_n|\mathbf{E}\rangle. \end{aligned} \tag{61}$$

To show that (58) works as well note that

$$H_0|\mathbf{E}\rangle = E_n|\mathbf{E}_0\rangle + \omega_n^2 v|\mathbf{E}\rangle - E_nG_0\omega_n^2 v|\mathbf{E}\rangle. \tag{62}$$

Similarly as above one iterates this equation, now with the help of (58), and finds

$$\begin{aligned} (H_0 - \omega_n^2 v)|\mathbf{E}\rangle &= E_n(1 - G_0\omega_n^2 v \\ &\quad + G_0\omega_n^2 vG_0\omega_n^2 v - \cdots)|\mathbf{E}_0\rangle \\ &= E_n\frac{1}{1 + G_0\omega_n^2 v}\,|\mathbf{E}_0\rangle = E_n|\mathbf{E}\rangle \end{aligned} \tag{63}$$

that is equivalent to (44).

To show the transversality of the solutions note that by applying $\boldsymbol{\nabla}\cdot$ on (59) one finds by using the second of relations (50)

$$\boldsymbol{\nabla}\cdot|\mathbf{E}\rangle = \boldsymbol{\nabla}\cdot|\mathbf{E}_0\rangle + \frac{1}{z}\boldsymbol{\nabla}\cdot(\Gamma\,|\mathbf{E}\rangle). \tag{64}$$

Now

$$\Gamma\,|\mathbf{E}\rangle = -\frac{v}{\epsilon_0}H\,|\mathbf{E}\rangle = -\omega_n^2 v|\mathbf{E}\rangle, \tag{65}$$

and

$$\boldsymbol{\nabla}\cdot(\epsilon\,|\mathbf{E}\rangle) = \epsilon_0\boldsymbol{\nabla}\cdot|\mathbf{E}_0\rangle. \tag{66}$$

Similarly, one shows the transversality for the solutions of (58),

$$\boldsymbol{\nabla}\cdot|\mathbf{E}\rangle = \boldsymbol{\nabla}\cdot|\mathbf{E}_0\rangle - \frac{1}{\epsilon_0}\boldsymbol{\nabla}\cdot(v|\mathbf{E}\rangle),$$

i.e.,

$$\boldsymbol{\nabla}\cdot(\epsilon\,|\mathbf{E}\rangle) = \epsilon_0\boldsymbol{\nabla}\cdot|\mathbf{E}_0\rangle. \tag{67}$$

Thus if one takes $|\mathbf{E}_0\rangle$ to be transverse then $|\mathbf{E}\rangle$ will be transverse too. In other words, both, operator $(1 - G_0\Gamma)^{-1}$ and $(1 + G_0\omega^2 v)^{-1}$, map transverse eigenfunctions of H_0 onto transverse eigenfunctions of H. Provided the operator $(1 - G_0\Gamma)^{-1}$ or $(1 + G_0\omega^2 v)^{-1}$ exists then H has an eigenfunction $|\mathbf{E}\rangle$,

$$|\mathbf{E}\rangle = \frac{1}{1 - G_0\Gamma}\,|\mathbf{E}_0\rangle = \frac{1}{1 + G_0\omega^2 v}\,|\mathbf{E}_0\rangle, \tag{68}$$

of the same eigenenergy E_n as $|\mathbf{E}_0\rangle$, which can be constructed by the Fredholm method.[23] One can show that $[1 + G_0(E_n + i0)\omega_n^2 v]^{-1}$ coincides with the restriction of $[1 - G_0(E_n + i0)\Gamma]^{-1}$ on the space of the eigenfunctions of H_0 with eigenenergy $E_n = \omega_n^2\epsilon_0$. By using the identity $[1 - G_0\Gamma]^{-1} = 1 + G\Gamma$ one finds

$$\begin{aligned} \frac{1}{1 - G_0(E_n + i0)\Gamma}|\mathbf{E}_0\rangle &= [1 + G(E_n + i0)\Gamma]|\mathbf{E}_0\rangle \\ &= [1 - \tilde{G}(\omega_n^2 + i0)\omega_n^2 v]|\mathbf{E}_0\rangle, \end{aligned} \tag{69}$$

where $\tilde{G}(\omega_n^2 + i0)$ is defined by (45). On the other hand,

$$\begin{aligned} \frac{1}{1 + G_0\omega_n^2 v} &= 1 - \frac{1}{\omega_n^2\epsilon_0 + i0 - (\mathrm{H}_0 - \omega_n^2 v)}\omega_n^2 v \\ &= 1 - \tilde{G}(\omega_n^2 + i0)\omega_n^2 v. \end{aligned} \tag{70}$$

So far we have not addressed the question of convergence of the Rayleigh-Schrödinger perturbation series that occur, for example, in (61) and (63). For those who are interested in this question we refer to Ref. 27 where an improvement of the Rayleigh-Schrödinger perturbation theory is given by the help of a generalization of the Borel summability method.

After the decomposition (49) one can repeat all standard techniques known for the Schrödinger equation. One defines the T matrix by the Lippmann-Schwinger equation,

$$\begin{aligned} T &= \Gamma + \Gamma G_0^+ T = \Gamma + TG_0^+\Gamma = \Gamma(1 - G_0^+\Gamma)^{-1} \\ &= (1 - \Gamma G_0^+)^{-1}\Gamma, \end{aligned} \tag{71}$$

with G_0^+ satisfying the outgoing boundary conditions. Sometimes it is more convenient to work with Hermitian quantity as the K matrix. The K matrix is defined essentially in the same manner as the T matrix,

$$\begin{aligned} K &= \Gamma + \Gamma G_0^0 K = \Gamma + KG_0^0\Gamma = \Gamma(1 - G_0^0\Gamma)^{-1} \\ &= (1 - \Gamma G_0^0)^{-1}\Gamma. \end{aligned} \tag{72}$$

The Green function G_0^0 here is, however, the real or the Hermitian part of G_0^+,

$$G_0^+ = G_0^0 - iD, \tag{73}$$

and D is a solution of the homogeneous equation. The T matrix can be expressed in terms of K matrix and vice versa,

$$T = K(1 + iDK)^{-1}, \qquad K = T(1 - iDT)^{-1}. \tag{74}$$

For spherically symmetric scatterer the channel $\mathbf{S}_L$ matrix can be expressed as

$$\mathbf{S}_L = \frac{1 - iK_L}{1 + iK_L} = 1 - 2iT_L = e^{2i\eta_l}, \tag{75}$$

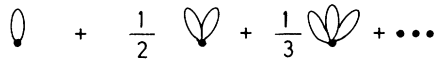

FIG. 1. Single-site tadpole diagrams.

where

$$T_L = -\sin\eta_l e^{i\eta_l}. \tag{76}$$

Here η_l is the phase shift, which in this special case does not depend on the magnetic quantum number.[1]

IV. DENSITY OF STATES CALCULATIONS

We now turn on to the calculation of DOS's in a system of nonoverlapping scattering centers. In the next we shall follow the original calculations of Lloyd and Smith for the DOS of electrons.[1] When considering the thermodynamic limit $\Omega \to \infty$ and $N \to \infty$ such that the density of scatterers N/Ω stays finite one can take one of two fundamentally different points of view: either the system has an infinity volume Ω and thus occupies all space, or the system is situated in a much larger volume Ω_∞ with the limits being taken so that $\Omega_\infty \to \infty$ before $\Omega \to \infty$ and $\Omega/\Omega_\infty \to 0$ even though the volume Ω becomes infinite. In the first case the integrated density of states (IDOS's) $N(E)$ is found from the formula

$$\begin{aligned} N(E) &= -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln[E_+ - H] \\ &= N_0(E) - \frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln[1 - G_0^+\Gamma], \end{aligned} \tag{77}$$

with $\Gamma = \sum_i \Gamma_i$, where the sum runs over all scatterers.[1] In the second case the IDOS is determined directly by the $\mathbf{S}$ matrix of the system via the Krein-Friedel formula

$$N(E) = N_0(E) + \frac{1}{2\pi i}\mathrm{Tr}\ln\mathbf{S} = N_0(E) + \frac{1}{2\pi}\mathrm{Im}\mathrm{Tr}\ln\mathbf{S}. \tag{78}$$

To calculate the change of the IDOS induced by the presence of scatterers and establish the equivalence of (77) and (78) one expands the logarithm in (77),

$$\begin{aligned} \triangle N(E) &= -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left[1 - G_0^+\Gamma\right] \\ &= \frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\sum_{n=1}^{\infty}\frac{1}{n}(G_0^+\Gamma)^n, \end{aligned} \tag{79}$$

and substitutes $\Gamma = \sum_i \Gamma_i$. A generic term of the expansion is given by

$$\frac{1}{n}\mathrm{Tr}\,(A_{i_1}A_{i_2},\ldots,A_{i_n}) \tag{80}$$

with $A_{i_k} = G_0^+\Gamma_{i_k}$ where the indices i_k may equal. The diagram corresponding to this term is constructed by connecting vertices $i_1, i_2, \ldots, i_n$ in subsequent order. Because of the trace operation the vertices i_n and i_1 are connected, too. If some pair of vertices is equal one draws a tadpole which starts and terminates at the vertex (see Fig. 1). If in some p-tuple of vertices all the vertices have the same label then $p-1$ tadpoles are drawn from the given vertex. To each vertex i_k corresponds the scattering potential Γ_{i_k} and to each line connecting subsequent vertices the propagator $G_0^+(i_k - i_{k+1})$.

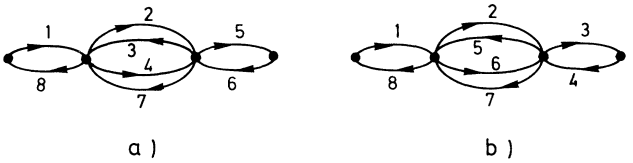

FIG. 2. Two different closed trajectories which give different contributions to $\Delta N(E)$ but lead to the same diagram. The numbers indicate successive paths betwen different scatterers from which given closed trajectories are composed.

In what follows it is convenient to imagine the term (80) as a closed trajectory. It is clear that any closed trajectory of nth order with at least two different vertices occurs exactly n times in the expansion (79): any term $A_{i_1}A_{i_2},\ldots,A_{i_n}$ with cyclic permutation of indices $i_1 i_2 \ldots i_n$ gives the same trajectory. The main reason to speak about the trajectories is that sometimes *different* closed trajectories leading to the *same* diagram may give a *different* contribution. An example of this are trajectories $(1,2,3,2,3,4,3,2)$ and $(1,2,3,4,3,2,3,2)$ (see Fig. 2). They are different modulo cyclic permutation of indices, nonetheless they give rise to the same diagram. If one then follows the rules to calculate the contribution of the trajectories one finds that they are different if the scatterers are not identical or not of the same distance each from other since then

$$\mathrm{Tr}\,(A_1A_2A_3A_2A_3A_4A_3A_2) \neq \mathrm{Tr}\,(A_1A_2A_3A_4A_3A_2A_3A_2), \tag{81}$$

the fact that seems to have been unnoticed so far.

As shown by Lloyd and Smith[1] all tadpole diagrams that give multiple scattering from the same site can be summed over. One first resums the tadpole diagrams with a single-site (see Fig. 1). The result for the site j is simply

$$-\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left[1 - G_0^+\Gamma_j\right]. \tag{82}$$

It can be rewritten to the more familiar Friedel form

$$-\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left[1 - G_0^+\Gamma_j\right] = \frac{1}{2\pi}\mathrm{Im}\mathrm{Tr}\ln\mathbf{S}^j = \frac{1}{\pi}\sum_{AL}\eta^j_{AL,AL}, \tag{83}$$

where $\mathbf{S}^j$ is the single-site $\mathbf{S}$ matrix on the site j, and $\eta^j_{AL,A'L'}$ are the corresponding phase shifts.[1] One obtains the result under the hypothesis that $(1 - G_0^0\Gamma_j)$ has no zeros and poles on the real axis. It is known that if $F(E)$ is an analytical function in a strip $E + is$ of the upper half-plane, which is real when E is real and which has zeros E_z and poles E_p on the real axis, then

$$\lim_{s\to 0}\mathrm{Im}\ln F(E+is) = -\pi\sum_z \Theta(E-E_z) + \pi\sum_p \Theta(E-E_p), \quad (84)$$

where $\Theta(x)$ is the Heaviside step function.[12] Thus, if the above hypothesis is satisfied then $\mathrm{Im}\mathrm{Tr}\ln\left[1-G_0^0\Gamma_j\right]=0$ and

$$-\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left[1-G_0^+\Gamma_j\right] = -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left[1+iDk^j\right], \quad (85)$$

where k^j is the single-site k matrix. In the angular momentum representation[1,28]

$$D_{AL,A'L'}(\mathbf{R})|_{\mathbf{R}=0} = \delta_{LL'}\delta_{AA'}. \quad (86)$$

Since $k^j_{AL,A'L'}$ is real, $\mathrm{Im}\ln[1-ik^j_{AL,A'L'}] = -\mathrm{Im}\ln[1+ik^j_{AL,A'L'}]$, and using the relation (75) one finally establishes (83). Therefore, the change of the IDOS can be expressed as

$$\triangle N(E) = \frac{1}{\pi}\sum_{j=1}^{N}\sum_{AL}\eta^j_{AL,AL} + \triangle N^{(1)}(E), \quad (87)$$

where $\triangle N^{(1)}(E)$ is entirely due to the presence of *multiple scatterers* and *multiple-scattering effects*. In order to calculate $\triangle N^{(1)}(E)$ one sums over tadpoles in the remaining diagrams. The summation results in replacing the vertex contribution Γ_j by the single-site t matrix t^j,

$$\Gamma_j \to t^j = \Gamma_j\frac{1}{1-G_0^+\Gamma_j}. \quad (88)$$

For example, for two different vertices $i_1=1$ and $i_2=2$ one has

$$\mathrm{Tr}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} G_0^+\Gamma_1(G_0^+\Gamma_1)^{m-1}G_0^+\Gamma_2(G_0^+\Gamma_2)^{n-1} = \mathrm{Tr}\,G_0^+\Gamma_1\frac{1}{1-G_0^+\Gamma_1}G_0^+\Gamma_2\frac{1}{1-G_0^+\Gamma_2}. \quad (89)$$

$\triangle N^{(1)}(E)$ is then written as

$$\triangle N^{(1)}(E) = \frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\left(\frac{1}{2}\sum_i\sum_{j\neq i}G_0^+t^iG_0^+t^j + \frac{1}{3}\sum_i\sum_{j\neq i}\sum_{k\neq i,j}G_0^+t^iG_0^+t^jG_0^+t^k+\cdots\right),$$

where any two subsequent (with regard to the trace) t matrices have a different label.

By virtue of the nonoverlapping condition the trace can be taken either in the basis of spherical harmonics in the case of electrons, or, of electric and magnetic multipoles in the case of photons. Because of the trace operation any closed trajectory becomes a closed trajectory in the symbolic phase space and the diagrammatic rules to calculate $\triangle N^{(1)}(E)$ can be formulated as follows on the energy shell.

(1) Draw all possible closed trajectories (orbits). Any intermediate path has to connect different sites but it can return back to the original site after visiting some different site.

(2) To any orbit corresponds a diagram with vertices given by the single-site t matrices $t^j_{AL,A'L'}$. To the line connecting the jth and nth sites corresponds the propagator matrix $G^{jn}_{AL,A'L'} = G^+_{AL,A'L'}(\mathbf{R}_n-\mathbf{R}_j)$.

(3) The contribution of a given orbit is obtained by taking the trace of a matrix which results by multiplying t and G matrices in the order that is determined by tracing the orbit.

(4) The total contribution to the density of states is given by summing over all orbits and by adding the Friedel sum (83) for each scatterer.

All the above rules can be summarized by the analytical expression (cf. Ref. 1)

$$\triangle N(E) = \frac{1}{\pi}\sum_{j=1}^{N}\sum_{AL}\eta^j_{AL,AL} - \frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left[\delta_{LL'}\delta_{AA'}\delta_{jn} - \sum_{A_1L_1}\mathcal{G}^{jn}_{AL,A_1L_1}t^n_{A_1L_1,A'L'}\right], \quad (90)$$

where $\sum_{A_1L_1}\mathcal{G}^{jn}_{AL,A_1L_1}t^n_{A_1L_1,A'L'}$ is the matrix with three pairs of indices: angular momentum LL', multipole AA', and spatial ones jn. The trace is then taken over all the pairs of indices. The Green function (propagator) $\mathcal{G}^{jn}_{AL,A'L'}$ here equals $G^{+jn}_{AL,A'L'}$ except for $j=n$ where it is zero. It is the familiar structure constant of Sec. II. Formally, one can write

$$\mathcal{G}^{jn}_{AL,A'L'} = \alpha_jG^{+jn}_{AL,A'L'} \quad (91)$$

where α_j is a Grassmann-like variable on the site j (Grassmann-like because $\alpha_j^2=0$ but neither commutation nor anticommutation of α_j and α_n are defined).

Sometimes it is more convenient to rewrite (90) to a slightly different form in terms of k matrix. By combining (83) and (85) one can write

$$\frac{1}{\pi}\sum_{AL}\eta^j_{AL,AL} = -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left\{\left[\delta_{LL'}\delta_{AA'}+ik^j_{AL,A'L'}\right]\delta_{jn}\right\}. \quad (92)$$

Afterwards both term in (90) are written in the similar matrix form, one can sum the logarithms by multiplying their arguments as matrices, and obtain

$$-\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\ln\left\{\delta_{LL'}\delta_{AA'}\delta_{jn}+ik^j_{AL,A'L'} - \sum_{ALA_2L_2}\mathcal{G}^{jn}_{AL,A_2L_2}t^n_{A_2L_2,A'L'} - i\sum_{A_1L_1A_2L_2}k^j_{AL,A_1L_1}\mathcal{G}^{jn}_{A_1L_1,A_2L_2}t^n_{A_2L_2,A'L'}\right\}. \quad (93)$$

After using the relations (74), (86), (91) and the cyclicity property of trace one arrives at

$$\triangle N(E) = -\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln\left[\delta_{LL'}\delta_{AA'}\delta_{jn} - \sum_{A_1L_1} G^{+jn}_{AL,A_1L_1}k^n_{A_1L_1,A'L'}\right]. \quad (94)$$

The formalism is well suited for a finite cluster of scatterers. If the number N of scatterers tends to infinity one defines the integrated density of states $\bar{N}(E) = N(E)/V$ per unit volume. After a suitable averaging over the position of scatterers the formalism has also been applied by Lloyd to describe liquids.[29] If the scatterers are identical and arranged in a periodic manner a useful tool to perform the summation over lattice sites in the expansion of (90) is to use the lattice Fourier transform,

$$\mathcal{G}_{AL,A_1L_1}(\mathbf{k}) = \sum_{\mathbf{n}\in\Lambda}\mathcal{G}^{jn}_{AL,A_1L_1}e^{i\mathbf{k}\cdot(\mathbf{n}-\mathbf{j})} = \sum_{\mathbf{n}\in\Lambda}\mathcal{G}^{nj}_{AL,A_1L_1}e^{i\mathbf{k}\cdot(\mathbf{j}-\mathbf{n})}, \quad (95)$$

where the sum runs over all points of the lattice Λ and $\mathbf{k}$ is the Bloch momentum. Because of the cyclicity of the trace operation in (90) the trace does not change under the substitution

$$\mathcal{G}^{jn}_{AL,A_1L_1} \to \mathcal{G}^{jn}_{AL,A_1L_1}e^{i\mathbf{k}\cdot(\mathbf{n}-\mathbf{j})}. \quad (96)$$

In summing term by term in the expansion of (90) one fixes one lattice index. The summation over the remaining lattice indices then gives the Fourier transform of $\mathcal{G}^{jn}_{AL,A_1L_1}$. Eventually, one finds the change of the integrated density of states $\triangle\bar{N}(E)$ per lattice site (unit cell volume V) to be

$$\triangle\bar{N}(E) = \frac{1}{\pi}\sum_{AL}\eta_{AL,AL}(E) - \frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln\left[\delta_{LL'}\delta_{AA'} - \sum_{A_1L_1}\mathcal{G}_{AL,A_1L_1}(\mathbf{k})t_{A_1L_1,A'L'}\right] \quad (97)$$

[cf. (36)]. Although we have been interested in the three-dimensional MST and KKR our diagrammatic rules remain intact in two dimensions. The only change concerns the set of indices over which the trace is taken. For example, in the case of electrons the multi-index $L = lm$ is simply reduced to l. As a self-consistency check note that in the case of an *empty* lattice both the phase shifts $\eta_{AL,A'L'}$ and the t matrix [cf. (76)] are *zero* and hence, according to (97), $\Delta\bar{N}(E) = 0$. To get full IDOS $N(E)$ in three dimensions one has to add (97) to

$$N_0(E) = \frac{Vp^3}{3\pi^2\hbar^3} = \frac{V(2mE)^{3/2}}{3\pi^2\hbar^3} \quad (98)$$

in the case of electrons, and

$$N_0(E) = \frac{Vk^3}{3\pi^2} = \frac{VE^{3/2}}{3\pi^2} \quad (99)$$

in the case of photons.

Apart from the band structure calculations the expression (97) for $\triangle\bar{N}(E)$ can be used directly to calculate the IDOS of a quantum billiard on a torus after one has set $\mathbf{k} = \mathbf{0}$ (this is equivalent to impose the periodic boundary conditions). In the special case of a two-dimensional billiard on a torus the relation (97) gives the result that is equivalent to Eq. (6.11) of Ref. 12 without applying (84) on the KKR determinant (36) and without using a particular form of the structure constants. A useful methodological tool to study the semiclassical DOS of classically ergodic systems is the Gutzwiller trace formula,[16]

$$\mathrm{Tr}\,G(\mathbf{r},\mathbf{r},E) = \sum_j\frac{1}{E-E_j} = \bar{g}(E) + \frac{1}{i\hbar}\sum_\gamma\sum_{n=1}^{\infty}A_{n\gamma} \times \exp\left(inS_\gamma(E)/\hbar - i\pi n\nu_\gamma/2\right), \quad (100)$$

where the amplitude A_γ is defined as

$$A_{n\gamma} = \oint d\tau_\gamma|\det(M^n_{\gamma(\tau)} - I)|^{-1/2}. \quad (101)$$

The term $\bar{g}(E)$ is a smooth function giving the mean density of states. The double sum runs over all distinct periodic orbits in a phase space, labeled by γ, and over n, the number of retracing each orbit. The integer ν_γ is a phase shift: in the case of finite systems with the Dirichlet boundary conditions it counts the number of focal points and twice the number of reflections off the walls. $S_\gamma(E)$ is the action and the stability (monodromy) matrix $M_{\gamma(\tau)}$ records the sensitivity of the trajectory γ at its given point $\gamma(\tau)$ to changes in initial conditions.[16]

The full power of the Gutzwiller approach has been demonstrated in the discussion of the anisotropic Kepler problem,[16] the scattering of a point particle from three hard discs fixed on a plane—the so-called three disc repellor,[30] hydrogen energy levels in a strong magnetic field,[31] and by the quantization of energy levels of the helium atom.[32] It is interesting to compare our diagrammatic rules with the semiclassical Gutzwiller trace formula now. One sees immediately that the number of periodic orbits is substantionally suppressed in the exact expression. To visualize (90) "semiclassically" each sphere V_j containing a single scatterer is replaced by its center with regard to which the single-site t matrix is defined. Then it is natural that only the isolated orbits (in the terminology of Ref. 12) are considered which connect centers of different scatterers. Nonisolated orbits do not enter the exact expression, for we have been interested in the calculation of the *change* of the DOS and not of the DOS itself as in Refs. 12 and 16. This might be a sign that the convergence properties of the Gutzwiller trace formula at the special case of quantum billiards on a torus might be improved if one calculates the semiclassical expansion of the change of DOS directly. This does not concern finite systems with the Dirichlet boundary conditions imposed that are nonintegrable even without the presence of scatterers such as the Bunimovitch stadium or quantum cavities.[33]

V. SUMMARY AND CONCLUSIONS

To summarize, the photonic structure constants $G^{jn}_{AL,A'L'}$ have been calculated and basic MST and KKR equations for photons have been derived. Our result for the structure constants (31) is more symmetric than that in Ref. 21 where, probably, the trace was not kept whether the inward or outward formalism was used.

A formal operator formalism for the Maxwell equation has been presented. The essential difference of the Maxwell equation (2) with regard to the Schrödinger equation is that, in the former case, the potential from the point of view of the Schrödinger equation is energy dependent. It was shown [see (48) and (49)] how to perform the separation $H = H_0 + \Gamma$ such that Γ be energy independent. The price one pays for the decomposition is that the potential Γ is itself a differential operator multiplied by a spatially varying function [see (49)]. It reduces, however, to a multiplicative operator on eigenfunctions of both, H and H_0. The decomposition is necessary in order that the Green function gives the density of states by the same formula as in the Schrödinger case. The Lippmann-Schwinger equations have been analyzed within the operator formalism and properties of the Greens function have been discussed.

The Lloyd and Smith on-the-energy-shell multiple-scattering formalism[1] for the calculations of the change $\triangle N(E)$ of the integrated density of states induced by the presence of scatterers has been analyzed in the spirit of the Gutzwiller approach.[16] The important message of our paper is that one must not look for the diagrams of Ref. 1 but for closed orbits in phase space: there are different orbits which give different contributions to $\triangle N(E)$ but are described by the same diagram. As a result, diagrammatic rules have been interpreted in terms of closed orbits.

Our expression (90) shows that in the case of electromagnetic waves the Krein-Friedel formula[17] can be used as well. Formula (90) gives $\triangle N(E)$ as the sum of two contributions: one that is determined solely in terms of single-scattering properties, and the second that is due to multiple-scattering effects. Therefore, in addition to the separation of purely geometric and purely scattering properties as in the standard KKR method one can separate the single-scattering and the multiple-scattering contributions to the IDOS. A comparison of the exact expression (90) for $\triangle N(E)$ with the semiclassical Gutzwiller trace formula (100) (Ref. 16) has been made. The comparison shows that, in the special case of quantum billiards on a torus, the number of closed orbits in the exact expression to be summed over is significantly reduced.

An application of the above results to study the band structure of photons and impurities in a photonic crystal will be given elsewhere.[28]

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APPENDIX A: NOTATIONS AND DEFINITIONS

Scalar spherical harmonics Y_L are used as defined by Ref. 22, i.e., satisfying the *Condon-Shortley* convention, in which

$$Y^*_{lm}(\theta,\phi) = (-1)^m Y_{l,-m}(\theta,\phi), \qquad Y_{lm}(-\theta,-\phi) = Y_{l,-m}(\theta,\phi). \tag{A1}$$

Our definition of vector spherical harmonics coincides up to factor i with Ref. 23,

$$\mathbf{Y}^{(m)}_L = \mathbf{X}_L = \frac{1}{\sqrt{l(l+1)}}\mathbf{L}\,Y_L, \tag{A2}$$

$$\mathbf{Y}^{(e)}_L = (\mathbf{r}_0 \times \mathbf{X}_L), \tag{A3}$$

$$\mathbf{Y}^{(o)}_L = iY_L\mathbf{r}_0, \tag{A4}$$

where $\mathbf{L}$ is the orbital angular momentum operator and $\mathbf{r}_0$ unit radius vector. They are all *normalized*

$$\langle \mathbf{Y}^{(a)}_L | \mathbf{Y}^{(a')}_{L'} \rangle = \delta_{aa'}\delta_{LL'}, \tag{A5}$$

and satisfy

$$\partial_r \mathbf{Y}^{(a)}_L = 0. \tag{A6}$$

One can show[28] that

$$\boldsymbol{\nabla} \times \mathbf{X}_L = \frac{1}{r}\mathbf{Y}^{(e)}_L + \frac{\sqrt{l(l+1)}}{r}\mathbf{Y}^{(o)}_L, \tag{A7}$$

$$\langle Y_{l'm'} | \mathbf{Y}^{(m)\alpha}_{lm} \rangle = \frac{1}{\sqrt{l(l+1)}}\delta_{l'l}\delta_{m'm+\alpha}T^{\alpha}_{lm}, \tag{A8}$$

$$\langle Y_{l'm'} | \mathbf{Y}^{(e)\alpha}_{lm} \rangle = -i\delta_{m'm+\alpha}\{\sqrt{l+1}\,C^{\alpha}(l-1,m+\alpha,l,m)\delta_{l'l-1} + \sqrt{l}\,C^{\alpha}(l+1,m+\alpha,l,m)\delta_{l'l+1}\}, \tag{A9}$$

$$\langle Y_{l'm'} | \mathbf{Y}^{(o)\alpha}_{lm} \rangle = -i\delta_{m'm+\alpha}\{\sqrt{l}\,C^{\alpha}(l-1,m+\alpha,l,m)\delta_{l'l-1} - \sqrt{l+1}\,C^{\alpha}(l+1,m+\alpha,l,m)\delta_{l'l+1}\}. \tag{A10}$$

Constants T^{α}_{lm}'s are defined by the action of spherical components of $\mathbf{L}^{\alpha}$ on spherical harmonics,

$$\mathbf{L}^{\alpha}Y_L = T^{\alpha}_{lm}Y_{lm+\alpha}. \tag{A11}$$

$C^{\alpha}(l'm'lm)$ are defined by

$$\langle l'm'|V^{\alpha}|lm\rangle = C^{\alpha}(l'm'lm)\langle l'm'||V^{\alpha}||lm\rangle, \tag{A12}$$

where $\langle l'm'||V^{\alpha}||lm\rangle$ is the reduced matrix element[34] that does not depend on m and m'. They can be expressed via $3j$ *symbols*,[34]

$$C^{\alpha}(l'm'lm) = (-1)^{l'-m'}\begin{pmatrix} l' & 1 & l \\ -m' & \alpha & m \end{pmatrix}. \tag{A13}$$

In all the above formulas $l \geq 1$ for there is neither electric nor magnetic multipole with $l = 0$.

The *Gaunt number* $C^{L_3}_{L_2L_1}$ is the matrix element[2]

$$C^{L_3}_{L_2L_1} = \langle Y_{L_1}|Y_{L_2}|Y_{L_3}\rangle = \oint Y^*_{L_1}Y_{L_2}Y_{L_3}do = (-1)^{m_1}\left[\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right]^{1/2}\begin{pmatrix} l_1 & l_2 & l_3 \\ -m_1 & m_2 & m_3 \end{pmatrix}\begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}. \tag{A14}$$

In the Condon-Shortley convention (A1) that is adopted here they are all *real* numbers. Due to the symmetry of $3j$ symbols one has

$$C^{L_3}_{L_2L_1} = C^{L_2}_{L_3L_1} = (-1)^{m_3}C^{l_3,-m_3}_{L_1L_2} = C^{l_3,-m_3}_{l_1,-m_1;l_2,-m_2}. \tag{A15}$$

The first equality can be deduced straightforwardly from the form of the integral in (A14). The second uses the fact that

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = 0 \tag{A16}$$

whenever $J = j_1 + j_2 + j_3$ is *odd*. For J *even* one has[34]

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = (-1)^{J/2}\left[\frac{(J-2j_1)!(J-2j_2)!(J-2j_3)!}{(J+1)!}\right]^{1/2}\frac{(J/2)!}{(J/2-j_1)!(J/2-j_2)!(J/2-j_3)!}. \tag{A17}$$

If $C^{L_3}_{L_2L_1}$ is nonzero then $(-1)^{l_1+l_2+l_3} = (-1)^{m_1+m_2+m_3} = 1$. Due to the properties (A15) of the Gaunt numbers and spherical harmonics (A1) one can write (24) in several equivalent forms,

$$\begin{aligned} g_{L'L}(\mathbf{R}) &= -(-1)^l i^{l+l'+1}4\pi\sigma\sum_{L_1}C^{L_1}_{L'L}i^{l_1}h^+_{l_1}(\sigma R)Y^*_{L_1}(\mathbf{R}) \\ &= -(-1)^l i^{l+l'+1}4\pi\sigma\sum_{L_1}C^{L_1}_{LL'}i^{l_1}h^+_{l_1}(\sigma R)Y_{L_1}(\mathbf{R}) \\ &= -(-1)^{l'}i^{l+l'+1}4\pi\sigma\sum_{L_1}C^{L_1}_{LL'}i^{l_1}h^+_{l_1}(\sigma R)Y_{L_1}(-\mathbf{R}). \end{aligned} \tag{A18}$$

APPENDIX B: BASIC MST IDENTITIES

$$W(j_l, h^+_l) = iW\left[j_l(\sigma r), n_l(\sigma r)\right] = \frac{i}{\sigma r^2}, \tag{B1}$$

$$\langle \mathbf{J}^{\alpha}_{AL}|\mathbf{J}^{\alpha}_{A'L'}\rangle = \delta_{AA'}\delta_{LL'}N^l_A = \delta_{AA'}\delta_{LL'}\begin{cases} j^2_l, & A = M \\ \frac{1}{(2l+1)}\left[(l+1)j^2_{l-1} + lj^2_{l+1}\right], & A = E, \end{cases} \tag{B2}$$

$$\langle \mathbf{J}^{\alpha}_{ML}|Y_{L'}\rangle = j_l\frac{1}{\sqrt{l(l+1)}}T^{\alpha}_{lm}\delta_{l'l}\delta_{m'm+\alpha}, \tag{B3}$$

$$\begin{aligned} \langle \mathbf{J}^{\alpha}_{EL}|Y_{L'}\rangle &= \delta_{m'm+\alpha}\{\sqrt{l+1}\,j_{l-1}C^{\alpha}(l-1,m+\alpha,l,m)\delta_{l'l-1} - \sqrt{l}\,j_{l+1}C^{\alpha}(l+1,m+\alpha,l,m)\delta_{l'l+1}\} \\ &= \delta_{m'm+\alpha}\left\{j_{l-1}\bar{C}^{\alpha}(l,-1,m)\delta_{l'l-1} + j_{l+1}\bar{C}^{\alpha}(l,1,m)\delta_{l'l+1}\right\}. \end{aligned} \tag{B4}$$

All the above formulas follow directly from the definitions of magnetic (14) and electric (15) multipoles and scalar product formulas of the preceding appendix. Now, one can show that

$$\langle Y_{L'}|j_{l'}\partial_r - j'_{l'}|\mathbf{J}^{\alpha}_{AL}\rangle = \langle Y_{L'}|W(j_{l'},\mathbf{J}^{\alpha}_{AL})\rangle = \langle Y_{L'}|W(h^{+}_{l'},\mathbf{H}^{+}_{AL})\rangle = 0. \tag{B5}$$

For magnetic multipoles the result is zero for $l \neq l'$ as the consequence of scalar product formula, and zero for $l' = l$ for it is proportional to the Wronskian of identical functions. Similarly, for electric multipoles one needs to check only the case of $l' = l \pm 1$ since otherwise the result is, as above, zero due to scalar product formulas. In the case of $l' = l + 1$, for example, one finds in principle terms that are either proportional to $W(j_{l+1}, j_{l+1})$ or $W(j_{l+1}, j_{l-1})$. The former then vanish because of vanishing Wronskian, the latter because of vanishing of the numerical prefactor in front of it. As a direct consequence of the above considerations one has

$$\langle Y_{L'}|W(h^{+}_{l'},\mathbf{J}_{AL})\rangle = -\langle Y_{L'}|W(j_{l'},\mathbf{H}^{+}_{AL})\rangle, \tag{B6}$$

$$\langle Y_{L'}|j_{l'}\partial_r - j'_{l'}|\mathbf{H}^{+\alpha}_{ML}\rangle = \frac{i}{\sigma r^2}\frac{1}{\sqrt{l(l+1)}}T^{\alpha}_{lm}\delta_{l'l}\delta_{m'm+\alpha}, \tag{B7}$$

$$\begin{aligned}\langle Y_{L'}|j_{l'}\partial_r - j'_{l'}|\mathbf{H}^{+\alpha}_{EL}\rangle &= \frac{i}{\sigma r^2}\delta_{m'm+\alpha}\left[\sqrt{l+1}\,C^{\alpha}(l-1,m+\alpha,l,m)\delta_{l'l-1} - \sqrt{l}\,C^{\alpha}(l+1,m+\alpha,l,m)\delta_{l'l+1}\right]\\ &= \frac{i}{\sigma r^2}\delta_{m'm+\alpha}\left[\bar{C}^{\alpha}(l,-1,m)\delta_{l'l-1} + \bar{C}^{\alpha}(l,1,m)\delta_{l'l+1}\right].\end{aligned} \tag{B8}$$

Ignoring for a while j_l terms and multiplicative factors one finds by using the above formulas that $\langle Y_{L'}|W(j_{l'},\mathbf{H}^{+}_{AL})\rangle = \langle Y_{L'}|\mathbf{J}_{AL}\rangle$. This indicates that, by using (B6),

$$\sum_{L''}\langle \mathbf{J}_{AL}|Y_{L''}\rangle \cdot \langle Y_{L''}|W(h^{+}_{l''},\mathbf{J}_{A'L'})\rangle$$

$$= \sum_{L''}\langle \mathbf{J}_{AL}|Y_{L''}\rangle \cdot \langle Y_{L''}|\mathbf{J}_{A'L'}\rangle = \langle \mathbf{J}_{AL}|\mathbf{J}_{A'L'}\rangle. \tag{B9}$$

Including all the factor one indeed confirms that

$$\sum_{L''} j_{l''}\langle \mathbf{J}_{AL}|Y_{L''}\rangle \cdot \langle Y_{L''}|W(h^{+}_{l''},\mathbf{J}_{A'L'})\rangle$$

$$= -\frac{i}{\sigma r^2}\delta_{AA'}\delta_{LL'}N^{l}_{A}. \tag{B10}$$

The result is a consequence of two identities,

$$\sum_{\alpha=-1}^{1}\bar{C}^{\alpha 2}(l,1,m) = \frac{l+1}{2l+1}$$

and

$$\sum_{\alpha=-1}^{1}\bar{C}^{\alpha 2}(l,-1,m) = \frac{l}{2l+1}. \tag{B11}$$

They immediately imply

$$\sum_{\substack{p=-1\\ p\neq 0}}^{1}\sum_{\alpha=-1}^{1}\bar{C}^{\alpha}(l,p,m)^2 = 1. \tag{B12}$$

Similarly, one can find that

$$\sum_{\alpha=-1}^{1}\bar{T}^{\alpha\ 2}_{lm} = 1. \tag{B13}$$

The last two identities then prove the "unitarity" of τ and $\mathbf{c}$ matrices.

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