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The authors present a closed formulation of resonant point scatterers for classical-wave propagation problems. A Green's-function approach is employed in which all the small-distance singularities are regularized. Application of point scatterers considerably simplifies multiple-scattering calculations needed, for instance, for understanding the optical properties of dense cold gases and optical lattices. In the case of the vector description of light, it is shown that two different regularization parameters are required in order to obtain physically meaningful results. One parameter is related to the physical size of the pointlike scattering particle, while the other is connected to its dynamic properties. All parameters involved are defined in terms of physical observables leading to a complete and self-consistent treatment. The applicability of the point-scatterer model to several physical models is demonstrated. We calculate the local density of states of waves in the presence of one resonant point scatterer. For the vector case, the bare polarizability is shown to enter the local density of states. For a collection of resonant point dipoles, the Lorentz-Lorenz relation for the dielectric constant is derived for cubic lattices and for disordered arrangements. [S0034-6861(98)00302-X]

CONTENTS

I. INTRODUCTION

When describing interactions between light and matter one has to deal with both the radiative and the material degrees of freedom. Treating both types of degrees of freedom on the same footing is often cumbersome, and one would like to integrate out one of the two worlds. The choice for one or the other depends on experimental and on theoretical considerations, but also, to some degree, on taste. In atomic physics, for example, one often chooses to enwrap or dress the atomic properties with the (zero-point) radiative degrees of freedom. Matter is then described by an effective microscopic Hamiltonian and the radiative degrees of freedom are reflected in the natural lifetimes and the Lamb shifts of the atomic levels. A popular line of approach is the further simplification of the electronic structure of the atom into a two-level atom. In this ''all-matter'' representation interactions are also fully described in the space of the atomic degrees of freedom. At not too large interparticle distances, two ground-state atoms experience the van der Waals interaction and an atom in the excited state and an atom in the ground state feel the (resonant) dipole-dipole interaction. Retardation effects become appreciable at large distances and they require another approach than simply integrating out the degrees of freedom of light.

If the response of a microscopic many-body system to an external light source is studied, it makes more sense to treat the material degrees of freedom in some effective manner by capturing them in physical quantities such as the polarizability and conductivity that subsequently enter the equations of motion governing the wave dynamics. Interactions between atoms are then exposed as multiple-light-scattering phenomena. For instance, the recurrent scattering of classical waves from two polarizable particles can be mapped exactly on the interactions so familiar in atomic physics: induced dipole-dipole coupling, the van der Waals interaction,

and nonretarded and retarded Casimir forces (van Tiggelen *et al.*, 1990; van Tiggelen and Lagendijk, 1994; van Tiggelen, 1997).

Given the rapidly growing interest in more dense atomic systems, like Bose-condensed gases (Anderson *et al.*, 1995; Bradley *et al.*, 1995; Davies *et al.*, 1995) and optical lattices (Birkl *et al.*, 1995; Tan *et al.*, 1995; Weidemüller *et al.*, 1995), it is worthwhile to promote the usefulness of the ''all-light'' representation also in atomic physics. Many advances and discoveries made in other fields, predominantly condensed-matter physics, have their counterpart not only in ordered or disordered dielectric systems but also in atomic physics. The analogies in these diverse fields are understood to stem from the underlying wave nature of both (classical) waves and quantum particles. We shall mention a number of concepts that are all connected to multiple scattering of waves. Many of these might be measurable in cold atomic gases.

Photonic band-gap materials. In analogy with the formation of electronic band gaps in periodic solids leading to insulators and semiconductors, periodic dielectric structures have been investigated intensely as a means of creating a band gap for visible light (John, 1987; Yablonovitch, 1987; Soukoulis, 1996; Vos *et al.*, 1996). The resulting manipulation and suppression of spontaneous emission in such lattices is both of fundamental and of practical interest. Recent advances in the optical cooling of atomic gases have made possible the construction of lattices of cold atoms (Birkl *et al.*, 1995; Tan *et al.*, 1995; Weidemüller *et al.*, 1995). In completely filled lattices, band structures for light and even photonic band gaps have been suggested to exist (Deutsch *et al.*, 1995; Sprik *et al.*, 1996; van Coevorden *et al.*, 1996).

Anderson localization of waves. This phenomenon comprises the vanishing of any kind of propagation of classical and quantum-mechanical waves in a strongly scattering disordered sample due to interference (Anderson, 1958, 1985; Abrahams *et al.*, 1979; Akkermans and Maynard, 1985; Lagendijk *et al.*, 1986). As a precursor to Anderson localization, so-called weak-localization effects (Bergmann, 1984), such as enhanced backscattering of light from disordered media have been experimentally observed (Kuga and Ishimaru, 1984; van Albada and Lagendijk, 1985; Wolf and Maret, 1985) and subsequently explained theoretically (Akkermans *et al.*, 1986; Stephen and Cwilich, 1986; Akkermans *et al.*, 1988; MacKintosh and John, 1988; van der Mark *et al.*, 1988). The phenomenon of Anderson localization was first described for the scattering of electrons off impurities in solids (Anderson, 1958; Khmel'nitskii, 1984) and is one of the cornerstones of present-day condensed-matter physics. An unambiguous observation has, however, so far proven to be difficult due to the ubiquitious presence of electron-electron interactions. Anderson localization of light has not yet been reported. The propagation of near-resonant light through optical lattices that are partially filled with ultracold atoms could possibly exhibit Anderson localization. In dense cold atomic gases the phenomenon of enhanced backscattering might also be observable.

Universal conductance fluctuations. Genack (1987) has shown experimentally that speckles in the transmission of light through disordered systems exhibit interesting correlations, in analogy with conductance fluctuations for electrons (Lee and Stone, 1985). It was found theoretically (Feng *et al.*, 1988) that multiply scattered light could be decomposed into short, long, and infinite-range intensity correlations. This field is still an area of active research [see, for example, Sheng (1995)].

Random lasers. The question addressed in this new field is whether or not it is possible to combine laser action in an amplifying medium with multiple scattering. The gain in the system would be determined not by mirrors but by the multiple scattering of the light (Letokhov, 1967; Lawandy *et al.*, 1994).

Lorentz-Lorenz relation. The Lorentz-Lorenz relation (Born and Wolf, 1980) describes the optical response of a dielectric and is usually derived by employing the notion of the Lorentz cavity in combination with some, hitherto, implicit assumptions, rendering it an uncertain theoretical foundation. For a review of a large number of derivations see the work of van Kranendonk and Sipe (1977) and Schnatterly and Tarrio (1992). A reformulation of this problem into a genuine multiple-light-scattering situation has recently produced a rigorous microscopic derivation of the Lorentz-Lorenz relation and the Clausius-Mossotti equation for mixtures (Lagendijk *et al.*, 1997; also see Sec. V). This new approach permits a systematic refinement of the above relations.

Energy-transport velocity of light. It has been shown by van Albada *et al.* (1991) that the velocity determining the transport of diffusive light in a disordered dielectric medium may deviate appreciably from the phase and/or group velocity appropriate for coherent propagation. The marked differences in velocities were shown (Lagendijk and van Tiggelen, 1996) to be due to the occurrence of resonances in the scattering cross section. In gases the phenomenon of radiation trapping (Colbert and Wexler, 1993) is well known. However, radiation trapping is an incoherent process, whereas the phenomenon discussed here is coherent. ''Coherent'' radiation trapping might be observable in cold atomic gases.

Optical Hall effect. Investigation (van Tiggelen, 1995; van Tiggelen *et al.*, 1996) into the properties of multiple scattering of light in magnetic fields has revealed the existence of optical Hall currents. These currents appear as a consequence of the anisotropy of the scattering cross section of optically active atoms and materials.

All of the above phenomena allow for qualitative and quantitative analysis in terms of multiple-scattering theory. In practice the microscopic structures of the relevant scattering building blocks are so complicated that they give rise to rather cumbersome and technically complicated computations. The latter is true even for a spherical Mie scatterer. A tremendous simplification can be obtained by employing pointlike scattering objects as building blocks. In fact, many of the theoretical ad-

vances concerning the above-mentioned topics have been made possible by employing the notion of point scatterers (Lagendijk and van Tiggelen, 1996). The simplicity of the employed building block does not destroy the subtle interference properties that underlie most of these phenomena. The formulation of well-behaving pointlike objects is not straightforward, but given the enormous rewards if successful, this has to be pursued. Among the problems that arise are the singularities inherent in Green's functions when describing the propagation of waves scattering off pointlike scatterers.

In atomic physics pointlike objects have been used since the beginning of this century: In the interaction with light the atom is often treated in the dipole approximation, and this means it is treated as a point dipole. However, the problems we are dealing with here have never been fully addressed in atomic physics. In this paper a consistent procedure for the formulation and treatment of point dipoles will be presented. These point dipoles can represent finite-size dielectric or metallic spheres or finite-size systems with an internal degree of freedom such as atoms in regimes where the wavelength is much larger than any physical size. Clearly, some of the essential physics has to be contained when formulating and applying point scatterers. For example, when considering multiple scattering of light in a medium consisting of random dielectric objects of an arbitrary shape having a large number of geometrical resonances, one can adequately model such a system with randomly distributed point scatterers exhibiting one resonance. This approach is comparable to the use of an effective two-level system or atom in solid-state or semiclassical atomic physics. For frequencies ω close to the resonance frequency ω_0, the linear dynamic polarizability $\alpha(\omega)$ of our point scatterers will be shown to be equivalent to the well-known expression for a damped harmonic oscillator or a two-level system,

$$\alpha(\omega)=\alpha(0)\times\frac{\omega_0^2}{\omega_0^2-\omega^2-i\Gamma\omega}, \tag{1}$$

where Γ is the linewidth of the corresponding resonance. For single atoms, Γ equals the rate of spontaneous emission or Einstein A coefficient.

In this work we employ the Green's-function formalism to construct the T matrix (or dynamic polarizability) describing the scattering of waves from a pointlike particle. We treat both scalar and vector descriptions of electromagnetic waves. Contrary to the case of infinite- and finite-range potentials, the use of a point interaction leads to a T matrix of a single scatterer that has a mathematically simple form in both coordinate and momentum space. This T matrix is therefore very suitable to serve as a building block in multiple-scattering theory. In coordinate space, singularities at $r=0$ of scalar and dyadic Green's functions are encountered. These singularities are inherent in continuum-space Green's functions. They are not present in Green's functions defined on lattices due to the finite support in momentum space of the corresponding Brillouin zone. For a proper and self-consistent formulation of point scatterers these singularities have to be regularized. We shall show that two different regularization parameters have to be introduced in the case of vector waves in order to obtain physically relevant scattering objects. All parameters involved in both the formulation of the point scatterers and the regularization of the Green's functions will be related to physical quantities. Thus no free, adjustable parameters will remain and a complete and self-consistent description will be obtained.

When employing point scatterers the singularities at $r=0$ of the Green's functions may also show up explicitly in the computation of coordinate-dependent physical quantities. For example, in our approach they appear in the local density of states (DOS) of waves in the presence of at least one point scatterer. In the case of vector waves the latter singularities are nonintegrable and thus unphysical. The same problem arises in the normalization of the scattering solutions for vector waves. It is therefore expedient to remove the singularities in such a way that one obtains regularized expressions for Green's functions valid not only for $r=0$, but also for $r\neq 0$. With respect to the latter we adopt a practical approach. For the typical applications that we consider, in which the wavelength of light is very much larger than the spatial extent of the scatterer, the finer details of the interaction region are not easily accessible. In the following, where we represent a finite-size scatterer by a point scatterer, the scattering solutions to be obtained will not be required to be exact *within* the interaction region (size being comparable to physical size). Hence employing regularized Green's functions for $r\neq 0$ as well can be considered to be consistent with the simultaneous use of a point interaction.

In quantum mechanics the use of point interactions has been studied extensively. For a review see, for example, the monograph by Albeverio *et al.* (1988). Existing literature on the scattering of electromagnetic waves from pointlike objects has primarily focused on the formulation of a physical (nonzero) scattering amplitude (Wu, 1984; van Diejen and Tip, 1991; Nieuwenhuizen *et al.*, 1992). Pioneering work was done by Wu, who generalized the Fermi pseudopotential originally designed for quantum particles to the electromagnetic case (Wu, 1984). In his work the singularities of the dyadic Green's function are not treated, but are circumvented by properly modifying the point interaction (Wu, 1984). In contrast to our approach, the resulting Fermi pseudopotential leads to a T matrix that does not exhibit resonant behavior and, therefore, has only limited use.

In a different treatment of point scatterers (van Diejen and Tip, 1991), the ordinary Hilbert space is generalized to a Pontryagin space in which an inner product is formulated that is not positive definite. In the physical subspace the singularities of the Green's function can be dealt with and a unitary S matrix can be formulated. It must be noted that there the longitudinal component of the electric field is projected out. In earlier work on resonant point scatterers for light (Nieuwenhuizen *et al.*, 1992), the Green's function was regularized by introducing an upper cutoff in momentum space. There the regu-

larization was restricted to $r=0$ values of the Green's function. Moreover, the distinction between a transverse and a longitudinal regularization parameter in the case of vector waves was not fully recognized.

This review is organized as follows. In Sec. I the Green's-function scattering theory for a point scatterer is treated and a scattering solution in terms of the T matrix is obtained. The singularities of the Green's functions are discussed and procedures for regularizing them are given and employed. In Sec. III the T matrix of a point scatterer is treated in detail. For vector waves it is found that the regularization parameter corresponding to the longitudinal part of the dyadic Green's function is connected to the physical size of the microscopic scattering object, while the transverse parameter is connected to the dynamic quantities ω_0 and Γ. The relevance of the resulting T matrix for one point scatterer is discussed in connection with behavior in certain regimes of several physical one-particle models. The usefulness of the regularized Green's function approach is demonstrated in Sec. IV by calculating the local DOS of waves in the presence of one point scatterer. Results are given for the various contributions that can be distinguished in the local DOS. In the case of vector waves, the static polarizability $\alpha(0)$ that one measures in a scattering experiment is unequal to the polarizability α_B defining the "bare" coupling between the waves and the point scatterer that enters the Maxwell equations. Both polarizabilities are shown to appear explicitly in the local DOS. The Lorentz-Lorenz relation for the dielectric constant is derived in Sec. V for two cases: a cubic and a disordered arrangement of resonant point dipoles. The derivation for the former case is valid in the long-wavelength limit and follows quite straightforwardly employing the notion of point scatterers. For the latter case, the dielectric constant is obtained from a rigorous microscopic multiple-scattering calculation, which includes particle correlations up to infinite order in the density (Lagendijk *et al.*, 1997). In Sec. VI we conclude with a summary of our results. Some computational details are shown in the Appendix.

II. GREEN'S-FUNCTION FORMALISM

A. Maxwell-Helmholtz equation

In scattering theory one identifies some zeroth-order dynamics of which the *exact* solution is subsequently used to analyze the properties of the wave problem of interest. We first consider the dynamics of electric vector fields having a velocity of light c in a translationally invariant medium (not necessarily a vacuum). The Green's-function formalism is employed. In the scalar description of light, in which the polarization dependence is not regarded, the scalar Green's function g_0 obeys the inhomogeneous Maxwell-Helmholtz equation

$$\left[\frac{\omega^2}{c^2}+i\epsilon+\nabla^2\right]g_0(\omega^+,\mathbf{r}-\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}'). \tag{2}$$

We have used the fact that in translationally invariant media $g_0(\mathbf{r},\mathbf{r}')=g_0(\mathbf{r}-\mathbf{r}')$. To ensure the correct analytical properties of g_0 in the complex frequency plane, or equivalently, to obtain retarded outgoing field solutions, an infinitesimally small and positive imaginary part has been included: $\omega^+\equiv\omega+i\epsilon$. The well-known solutions of Eq. (2) in Fourier and coordinate space are ($k^+\equiv\omega^+/c$)

$$g_0(\omega^+,\mathbf{p})=\frac{1}{k^2-p^2+i\epsilon}, \tag{3}$$

$$g_0(\omega^+,\mathbf{r})=-\frac{e^{ik^+r}}{4\pi r}. \tag{4}$$

In coordinate space, g_0 is characterized by outgoing spherical waves and a $1/r$ singularity which is square integrable at $r=0$.

The dyadic Green's function $\mathcal{G}_0$ satisfies the inhomogeneous dyadic Maxwell-Helmholtz equation

$$\left[\left(\frac{\omega^2}{c^2}+i\epsilon\right)\mathcal{I}-\nabla\times\nabla\times\right]\mathcal{G}_0(\omega^+,\mathbf{r}-\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')\mathcal{I}, \tag{5}$$

where $\mathcal{I}$ is the 3×3 unit tensor in polarization space. Making use of the product rule $\nabla\times\nabla\times=\nabla\otimes\nabla-\nabla^2\mathcal{I}$, in which $\otimes$ defines a dyad or tensor product, and Fourier-transforming Eq. (5) to momentum space gives

$$\begin{aligned}\mathcal{G}_0(\omega^+,\mathbf{p})&=\frac{1}{(k^2+i\epsilon)\mathcal{I}-p^2\boldsymbol{\Delta}_p}\\&=\frac{1}{k^2-p^2+i\epsilon}\,\boldsymbol{\Delta}_p+\frac{1}{k^2}\,\hat{\mathbf{p}}\otimes\hat{\mathbf{p}}\\&\equiv\mathcal{G}_0^T(\omega^+,\mathbf{p})+\mathcal{G}_0^L(\omega^+,\mathbf{p}).\end{aligned} \tag{6}$$

Here $\Delta_{\mathbf{p}}\equiv\mathcal{I}-\hat{\mathbf{p}}\otimes\hat{\mathbf{p}}$ represents a projector upon the space normal to the unit vector $\hat{\mathbf{p}}\equiv\mathbf{p}/p$. The Green's function (6) can be decomposed into a transverse (T) and longitudinal (L) part with respect to the momentum $\mathbf{p}$. The former describes transverse propagating modes, whereas the latter, having a pole at $k=0$, describes the nonpropagating (electrostatic) modes.

The dyadic solution of Eq. (5) in coordinate space reads (see the Appendix)

$$\mathcal{G}_0(\omega^+,\mathbf{r})=-\left(\mathcal{I}+\frac{1}{k^2}\,\nabla\otimes\nabla\right)\frac{e^{ik^+r}}{4\pi r}, \tag{7}$$

$$=-\frac{e^{ik^+r}}{4\pi r}\,[P(ikr)\mathcal{I}+Q(ikr)\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}]+\frac{\delta(\mathbf{r})}{3k^2}\,\mathcal{I}, \tag{8}$$

in which the functions P and Q are defined by

$$P(z)\equiv\left(1-\frac{1}{z}+\frac{1}{z^2}\right),\quad Q(z)\equiv\left(-1+\frac{3}{z}-\frac{3}{z^2}\right). \tag{9}$$

Following Eq. (6) the decomposition into a transverse and a longitudinal part in momentum space leads to (see the Appendix)

$$\mathcal{G}_0^T(\omega^+,\mathbf{r}) = -\frac{\mathcal{I}-3\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}}{4\pi k^2 r^3} - \frac{e^{ik^+r}}{4\pi r}\,[P(ikr)\mathcal{I} + Q(ikr)\hat{\mathbf{r}}\otimes\mathbf{r}], \tag{10}$$

and

$$\mathcal{G}_0^L(\omega,\mathbf{r}) = \frac{\mathcal{I}-3\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}}{4\pi k^2 r^3} + \frac{\delta(\mathbf{r})}{3k^2}\,\mathcal{I}. \tag{11}$$

In the far-field regime $kr \gg 1$, the transverse Green's function (defined with respect to momentum) also becomes transverse with respect to $\mathbf{r}$: $\mathcal{G}_0^T(\omega^+,\mathbf{r}) \approx -\exp(ik^+r)\Delta_{\mathbf{r}}/4\pi r$. In the static limit $\omega\to 0$, or for $r\to 0$, the "dipole" parts proportional to $1/r^3$ in $\mathcal{G}_0^T$ cancel and terms $\propto(\mathcal{I}+\hat{\mathbf{r}}\otimes\hat{\mathbf{r}})/r$ remain. Moreover, in the static limit $k\mathcal{G}_0^T(\omega^+,r)\to 0$. The transverse part of $\mathcal{G}_0$, therefore, has the same singularity in $r=0$ as the scalar Green's function (3). The longitudinal part of $\mathcal{G}_0$ exhibits a nonintegrable $1/r^3$ singularity. The occurrence of the delta function in $\mathcal{G}_0^L$ is completely analogous to the well-known case in electrostatics (Jackson, 1975, p. 141), where it ensures that the average field over a small sphere including a static point dipole is nonzero. The delta function (Weiglhofer, 1989) in Eqs. (8) and (11), which in the literature is often ignored and has to be added by hand, ensures that certain "sum" rules are satisfied. For example, $\int d\mathbf{r}\mathcal{G}_0(\omega^+,\mathbf{r}) = \mathcal{G}_0(\omega^+,\mathbf{p}=0) = \mathcal{I}/k^2$ [the angular average of $\mathcal{G}_0(\omega^+,\mathbf{r})$ excluding the delta function gives $\frac{2}{3}g_0(\omega^+,r)\mathcal{I}$].

The Green's functions or propagators g_0 and $\mathcal{G}_0$ carry the complete information about the spectrum and dynamics of electric scalar or vector fields described by the corresponding homogeneous scalar or vector Maxwell-Helmholtz equation. Electric fields $\mathbf{E}(\omega^+,\mathbf{r})$ resulting from introducing a source term $\mathbf{S}(\omega,\mathbf{r})$ in the homogeneous vector Maxwell-Helmholtz equation are then given by

$$\mathbf{E}(\omega^+,\mathbf{r}) = \int d\mathbf{r}'\,\mathcal{G}_0(\omega^+,\mathbf{r}-\mathbf{r}')\cdot\mathbf{S}(\omega,\mathbf{r}'). \tag{12}$$

A similar equation holds for the scalar case. The field solutions of the homogeneous Maxwell-Helmholtz equation can be added to Eq. (12).

The Green's functions g_0 and $\mathcal{G}_0$ describe the propagation of waves from an external δ-function source located at $\mathbf{r}'$ to the "observation" point $\mathbf{r}$. For example, see Jackson (1975, p. 395). Given an external oscillating dipole moment $\mathbf{d}\exp(-i\omega t)$ at $\mathbf{r}'$, the electric dipole field at $\mathbf{r}$ (containing radiative and longitudinal parts) is $\mathbf{E}(t,\mathbf{r}) = -(k^2/\varepsilon)\mathcal{G}_0(\omega^+,\mathbf{r}-\mathbf{r}')\cdot\mathbf{d}\exp(-i\omega t)$, where ε is the background permittivity. One should note that the dyadic Green's function $\mathcal{G}_0$ does obey the Maxwell equation

$$\boldsymbol{\nabla}\cdot\mathcal{G}_0(\omega^+,\mathbf{r}-\mathbf{r}') = \mathbf{0}, \tag{13}$$

because both the transverse electric-field solutions of the homogeneous vector Maxwell-Helmholtz equation and the dipole field (for $\mathbf{r}\neq\mathbf{r}'$) of a point dipole at $\mathbf{r}'$ do so. With the use of Eq. (12) and the delta function in $\mathcal{G}_0^L$ it follows that $\boldsymbol{\nabla}\cdot\mathbf{E}=0$ is satisfied for $\mathbf{r}=\mathbf{r}'$ if simultaneously $\boldsymbol{\nabla}\cdot\mathbf{S}=0$.

B. Scattering from a point particle

In this subsection we formulate the T matrix of a single scatterer, where the latter is regarded as a point particle. The former may be an atom or a dielectric sphere on/off resonance. The treatment will be given for vector waves; the differences from the case of scalar waves will be discussed in Sec. III.B. Our starting point is the introduction of a source term on the right-hand side of the dyadic Maxwell-Helmholtz equation (5). The Green's function $\mathcal{G}(\omega^+)$ for the full problem, written as a matrix in continuous coordinate space, obeys

$$\left[\left(\frac{\omega^2}{c^2}+i\epsilon\right)\mathcal{I}-\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\right]\mathcal{G}(\omega^+) = \mathbf{1}\otimes\mathcal{I} - \frac{\omega^2}{c^2}\,\mathcal{X}\mathcal{G}(\omega^+), \tag{14}$$

where $\mathbf{1}\otimes\mathcal{I}$ denotes the direct product of the unit matrices in coordinate and polarization space, $\mathbf{1}(\mathbf{r},\mathbf{r}') \equiv \delta(\mathbf{r}-\mathbf{r}')$, and $\mathcal{X}\equiv\mathcal{X}(\mathbf{r})\mathbf{1}$ is the (dimensionless) electric susceptibility. In the case of a spatially varying dielectric medium, $\mathcal{X}(\mathbf{r})\equiv\varepsilon(\mathbf{r})-\mathcal{I}$, where $\varepsilon(\mathbf{r})$ is the $\mathbf{r}$-dependent dielectric constant (relative to the one of a homogeneous medium with velocity of light c). In terms of a *frequency-dependent* potential $\mathcal{V}(\omega) \equiv -(\omega/c)^2\mathcal{X}$, Eq. (14) can be written as

$$\mathcal{G}(\omega^+) = \mathcal{G}_0(\omega^+) + \mathcal{G}_0(\omega^+)\mathcal{V}(\omega)\mathcal{G}(\omega^+). \tag{15}$$

This equation is the starting point of a (multiple-) scattering theory and is often called the Lippmann-Schwinger equation. In the case of disordered media and employing averaging techniques it is also called the Dyson equation. The frequency dependence of the potential constitutes a major difference from quantum-mechanical scattering theories and has some important consequences (Lagendijk and van Tiggelen, 1996).

We now define a point scatterer located at $r=0$ according to

$$\mathcal{V}(\omega,\mathbf{r}) \equiv -(\omega/c)^2\alpha_B\delta(\mathbf{r})\mathbf{1}\otimes\mathcal{I}, \tag{16}$$

where α_B (dimension of a volume) is the "bare" polarizability describing the strength of the coupling between the electromagnetic waves and where the pointlike particle represents effectively a microscopic finite-size scatterer. The "polarizability" α_B enters the equations of motion as a potential term and, generally, can be a tensor but is taken as scalar here for simplicity. As yet the value of α_B is still optional. In Sec. III particular choices for the bare coupling α_B will be discussed. We shall also show that α_B is related to the static polarizability $\alpha(0)$ that one measures in an experiment. Note (Lakhtakia, 1990) that the dipole moment $\mathbf{d}$ can be expressed by either $\mathbf{d}=\alpha(0)\mathbf{E}^{\text{exc}}$ or $\mathbf{d}=\alpha_B\mathbf{E}$, where $\mathbf{E}^{\text{exc}}$ is the electric field *exciting* the dipole and $\mathbf{E}$ is the field *including* depolarization effects. The scattering T matrix $\mathcal{T}$, defined by

$$\mathcal{G}(\omega^+) \equiv \mathcal{G}_0(\omega^+) + \mathcal{G}_0(\omega^+)\mathcal{T}(\omega^+)\mathcal{G}_0(\omega^+), \tag{17}$$

is given by the well-known Born series generated by iterating $\mathcal{G}_0$ in the integral equation (15),

$$\mathcal{T}(\omega^+)=\mathcal{V}(\omega)+\mathcal{V}(\omega)\mathcal{G}_0(\omega^+)\mathcal{V}(\omega)+\mathcal{V}(\omega)\mathcal{G}_0(\omega^+)\mathcal{V}(\omega)\mathcal{G}_0(\omega^+)\mathcal{V}(\omega)+\ldots,$$
$$=t(\omega^+)\,\delta(\mathbf{r})\mathbf{1}\otimes\mathcal{I}, \tag{18}$$

where the T-matrix element $t(\omega^+)$ is determined by

$$t(\omega^+)\mathcal{I}=-(\omega/c)^2\,\frac{\alpha_B}{\mathcal{I}+(\omega/c)^2\alpha_B\mathcal{G}_0(\omega^+,r=0)}. \tag{19}$$

The above Born series could be summed exactly, because of the simple form of the potential. For a point scatterer located at $\mathbf{r}=\mathbf{R}_P$ the T matrix, written out fully, reads

$$\mathcal{T}_P(\omega^+,\mathbf{r},\mathbf{r}')=t(\omega^+)\,\delta(\mathbf{r}-\mathbf{R}_P)\,\delta(\mathbf{r}'-\mathbf{R}_P)\mathcal{I}, \tag{20}$$

showing the extremely simple form of $\mathcal{T}$ that can be obtained employing point scatterers. The T matrix $\mathcal{T}(\omega^+,\mathbf{r},\mathbf{r}')$ describes the scattering of the electric field from position r to position $\mathbf{r}'$ by a particle located at $\mathbf{R}_P$. The dynamic polarizability $\alpha(\omega)$ of the point scatterer is given by [see also Eq. (23)]

$$\alpha(\omega)=-t(\omega)/(\omega/c)^2. \tag{21}$$

The T matrix given by Eq. (18), with the T-matrix element given by Eq. (19), describes the scattering exactly to all orders of the coupling α_B. The corresponding Green's function, following from Eq. (17),

$$\mathcal{G}(\omega^+,\mathbf{r},\mathbf{r}')=\mathcal{G}_0(\omega^+,\mathbf{r}-\mathbf{r}')+t(\omega)\mathcal{G}_0(\omega^+,\mathbf{r})\mathcal{G}_0(\omega^+,\mathbf{r}'), \tag{22}$$

is the exact solution exhibiting the dynamics of waves in the presence of one point scatterer located at $r=0$. Note that the point scatterer breaks the translational symmetry. The first term in Eq. (22) represents the unscattered propagation of waves from a source point at $\mathbf{r}'$ to the observation point $\mathbf{r}$. The second term describes the propagation from $\mathbf{r}'$ to the position of the point scatterer, the scattering process through t, and the subsequent propagation to $\mathbf{r}$. In the far-field regime the r-dependent factor of the latter term reads

$$t(\omega)\mathcal{G}_0(\omega^+,\mathbf{r})\overset{kr\gg1}{\rightarrow}-t(\omega)e^{ik^+r}\,\frac{\Delta_r}{4\pi r}+\alpha(\omega)\,\frac{3\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}-\mathcal{I}}{4\pi r^3}, \tag{23}$$

where we have used the relation (21) between $t(\omega)$ and $\alpha(\omega)$. In the static limit $\omega\rightarrow0$ only the "dipole" part remains. The Green's function $\mathcal{G}_0$ also represents the field response of an oscillating dipole (Jackson, 1975), so that Eqs. (22) and (23) demonstrate that a point scatterer is equivalent to a point dipole.

As we saw in the previous subsection, the matrix element of $\mathcal{G}_0$ at $r=0$ is infinite, rendering a zero T matrix. In order to retain a physical nonzero scattering and nonzero polarizability, we therefore have to replace $\mathcal{G}_0(\omega^+,r=0)$ by its regularized version. We shall now discuss how this can be achieved.

C. Regularization procedures

The singularities of the Green's functions at $r=0$ are connected to the large-p behavior in Fourier space. So, in order to remove the singularities, one can modify this behavior. The regularized scalar Green's function, denoted by $\tilde{g}_0$, that we use is defined according to

$$\tilde{g}_0(\omega^+,\mathbf{p})\equiv g_0(\omega^+,\mathbf{p})\times f(\Lambda,p),\quad f(\Lambda,p)\equiv\frac{\Lambda^2}{\Lambda^2+p^2}. \tag{24}$$

The regularization factor $f(\Lambda,p)$ moderates the large-p behavior of $g_0(\omega^+,\mathbf{p})$ and is appropriate provided one is not interested in variations over length scales smaller than the inverse of Λ, i.e., the finer details of the interaction region are not of specific interest. The factor $f(\Lambda,p)$ has been used among others in electrodynamics to regularize the so-called transverse delta function (Cohen-Tannoudji *et al.*, 1989). To have a relevant point-scatterer description and to alter the zeroth-order dynamics as little as possible, one has to take the cutoff momentum Λ sufficiently large relative to ω/c or the inverse length scales one is interested in. Observe that, for $p\ll\Lambda$, $f(\Lambda,p)\rightarrow1$. The volume integral of $\tilde{g}_0(\omega^+,r)$, therefore, will equal the volume integral over g_0, giving $g_0(p=0)=1/k^2$. In coordinate space one obtains

$$\tilde{g}_0(\omega^+,r)=-\frac{e^{ik^+r}-e^{-\Lambda r}}{4\pi r}\times f(\Lambda,k), \tag{25}$$

which is a continuous function of r and converges exponentially to the unregularized Green's function. The real and imaginary parts of $\tilde{g}_0$ still satisfy the well-known Kramers-Kronig relations (Born and Wolf, 1980) expressing the inherent causal properties of the Green's function (25) in the complex frequency plane. The small-r behavior of $\tilde{g}_0$ has now indeed become finite,

$$\tilde{g}_0(\omega^+,r=0)=-\left(\frac{\Lambda}{4\pi}+i\,\frac{k}{4\pi}\right). \tag{26}$$

Anticipating a description of point scatterers for appropriate frequency values only, we take $k/\Lambda\ll1$ and therefore have set $f(\Lambda,k)=1$ in Eq. (26). Note that the singular behavior of $g_0(\omega^+,r)$ pertains solely to its real part and that for the frequencies of interest $k/\Lambda\ll1$, similarly, only the real part of $\tilde{g}_0(\omega^+,r)$ will reflect the cutoff momentum Λ.

The employed regularization procedure is of course not unique, but it suffices for our purposes. The regulator $\theta(\Lambda-p)$, where θ is the Heaviside step function expressing a sharp momentum cutoff, could also have been used [see, for example, Nieuwenhuizen *et al.* (1992)]. This choice leads to the same result as in Eq. (26). Evidently, the form of the regularized g_0 for $r\neq0$ would be markedly different from that of Eq. (25), viz., $\tilde{g}_0=g_0-Si(r\Lambda)/2\pi^2r$, where Si is the sine-integral. The latter term vanishes as $1/\Lambda$ for large Λ. Our choice of Eq. (24) leads to a simpler expression for $\tilde{g}_0$ for $r\neq0$, which in addition converges exponentially to g_0.

We now turn to the vector case. Because the singularities of $\mathcal{G}_0^T$ and $\mathcal{G}_0^L$ differ, we allow for two regularization procedures with different parameters, Λ_T and Λ_L:

$$\widetilde{\mathcal{G}}_0^T(\omega^+,\mathbf{p}) \equiv \mathcal{G}_0^T(\omega^+,\mathbf{p}) \times f(\Lambda_T,p),$$

$$\widetilde{\mathcal{G}}_0^L(\omega^+,\mathbf{p}) \equiv \mathcal{G}_0^L(\omega^+,\mathbf{p}) \times \frac{\Lambda_L^4}{\Lambda_L^4+p^4}. \tag{27}$$

In coordinate space one obtains (see the Appendix)

$$\widetilde{\mathcal{G}}_0^T(\omega^+,\mathbf{r}) = -\frac{\mathcal{I}-3\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}}{4\pi k^2 r^3} - \left\{ \frac{e^{ik^+ r}}{4\pi r}\left[P(ikr)\mathcal{I} + Q(ikr)\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}\right] - \frac{e^{-\Lambda_T r}}{4\pi r}\left[P(-\Lambda_T r)\mathcal{I} + Q(-\Lambda_T r)\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}\right]\right\} f(\Lambda_T,k), \tag{28}$$

and

$$\widetilde{\mathcal{G}}_0^L(\omega,\mathbf{r}) = \frac{\mathcal{I}-3\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}}{4\pi k^2 r^3} \times \{1 - e^{-\Lambda_L r}[\cos\Lambda_L r + \Lambda_L r(\cos\Lambda_L r + \sin\Lambda_L r)]\} + \frac{\Lambda_L^2 e^{-\Lambda_L r}\sin\Lambda_L r}{2\pi k^2 r}\,\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}, \tag{29}$$

where we have absorbed a factor $1/\sqrt{2}$ in Λ_L. It can again be seen that the regularized Green's functions converge exponentially to their unregularized counterparts. The sum rule given by the volume integral over $\widetilde{\mathcal{G}}_0^T + \widetilde{\mathcal{G}}_0^L$ now exactly amounts to $\mathcal{I}/k^2$, so that a delta-function contribution is no longer required. Now, taking powers of the Green's function does not give rise to awkward terms for $r \to 0$. We retrieve the original transverse and longitudinal Green's function (10) and (11) by letting $\Lambda_T, \Lambda_L \to \infty$. The finite values of $\widetilde{\mathcal{G}}_0^T$ and $\widetilde{\mathcal{G}}_0^L$ at $r=0$ are given by

$$\widetilde{\mathcal{G}}_0^T(\omega,r=0) = -\left(\frac{\Lambda_T}{6\pi} + i\,\frac{k}{6\pi}\right)\mathcal{I}, \tag{30}$$

$$\widetilde{\mathcal{G}}_0^L(\omega,r=0) = \frac{\Lambda_L^3}{6\pi k^2}\,\mathcal{I}, \tag{31}$$

where just as for the scalar case we have set $f(\Lambda_T,k)=1$. Equations (26), (30), and (31) are now properly behaved and can be employed in the formulation of a physical nonzero T matrix. The exponent of the regularization parameter reflects the order of the singularity in $r=0$. Results comparable to Eqs. (29) and (31) can be obtained using $f_{\Lambda_L}^2$ as a regularization factor instead of $\Lambda_L^4/(\Lambda_L^4+p^4)$. The trigonometric terms in Eq. (29) would then be replaced by polynomial ones, resulting only in a different numerical prefactor in Eq. (31).

The result Eq. (31) can also be derived using the following argument, which in addition allows for an interpretation of the momentum cutoff Λ_L. Maxwell's equations are basically a macroscopic theory, so pointlike objects in fact represent some microscopic structure that cannot be resolved on the scale of the wavelength of light. The $1/r^3$ behavior of $\mathcal{G}_0^L$ in Eq. (11), when appearing in combination with a T-matrix expression, can then be considered to apply only for $r>a$, where a is some microscopic length, while the delta function can be replaced by a constant being the inverse of the volume $V_0 = 4\pi a^3/3$. In this way it follows that the parameter Λ_L is inversely proportional to a (static) microscopic length

$$\frac{\Lambda_L^3}{6\pi} = \frac{1}{3V_0}. \tag{32}$$

In the next section we show that the transverse parameter Λ_T, or Λ for scalar waves, can be related to the dynamic quantities ω_0 and Γ of a resonance at finite frequency.

Note that regularization *and* setting $f(\Lambda,k)=1$ and $f(\Lambda_T,k)=1$ for the frequency values of interest essentially modifies only the real part of g_0 and $\mathcal{G}_0$. Since the imaginary part of the Green's functions (see Sec. IV) describes the continuous-wave spectrum, the low-frequency eigenvalues of the scalar and dyadic Maxwell-Helmholtz equations (2) and (5) remain practically unchanged. For low frequencies, the regularization procedure has primarily affected the behavior of the eigenfunctions on very small length scales such that $kr \ll 1$, $r\Lambda \ll 1$, and $r\Lambda_{T,L} \ll 1$.

We have thus defined zeroth-order dynamics ($\widetilde{g}_0$ and $\widetilde{\mathcal{G}}_0$) for both scalar and vector waves. The regularized versions are appropriate for setting up a (multiple-) scattering theory that can accommodate point interactions for relevant frequencies.

III. *T* MATRIX FOR A POINT SCATTERER

A. General solution for vector waves

In this subsection we continue the treatment of Sec. II.B and give the physical and exact solution for the T matrix of a point scatterer. To this end, we replace in Eq. (19) the Green's function at $r=0$ by $\widetilde{\mathcal{G}}_0(\omega^+,r=0)$, which we calculated above. In this manner a physical nonzero T matrix can be formulated. Neglecting terms of higher order than $\omega/c\Lambda_T$, i.e., setting $f(\Lambda_T,k)=1$, we obtain from Eqs. (19), (30), and (31)

$$t(\omega) = -\frac{(\omega/c)^2}{\alpha_B^{-1} + \Lambda_L^3/6\pi - (\omega/c)^2\Lambda_T/6\pi - i(\omega/c)^3/6\pi}. \tag{33}$$

Note that in Eq. (19) α_B is taken to be a scalar that is yet to be chosen. We first treat the case of a frequency-independent α_B. In Secs. III.E and III.F the extension to a frequency-dependent bare coupling will be discussed.

Next, we relate the parameters in the resulting T-matrix element with the appropriate physical quantities of the finite-size scatterer we wish to represent by employing a point-scatterer model. Let us first note that in the denominator of Eq. (33) the terms proportional to

α_B^{-1} and Λ_L^3 are independent of frequency. Consequently, with Eqs. (21) and (23) the parameters α_B and Λ_L can be related to an experimentally accessible static polarizability $\alpha(0)$ as

$$\alpha(0)=\frac{\alpha_B}{1+\alpha_B\Lambda_L^3/6\pi}. \tag{34}$$

In the T-matrix element $t(\omega)$ a Lorentzian-type resonance can be identified with resonance frequency ω_0 and linewidth Γ given by

$$(\omega_0/c)^2\equiv\frac{6\pi}{\Lambda_T\alpha(0)},\quad \Gamma=\frac{\omega_0^2}{c\Lambda_T}. \tag{35}$$

In terms of the quality factor $Q\equiv\omega_0/\Gamma$ of the resonance, the transverse regularization parameter is determined by

$$\Lambda_T=\omega_0 Q/c. \tag{36}$$

Observe that Λ_L and Λ_T are related to static and dynamic quantities, respectively. Note that the imaginary term in $t(\omega)$ results from the coupling of the point scatterer with transverse modes described by $\mathcal{G}_0^T$: i.e., the finite width of the resonance is due to radiative damping.

Having expressed the parameters α_B, Λ_L, and Λ_L in terms of the physical quantities pertaining to an effective two-level system, we finally arrive at

$$t(\omega)=-(\omega/c)^2\alpha(0)\times\frac{\omega_0^2}{\omega_0^2-\omega^2-i(\Gamma\omega^3/\omega_0^2)}, \tag{37}$$

where the set $\{\omega_0,\Gamma,\alpha(0)\}$ consists of two independent quantities determining the point scatterer. The corresponding polarizability is in agreement with Eq. (1) and relates to the case of a two-level system or an atom exhibiting one resonant (electric dipole) transition. The T matrix (18) is diagonal in polarization space, but it can be generalized straightforwardly for tensorial α_B. At resonance one obtains an imaginary T-matrix element $t(\omega_0)=-i(\omega_0/c)^2\alpha(0)Q$. Equations (37) and (18) describe a Rayleigh scatterer: at low frequency the cross section (see below) vanishes as ω^4 and the anisotropically scattered intensity exhibits the angular distribution $(1+\cos^2\theta)$. An important property of $t(\omega)$ is that it obeys the optical theorem (Newton, 1982; Lagendijk and van Tiggelen, 1996)

$$-\frac{\mathrm{Im}\,t(\omega)}{k}=\frac{|t(\omega)|^2}{6\pi}=\sigma_{\mathrm{scat}}(\omega). \tag{38}$$

This relation says that the extinction (left-hand side) from the incoming light is transformed entirely into scattered intensity, given by the scattering cross section σ_{scat}, i.e., there is no absorption. It also confirms that Eq. (37) features only two independent quantities, which was already implicit in Eq. (35). For the optical theorem to hold, the physical observables in Eq. (37) should satisfy

$$Q=\frac{6\pi}{\alpha(0)(\omega_0/c)^3}. \tag{39}$$

For atoms the quality factor is very high, $Q\gg1$, so that Eq. (39) indicates that the ratio of the resonantly enhanced scattering cross section and the geometrical cross section of the point scatterer (associated with the static polarizability) is very large. Indeed, at resonance we have ($\lambda_0\equiv2\pi c/\omega_0$)

$$\sigma_{\mathrm{scat}}(\omega_0)=\frac{3}{2}\frac{\lambda_0^2}{\pi}, \tag{40}$$

which is the unitarity limit of σ_{scat} (Newton, 1982). Note that Eqs. (34) and (39) together imply that $\alpha(0)$, Q, Λ_T, and Λ_L should satisfy the (equivalent) inequalities

$$0<\alpha(0)\leqslant6\pi/\Lambda_L^3\Rightarrow Q=c\Lambda_T/\omega_0\geqslant(c\Lambda_L/\omega_0)^3. \tag{41}$$

Since $c\Lambda_{T,L}/\omega_0\gg1$, one finds that $1/\Lambda_T<1/\Lambda_L$. In fact, $1/\Lambda_T$ can be much smaller than $1/\Lambda_L$ for specific cases.

It is interesting to compare Eq. (39) with Fermi's "golden rule" expression for the Einstein spontaneous emission coefficient of an atom in free space. The partial static polarizability in terms of the electric dipole matrix element μ of two atomic levels is $\alpha(0)=2|\mu|^2/\varepsilon_0\hbar\omega_0$. Inserting the latter in Eq. (39) gives the well-known result (Loudon, 1983) $\Gamma=\omega_0^3|\mu|^2/3\pi\varepsilon_0\hbar c_0^3$.

In order to describe simultaneously, for instance, two (overlapping) atomic transitions with resonance frequencies ω_1 and ω_2 and partial static polarizabilities $\alpha_1(0)$ and $\alpha_2(0)$ [such that $\alpha(0)=\alpha_1(0)+\alpha_2(0)$ is the total static polarizability of the atom], one may write the T-matrix element as a linear combination of the T matrices t_1 and t_2 of the form (37). In $t=t_1+t_2$, interference effects from the two transitions have then been neglected. The transverse regularization parameters $\Lambda_{T(1,2)}$ enter the appropriate Green's function, appearing in expressions of the form $(t\tilde{\mathcal{G}}_0)_{(1,2)}$ [see, for example, Eq. (61)], denoting the propagation of waves scattered off the atom. For both transitions the longitudinal parameter Λ_L is the same, i.e., Λ_L^{-1} is approximately equal to the atomic size.

We now return to Eq. (34) and discuss the determination of α_B and Λ_L. Generally, an experimentally determined static polarizability does not fix the values of both α_B and Λ_L. In Sec. IV it is shown that the bare polarizability explicitly enters expressions for the local DOS of waves providing another independent connection between α_B and a physical quantity. On the other hand, in the preceding section it was argued that Λ_L can be interpreted as an inverse microscopic length scale [see Eq. (32)]. Identifying this length scale with the actual size of a small finite particle, one obtains $\Lambda_L^3\approx V_0^{-1}$ with V_0 now being the volume of the scattering particle. If this volume is known, the static polarizability sets the value of α_B. For an atom, Λ_L^{-1} should then be related to the "size" of the electronic wave function, i.e., the Bohr radius. An alternative approach would be to use a microscopic theory to calculate *a priori* the source term $\mathcal{X}$ in

the Maxwell-Helmholtz equation. Subsequently, by an appropriate length scaling, a suitable coupling α_B may be derived for an effective point-scatterer description. A more rigorous identification for α_B and Λ_L can be made in the cases where our formulation of point scatterers is applied to small dielectric or perfectly conducting spheres. These cases will be treated in Secs. III.C and III.E.

Summarizing this subsection, we have obtained a self-consistent description of a point scatterer for classical waves with no adjustable parameters. The regularization parameters and bare polarizability have been connected with physically observable quantities. For vector waves it is important to distinguish between a static and a dynamic parameter.

B. Classical scalar and quantum-mechanical waves

We shall now indicate the differences between vector and scalar waves. Clearly, the most important difference is the absence of a longitudinal part in g_0 in Eq. (19). Hence the bare polarizability α_B entering the scalar version of the Maxwell equations equals the static polarizability $\alpha(0)$ that is measured in an experiment. The equations above (and below) remain valid for scalar waves provided one performs the substitutions $\Lambda_T \to \Lambda$, $\Lambda_L \to 0$, and $6\pi \to 4\pi$ (alternatively $\frac{3}{2} \to 1$). This makes $t(\omega)$, and correspondingly $\alpha(\omega)$, almost identical for scalar and vector waves. The restrictions (41) on $\alpha(0)$ and Q, however, do not apply to scalar waves. Furthermore, the physical size of the pointlike scatterer enters the scalar description only through $\alpha_B = \alpha(0)$.

In the case of quantum-mechanical wave scattering from a pointlike particle, described by a frequency-independent potential $V(\mathbf{r}) \equiv U_0 \delta(\mathbf{r})\mathbf{1}$ and U_0 a constant, an approach similar to the one above leads to a renormalization of U_0: $U = U_0/(1 + U_0 \Lambda/4\pi)$. The resulting T-matrix element $t(\omega) = 1/(1/U + ik/4\pi)$ obeys the optical theorem and goes to a nonzero constant for $\omega \to 0$ as expected. The parameter U is determined by the cross section σ_{scat}. The T-matrix element, however, does not exhibit any resonance.

C. Small dielectric sphere

In this subsection and those that follow, we compare our point-scatterer formalism to several physical models and elucidate under which conditions the latter may be described by our point-interaction model. We first treat the case of small dielectric spheres.

1. Electrostatics

For a dielectric sphere with volume $V = 4\pi a^3/3$ and (relative) dielectric constant ε it is well known from electrostatics (Jackson, 1975) that the experimentally observed polarizability is not the bare polarizability given by $\alpha_B = (\varepsilon - 1)V$, which enters the Maxwell-Helmholtz equation, but in fact

$$\alpha(0) = 3\frac{\varepsilon - 1}{\varepsilon + 2} V, \tag{42}$$

due to the boundary conditions on the surface of the sphere. Using Eq. (34) one finds that

$$\Lambda_L^3/6\pi = 1/3V. \tag{43}$$

One thus recovers Eq. (32) with $V = V_0$. Equation (34) can be written as

$$\alpha_B = \alpha(0)/[1 - \alpha(0)/3V], \tag{44}$$

indicating that Λ_L^3 expresses a geometrical depolarization effect. In the case of a perfectly conducting sphere, electrostatics (Jackson, 1975) gives the result $\alpha(0) = 3V$ (see also Sec. III.E). Observing that for a perfect conductor the effective dielectric constant $\varepsilon \to -\infty$ one finds $\alpha_B \to -\infty$ and Eq. (32) with $V = V_0$. Hence one can indeed rigorously relate Λ_L^{-1} to the actual physical size of pointlike scatterers. Note that for dielectric and conducting spheres resonances are of geometrical origin, while for atoms the resonances are internal ones, i.e., they correspond to an internal degree of freedom.

The exact scattering solution in terms of vector spherical harmonics is known for a finite-size dielectric sphere (van de Hulst, 1957; Bohren and Huffman, 1983). The Mie scattering coefficient $a_1(x, \varepsilon)$, corresponding to the electric dipole normal mode, is expressed in terms of the size parameter $x \equiv \omega a/c$, ε and Riccati-Bessel functions and satisfies the optical theorem for real ε. The T-matrix element of the above normal-mode solution is $t_{\text{Mie}}(\omega) = \mp i 6\pi c a_1/\omega$ (the sign depending on the definition of a_1 in the literature). By examining $t_{\text{Mie}}(\omega)$ for small size parameters and varying ε one may find behavior comparable to Eq. (37) in certain cases. Employing Eqs. (33) and (34), one can obtain expressions for Λ_L and Λ_T given that $\alpha_B = (\varepsilon - 1)V$. We now discuss the resonant and Rayleigh regimes.

2. Resonant regime

For small size parameters $x \ll 1$ and simultaneously large ε, the above t_{Mie} exhibits resonant behavior (van de Hulst, 1957). The size parameter at resonance is determined (van de Hulst, 1957) by $\sqrt{\varepsilon} x_0 = r_1/(1 + 1/\varepsilon)$ with r_1 being one of the roots of the spherical Bessel function j_1. Near the resonance frequency, behavior equivalent to t of Eq. (19) is found: $t_{\text{Mie}} = t(\omega)[1 + O(x_0^2)][1 + O(x_0 - x)]$. For large ε, α_B may be neglected, leading to

$$\frac{\Lambda_L^3}{6\pi} = \frac{\varepsilon x_0^2}{12\pi a^3}, \quad \frac{\Lambda_T}{6\pi} = \frac{\varepsilon}{12\pi a}. \tag{45}$$

It can be seen that $\Lambda_T \gg \Lambda_L \approx 1/a$.

3. Rayleigh regime

For $x \ll 1$ and $\sqrt{\varepsilon} x \ll 1$ no resonant scattering is obtained. The t matrix may simply be written as $t_{\text{Mie}} \simeq -k^2 \alpha(0)$, where $\alpha(0)$ is given by Eq. (42). To ensure

that the T matrix satisfies the optical theorem it may also be expressed in a form similar to Eq. (37),

$$t_{\mathrm{Mie}}=-k^2\alpha(0)\times\left\{1-\frac{\varepsilon-1}{\varepsilon+2}[(\varepsilon+10)x^2/10 +i2x^3/3]\right\}^{-1}[1+O(x^2)]. \tag{46}$$

The "resonance" lies at frequencies where the above approximation does not hold. From Eq. (46) one derives again Eq. (43) for Λ_L together with

$$\frac{\Lambda_T}{6\pi}=\frac{(\varepsilon+10)/10}{4\pi a}. \tag{47}$$

D. Lorentz model for an atom

For an atom, the parameter Λ_L should be related to the "size" of the electronic wave function. An adequate estimate of Λ_L in terms of the parameters of the atom can be obtained by considering the local depolarization field of the induced charge distribution. Using the harmonically bound electron or Lorentz model for an atom in a static external field, one gets for the ground state $\alpha(0)=e^2/m\omega_0^2\varepsilon_0$, where e and m are the charge and mass of the electron, respectively. To lowest order in an external field $E_{\mathrm{ext}}\hat{\mathbf{z}}$ the induced electronic charge distribution exerts a local or near field given by $-\alpha(0)E_{\mathrm{ext}}/(6\pi\ell^3)\hat{\mathbf{z}}$ with $\ell^2=\hbar/m\omega_0$. (The second moment of the unperturbed ground-state wave function is $\frac{3}{2}\ell^2$.) Equating this expression with $-\alpha(0)\Lambda_L^3E_{\mathrm{ext}}\hat{\mathbf{z}}/6\pi$ [see also Eq. (44)], one identifies $\Lambda_L=1/\ell$.

From the radiative damping of the Lorentz oscillator $\Gamma=\omega_0^2e^2/6\pi\varepsilon_0mc_0^3$ and using Eq. (35) one obtains

$$\frac{\Lambda_T}{6\pi}=\frac{1}{4\pi r_0}, \tag{48}$$

where $r_0=e^2/4\pi\varepsilon_0mc_0^2$ is the classical electron radius.

E. Fröhlich mode of a small metallic sphere

We now treat a case in which the bare polarizability entering the Maxwell-Helmholtz equation is frequency dependent. Consider a small metallic sphere with volume $V=4\pi a^3/3$ for which the skin depth is much larger than the radius a. Writing $\alpha_B(\omega^+)=[\varepsilon(\omega^+)-1]V$ with

$$\varepsilon(\omega^+)=1-\left(\frac{\omega_p}{\omega^+}\right)^2, \tag{49}$$

where ω_p is the (bulk) plasma frequency, one readily obtains

$$\alpha(\omega^+)=3V\times\frac{\omega_p^2/3}{\omega_p^2/3-(\omega^+)^2}, \tag{50}$$

where Eqs. (33) and (43) have been used. One recognizes that the static polarizability equals $3V$, as is known from electrostatics. The resonance frequency $\omega_0=\omega_p/\sqrt{3}$ of the so-called Fröhlich mode (Bohren and Huffman, 1983) corresponds with $\varepsilon(\omega_0)=-2$. For the latter value of the dielectric constant the Mie coefficient of the electric dipole normal mode exhibits a resonance with a *finite* width for a small sphere (Bohren and Huffman, 1983). The resonance and the width depend on the radius of the sphere. The resonance condition to second order in the size parameter x is $\varepsilon=-(2+12x^2/5)$. In our point-scatterer model the size-dependent shift of ω_0 can be taken into account by the term proportional to Λ_T in Eq. (33), giving

$$\frac{\Lambda_T}{6\pi}=\frac{1}{5\pi a}. \tag{51}$$

For the resulting T matrix Eqs. (35) and (36) are no longer valid due to the fact that Λ_T describes only the frequency shift. On the other hand, Eq. (39) still applies and the T matrix satisfies the optical theorem with $\Gamma=2\omega_0(\omega_0a/c)^3/3$.

F. Modeling an internal resonance

In this subsection we propose an improved approach for modeling an atomic or two-level resonance without recourse to an elaborate microscopic theory. In Secs. III.A, III.B, and III.D a resonance comes out *a posteriori* by means of the transverse regularization parameter Λ_T. The internal dynamics of a microscopic system can alternatively be captured by defining the frequency-dependent bare polarizability

$$\alpha_B(\omega^+)\equiv\alpha_B(0)\times\frac{\omega_B^2}{\omega_B^2-(\omega^+)^2}, \tag{52}$$

where ω_B is the (bare) resonance frequency in the absence of any coupling to radiative modes. With this definition, a T matrix of the form of Eq. (37) satisfying the optical theorem can be obtained. The coupling to the imaginary part of the transverse Green's function $\mathcal{G}_0$ leads to a resonance with a finite width (radiative line broadening): $\Gamma=\omega_0^4\alpha(0)/6\pi c^3$. Substituting Eq. (52) in (33) and employing Eq. (43) leads to Eq. (34) with α_B replaced by $\alpha_B(0)$ and to

$$\frac{\Lambda_T}{6\pi c^2}=\frac{1}{\omega_0^2}\left(\frac{1}{3V}+\frac{\omega_B^2-\omega_0^2}{\alpha_B(0)\omega_0^2}\right), \tag{53}$$

where ω_0 is the observed resonance frequency. The parameter Λ_T accounts for a frequency shift of the resonance. The relation $\Lambda_T=\omega_0Q/c$ consequently no longer holds, in fact $\Lambda_T\leqslant\omega_0Q/c$.

The above approach is more general than the one followed in Sec. III.A.

IV. LOCAL DENSITY OF STATES IN THE CASE OF ONE POINT SCATTERER

In this section we demonstrate the usefulness of our description of regularized Green's functions and T matrices by investigating the problem of how a point scat-

terer influences the wave spectrum in its environment. It is shown that removing the singularities of the Green's functions leads to a well-defined local DOS *at* the position of the point scatterer, in contrast to using unregularized Green's functions.

The complete information on the frequency eigenvalues and eigenfunctions of a system is contained in the corresponding Green's function. The imaginary part of the Green's function gives the (local) DOS belonging to the continuous or propagating spectrum (Economou, 1979). Before we proceed, an important distinction (Lagendijk and van Tiggelen, 1996) for classical waves has to be made due to the fact that the potential $\mathcal{V}=-(\omega/c)^2\mathcal{X}$ entering the integral equation (15) depends on the frequency eigenvalues. To properly count the number of eigenvalues $N(\omega^2)=\Sigma_j\delta(\omega^2-\omega_j^2)$ between ω^2 and $\omega^2+d\omega^2$ of a system with dielectric permeability $\varepsilon\equiv 1+\mathcal{X}$, one must introduce a suitably defined Green's function:

$$\hat{\mathcal{G}}\equiv\varepsilon^{1/2}\mathcal{G}\varepsilon^{1/2}. \tag{54}$$

Here $\mathcal{G}$ is the solution of Eqs. (14) and (15). The Green's function $\hat{\mathcal{G}}$ pertains to a properly symmetrized equation of motion, where ε is now connected to the Hermitian "kinetic-energy" term (Lagendijk and van Tiggelen, 1996),

$$\left[\left(\frac{\omega^2}{c^2}+i\epsilon\right)\mathcal{I}-\varepsilon^{-1/2}(\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times)\varepsilon^{-1/2}\right]\hat{\mathcal{G}}(\omega^+)=\mathbf{1}\otimes\mathcal{I}. \tag{55}$$

Since ε is diagonal in coordinate space, one obtains for the diagonal elements of $\hat{\mathcal{G}}$

$$\begin{aligned}\mathrm{tr}\hat{\mathcal{G}}(\omega^+,\mathbf{r},\mathbf{r})&=\mathrm{tr}[\varepsilon(\mathbf{r})\mathcal{G}(\omega^+,\mathbf{r},\mathbf{r})]=\mathrm{tr}\mathcal{G}(\omega^+,\mathbf{r},\mathbf{r})\\&\quad+\mathrm{tr}[\mathcal{X}(\mathbf{r})\mathcal{G}(\omega^+,\mathbf{r},\mathbf{r})],\end{aligned} \tag{56}$$

where tr denotes the trace operation in polarization space and use has been made of its cyclic property. The local DOS $N(\omega,r)$ can be written as (Economou, 1979)

$$N(\omega,\mathbf{r})=-\frac{2\omega}{\pi c^2}\,\mathrm{Im}\,\mathrm{tr}\hat{\mathcal{G}}(\omega^+,\mathbf{r},\mathbf{r}). \tag{57}$$

The Jacobian factor $2\omega/c^2$ originates from $d(\omega/c)^2=(2\omega/c^2)d\omega$. Equation (56) indicates a partitioning (Lagendijk and van Tiggelen, 1996) of the modes described by $\hat{\mathcal{G}}$ into radiative modes (rad) and modes representing the energy stored in the scattering matter (mat),

$$N(\omega,\mathbf{r})\equiv N_{\mathrm{rad}}(\omega,\mathbf{r})+N_{\mathrm{mat}}(\omega,\mathbf{r}), \tag{58}$$

where the radiative local DOS is defined by

$$N_{\mathrm{rad}}(\omega,\mathbf{r})\equiv-\frac{2\omega}{\pi c^2}\,\mathrm{Im}\,\mathrm{tr}\mathcal{G}(\omega^+,\mathbf{r}). \tag{59}$$

For real and scalar dielectric permeability $\varepsilon(\mathbf{r})$ and susceptibility $\chi(\mathbf{r})$ one sees that

$$\begin{aligned}N(\omega,\mathbf{r})&=\varepsilon(\mathbf{r})N_{\mathrm{rad}}(\omega,\mathbf{r}),\\N_{\mathrm{mat}}(\omega,\mathbf{r})&=\chi(\mathbf{r})N_{\mathrm{rat}}(\omega,\mathbf{r}).\end{aligned} \tag{60}$$

The local DOS N_{mat} equals the density of energy stored in the material degrees of freedom of the scatterer. Outside the scatterer $N_{\mathrm{mat}}=0$ and the local DOS is entirely given by N_{rad}. The local DOS N_{rad} can be shown (Snoeks *et al.*, 1995; Barnett *et al.*, 1996) to be the relevant part of the DOS entering Fermi's "golden rule" in descriptions of the rate of spontaneous radiative decay of atoms inside dielectrics.

We now calculate $N(\omega,r)$ for a point scatterer located at $r=0$ and described by the susceptibility $\mathcal{X}(r)$ [see Eq. (16)], the Green's function (22), and the T-matrix element given by Eq. (37). Since the solution $\mathcal{G}$ leads to nonintegrable singularities, we consider the following regularized version:

$$\widetilde{\mathcal{G}}(\omega^+,\mathbf{r},\mathbf{r}')=\mathcal{G}_0(\omega^+,\mathbf{r}-\mathbf{r}')+t(\omega)\widetilde{\mathcal{G}}_0(\omega^+,\mathbf{r})\widetilde{\mathcal{G}}_0(\omega^+,\mathbf{r}'), \tag{61}$$

where in the second term on the right-hand side $\mathcal{G}_0$ has been replaced by $\widetilde{\mathcal{G}}_0$. This replacement can also be introduced when considering the normalization of the scattering solutions corresponding to Eq. (22). Note that $\widetilde{\mathcal{G}}_0$ converges exponentially to $\mathcal{G}_0$ [see Eqs. (28) and (29)]. The local DOS corresponding to the zeroth-order dynamics of the system reads

$$N_0(\omega,\mathbf{r})=-\frac{2\omega}{\pi c^2}\,\mathrm{Im}\,\mathrm{tr}\mathcal{G}_0(\omega^+,r=0)=\frac{\omega^2}{\pi^2c^3}\equiv N_0(\omega). \tag{62}$$

The local DOS N_0 is constant in coordinate space, as expected, and is solely due to the transverse part of $\mathcal{G}_0$; see also Eqs. (30) and (31). As already observed in Sec. II.C, the singularities at $r=0$ appear only in the real part of the Green's functions and applied regularization procedures therefore do not primarily affect the imaginary part. Employing the susceptibility $\mathcal{X}(\mathbf{r})=\alpha_B\delta(\mathbf{r})\mathbf{1}\otimes\mathcal{I}$ gives the local DOS

$$N(\omega,\mathbf{r})=N_{\mathrm{rad}}(\omega,r)[1+\alpha_B\delta(\mathbf{r})]. \tag{63}$$

Note that the *bare* polarizability α_B has entered the local DOS. The second terms of Eqs. (56), (58), and (63) are nonzero only at the position of the point scatterer where $\mathcal{X}\neq 0$. Replacing the delta function for $r=0$ by a constant $1/V_0$ given by Eq. (32) and defining $\alpha_B\equiv(\varepsilon_{\mathrm{eff}}-1)V_0$, one obtains

$$N(\omega,r=0)=\varepsilon_{\mathrm{eff}}N_{\mathrm{rad}}(\omega,r=0). \tag{64}$$

We now focus on the calculation of N_{rad} using Eq. (59). Since $\widetilde{\mathcal{G}}_0$ consists of a transverse and a longitudinal part, the second term in the Green's function (22) gives rise to three contributions in the local DOS in Eq. (59): two contributions resulting from $\widetilde{\mathcal{G}}_0^T$ and $\widetilde{\mathcal{G}}_0^L$, respectively, and one "mixed" contribution. It can be shown that the volume integral of the latter contribution equals zero. The analytical result for $N_{\mathrm{rad}}(\omega,r=0)$ reads

$$N_{\mathrm{rad}}(\omega,r=0)=N_0(\omega)\,\frac{|\alpha(\omega)|^2}{\alpha_B^2}, \tag{65}$$

where the dynamic polarizability $\alpha(\omega)$ is given by Eq. (21). Note that α_B has again entered in an expression for

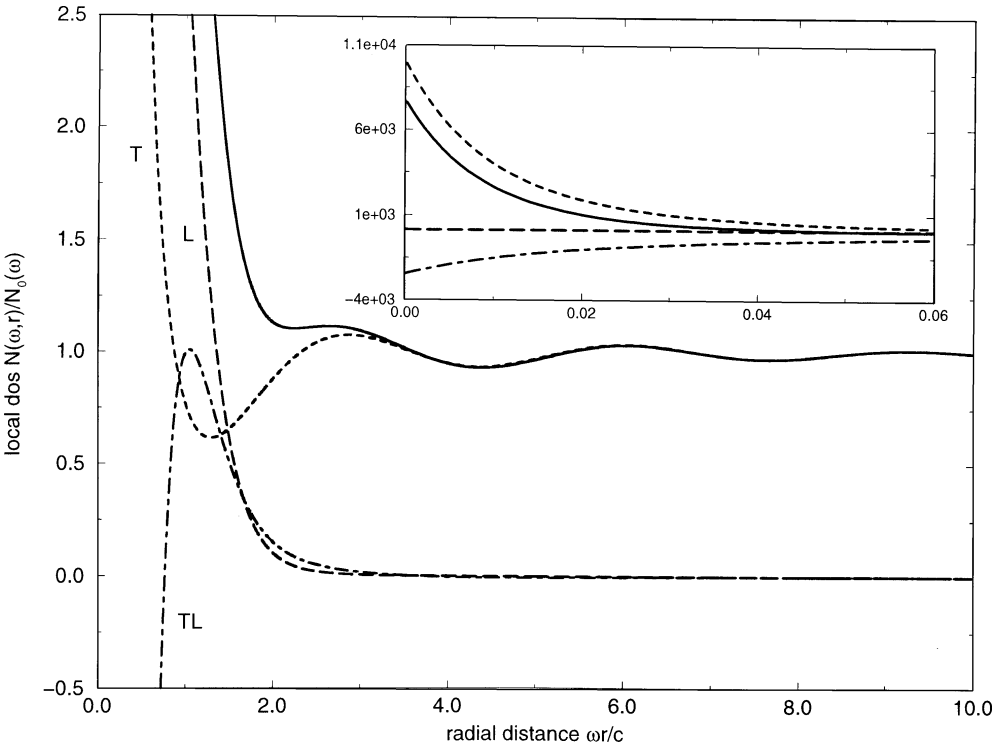

FIG. 1. Local DOS $N_{\rm rad}(\omega,r)/N_0(\omega)$ (solid line) for light scattering from one point scatterer at $r=0$ as a function of the scaled radial distance. The local DOS N_0 corresponds to the zeroth-order dynamics. The transverse (T, dashed line), longitudinal (L, long-dashed line), and "mixed" (TL, dot-dashed line) contributions are also shown. The inset displays the behavior near the origin. The chosen parameters are $\omega=\omega_0$, $Q=100$, $c\Lambda_T/\omega_0=100$, and $c\Lambda_L/\omega_0=2.3$.

a local DOS. Defining the contributions from the transverse and longitudinal parts of $\tilde{\mathcal{G}}_0$ according to $N_{\rm rad}(\omega,r=0)\equiv N_0(\omega)[D_T(\omega)+D_L(\omega)+D_{TL}(\omega)]$, one obtains

$$D_T(\omega)=Q^2\left|\frac{\alpha(\omega)}{\alpha(0)Q}\right|^2, \tag{66}$$

$$D_L(\omega)=(c\Lambda_L/\omega_0)^6\left|\frac{\alpha(\omega)}{\alpha(0)Q}\right|^2, \tag{67}$$

$$D_{TL}(\omega)=-2Q(c\Lambda_L/\omega_0)^3\left|\frac{\alpha(\omega)}{\alpha(0)Q}\right|^2. \tag{68}$$

The contribution from the unscattered part of the Green's function (22) is included in $D_T(\omega)$. Using the inequality (41) one derives $D_L(\omega)\leqslant D_T(\omega)$ and $-D_{TL}(\omega)\leqslant 2D_T(\omega)$. At resonance $|\alpha(\omega_0)/\alpha(0)Q|=1$. Remember that the static polarizability $\alpha(0)$ can be expressed in terms of ω_0/c and Q [see Eq. (39)] and that it is related to α_B and Λ_L through Eq. (34).

Neglecting the longitudinal part of $\tilde{\mathcal{G}}_0$ in $\tilde{\mathcal{G}}$ would result in the local DOS $N_{\rm rad}(\omega,r=0)$ being given by $N_0(\omega)|\alpha(\omega)/\alpha(0)|^2$. One might have expected the latter expression in Eq. (65). It is, however, known in solid-state physics (Mahan, 1981; Lagendijk and van Tiggelen, 1996) that due to certain conservation relations, i.e., the so-called Ward identities, dynamic corrections to bare parameters may or may not cancel one another, depending on the physical quantity under study. For example, the effective mass determining the group velocity of electrons in a medium does not enter the electronic conductivity, but the bare mass does (Mahan, 1981). The enhancement factor for the mass cancels against the one for the relaxation time.

Another argument for the appearance of α_B in Eq. (65) follows from noting that for dielectric spheres the quantity $\alpha(0)/\alpha_B=3/(\varepsilon+2)$ (Jackson, 1975; Born and Wolf, 1980); see also Eq. (42). This so-called Lorentz field factor expresses how the internal field differs from the macroscopic field outside the dielectric. Since the Green's function is a two-field correlation function, the local DOS [see Eq. (57)] should be proportional to $(\alpha(0)/\alpha_B)^2$.

Near a resonance the scattered intensity of light experiences strong delay or retardation effects, i.e., it takes time to accumulate and discharge energy in the dielectric matter. The dwell time $\tau_d(\omega)$ of light inside a scattering object S can be expressed (Lagendijk and van Tiggelen, 1996) as

$$\tau_d(\omega)=\frac{\int_S d\mathbf{r}N_{\rm mat}(\omega,\mathbf{r})}{N_0(\omega)\sigma_{\rm scat}(\omega)c}, \tag{69}$$

denoting the ratio of the stored energy and the current that carries energy away. Note that the maximal value of the cross section $\sigma_{\rm scat}$ is bounded by the unitarity limit in Eq. (40), which is independent of the value of Q. For our point scatterer one finds for the vector case, using Eqs. (21), (38), (62), and (63),

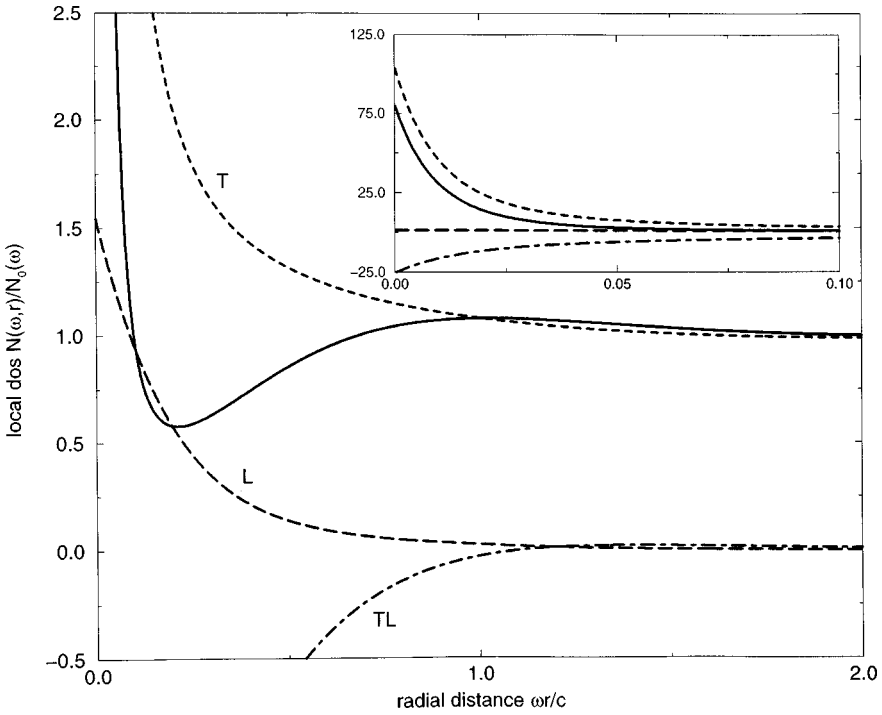

FIG. 2. As in Fig. 1, but for $\omega=0.95\omega_0$.

$$\tau_d(\omega)=\frac{6\pi c^3}{\alpha_B\omega^4}. \tag{70}$$

For scalar waves, $6\pi\rightarrow 4\pi$. It is interesting to observe that in the latter case equating $\tau_d(\omega=\omega_0)=1/\Gamma$ one exactly recovers Eq. (39) relating ω_0/c, Q, and $\alpha(0)$. Generally, for finite-size scatterers, the inverse dwell time near a resonance is of the order of the linewidth. Off resonance (except for $\omega\rightarrow 0$), the dwell time is much smaller. The dwell time enters expressions (Lagendijk and van Tiggelen, 1996) for the diffusion coefficient of light. Cancellation effects similar to those mentioned above for the electronic conductivity occur in the Einstein relation for light relating the conductivity or transmittance, describing steady-state transport in a disordered dielectric medium, to the product of the DOS and the frequency-dependent diffusion coefficient. The conductivity or transmittance are bounded from above, while the DOS for frequencies near a resonance may become very large ($\propto Q^2$). Necessarily, near a resonance the behavior of the diffusion coefficient must cancel that of the DOS, implying a very sharp decrease (Lagendijk and van Tiggelen, 1996) in the diffusive transport of light. The physical picture in the latter case is that near a resonance the dwell time becomes very large.

We give numerical results for the radiative local DOS as a function of the radial distance from the point scatterer using $c\Lambda_L/\omega_0=2.3$. In Figs. 1–3 we show the local DOS $N_{\rm rad}(\omega,r)/N_0(\omega)$ for various values of ω/ω_0 and Q. The contributions of $D_T(\omega,r)$, $D_L(\omega,r)$, and $D_{TL}(\omega,r)$ are also given. The insets show the finite values of these quantities at $r=0$, corresponding to Eqs. (66)–(68). The transverse contributions converge to unity for sufficiently large distances, whereas the longitudinal and "mixed" contributions decay to zero. Comparison of Figs. 1–3 demonstrates that at resonance ($\omega=\omega_0$) the amplitude of the spatial oscillations of the local DOS are maximal, in accordance with the unitarity limit (40) of the cross section $\sigma_{\rm scat}$. At resonance the local DOS also attains its maximal value proportional to Q^2. In Fig. 4 the local DOS $N_{\rm rad}(\omega,r)/N_0(\omega)$ is depicted for various values of Q. For sharper resonances (higher Q), the local DOS is "pulled" more towards the origin, i.e., the available mode density is increasingly concentrated near the scatterer. The vector and scalar cases are compared in Fig. 5. The scalar local DOS can be seen to follow closely the transverse contribution to the vector local DOS.

The analytical results above also apply to scalar waves using $N_0(\omega)=\omega^2/(2\pi^2c^3)$ and $\Lambda_L\rightarrow 0$. In addition, one now has $\alpha_B=\alpha(0)$. The local DOS $N_{\rm rad}(\omega,\mathbf{r})$ for the scalar case takes the form

$$\begin{aligned}\frac{N_{\rm rad}(\omega,\mathbf{r})}{N_0(\omega)}=1+(\omega/\omega_0)&\left|\frac{\alpha(\omega)}{\alpha(0)Q\omega_0 r/c}\right|^2\\ &\times\{Q[1-(\omega/\omega_0)^2][\sin 2kr-2e^{-\Lambda r}\sin kr]\\ &+(\omega/\omega_0)^3[\cos 2kr-2e^{-\Lambda r}\cos kr+e^{-2\Lambda r}]\},\end{aligned} \tag{71}$$

where $\Lambda=\omega_0Q/c$. The regularization terms cancel the $1/r^2$ singularity. Note the exponential behavior as a function of Λ, which is due to the exponential behavior of the regularized scalar Green's function (25).

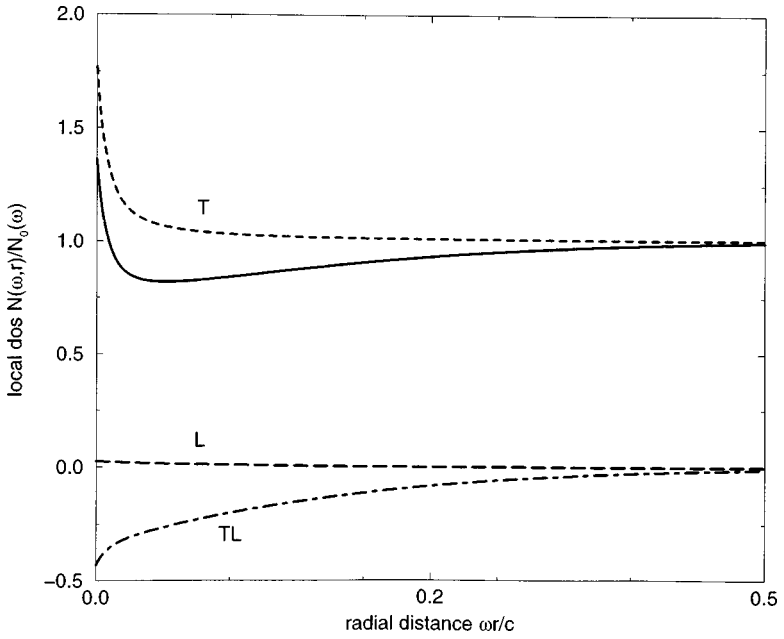

FIG. 3. As in Fig. 1, but for $\omega=0.5\omega_0$.

V. DIELECTRIC CONSTANT AND THE LORENTZ-LORENZ RELATION

In this section we consider the electromagnetic response of a collection of polarizable point particles. The cases of lattices with cubic symmetry and of configurationally disordered media such as gases and liquids will be treated. The dielectric constant is seen to satisfy the Lorentz-Lorenz relation (LLR; Born and Wolf, 1980). For cubic lattices the presented results are exact for low frequencies. In the case of disordered systems we discuss a rigorous microscopic derivation of the LLR (Lagendijk *et al.*, 1997), which includes particle correlations up to infinite order in the density.

A. Cubic lattices

Consider a periodic arrangement of identical point dipoles. Borrowing concepts from solid-state physics, one can express the electric field as

$$\mathbf{E}_{\mathbf{k}}(\omega,\mathbf{r})=\sum_{\mathbf{K}}\mathbf{E}(\omega,\mathbf{k}-\mathbf{K})e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}}, \tag{72}$$

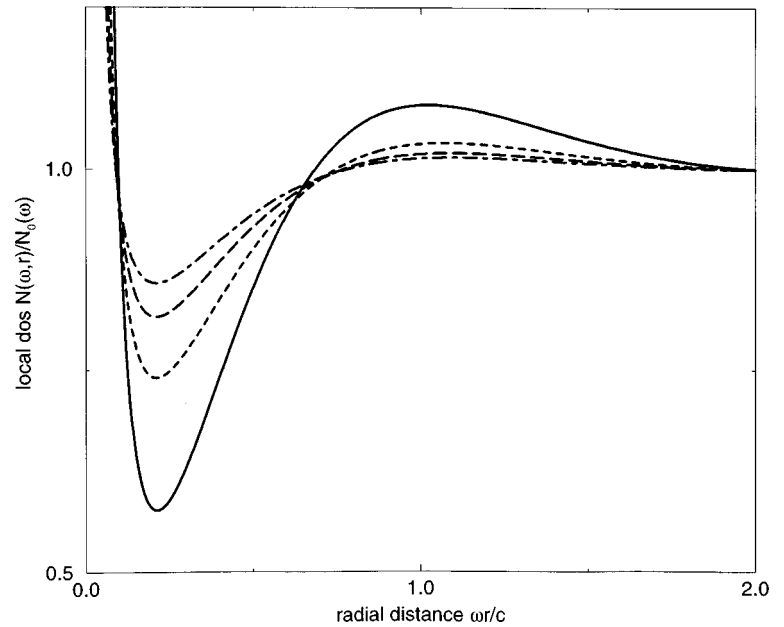

FIG. 4. The local DOS $N_{\mathrm{rad}}(\omega,r)/N_0(\omega)$ for various values of the quality factor Q. As in Fig. 2 we have $\omega=0.95\omega_0$. Solid line, $Q=100$; dashed line, $Q=200$; long-dashed line, $Q=300$; dot-dashed line, $Q=400$.

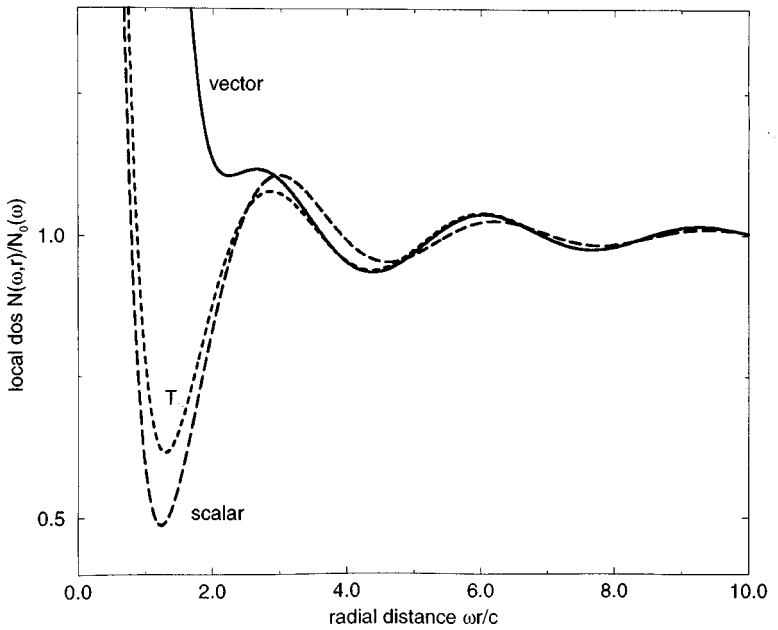

FIG. 5. Comparison of the vector and scalar cases for $\omega=\omega_0$ and $Q=100$. Vector case: solid line, local DOS; dashed line, transverse contribution (T); $c\Lambda_L/\omega_0=2.3$. Scalar case: long-dashed line, local DOS.

where $\mathbf{k}$ is the Bloch wave vector in the first Brillouin zone and $\{\mathbf{K}\}$ are reciprocal-lattice vectors. The periodic potential V, entering the vector Maxwell-Helmholtz equation for the electric field, can also be expanded in terms of $\mathbf{K}$ vectors,

$$V(\omega,\mathbf{r})\equiv-(\omega/c)^2\alpha_B\sum_{\mathbf{R}}\ \delta(\mathbf{r}-\mathbf{R})=\sum_{\mathbf{K}}\ V(\omega,\mathbf{K})e^{i\mathbf{K}\cdot\mathbf{r}},$$

$$V(\omega,\mathbf{K})=-(\omega/c)^2\,\frac{\alpha_B}{\Omega}, \tag{73}$$

in which $\{\mathbf{R}\}$ are lattice vectors and Ω is the volume of the primitive cell of the direct lattice. Note that for point dipoles $V(\omega,\mathbf{K})$ is independent of $\mathbf{K}$. The secular 3×3 determinant of the vector Maxwell-Helmholtz equation is now simply given by

$$\left\|\frac{1}{\Omega}\sum_{\mathbf{K}}\ \frac{1}{(\omega/c)^2\mathcal{I}-|\mathbf{k}-\mathbf{K}|^2\boldsymbol{\Delta}_{\mathbf{k}-\mathbf{K}}}+\frac{1}{(\omega/c)^2\alpha_B}\,\mathcal{I}\right\|=0, \tag{74}$$

which implicitly determines the dispersion law $\omega(\mathbf{k})$. The solutions $\omega(\mathbf{k})$ also follow from considering the poles of the T matrix of the entire lattice, which can be shown (Ziman, 1965) to be fixed by the Korringa-Kohn-Rostoker (KKR) condition in the case of muffin-tin-like potentials. In our case it reads

$$\left\|\sum_{\mathbf{R}\neq\mathbf{0}}e^{-i\mathbf{k}\cdot\mathbf{R}}\mathcal{G}_0(\omega,\mathbf{R})-t^{-1}(\omega^+)\mathcal{I}\right\|=0, \tag{75}$$

where $\mathcal{G}_0(\omega)\equiv\lim_{\epsilon\downarrow0}\mathcal{G}_0(\omega+i\epsilon)$ [see Eq. (8) and Kohn and Rostoker (1954)] and the T-matrix element t is defined by Eq. (19). Note that the properties pertaining to the lattice structure and the single-particle potential enter Eqs. (74) and (75) separately.

The equivalence of the two determinantal conditions can be understood by recognizing that the sum in Eq. (74) can be represented by (Kohn and Rostoker, 1954)

$$\frac{1}{\Omega}\sum_{\mathbf{K}}\ \frac{1}{(\omega/c)^2\mathcal{I}-|\mathbf{k}-\mathbf{K}|^2\boldsymbol{\Delta}_{\mathbf{k}-\mathbf{K}}}$$

$$=\sum_{\mathbf{R}}\ e^{-i\mathbf{k}\cdot\mathbf{R}}\mathcal{G}_0(\omega,\mathbf{R})\equiv\mathbf{G}_{\mathbf{k}}(r=0), \tag{76}$$

where $\mathbf{G}_{\mathbf{k}}(r=0)$ denotes the lattice Green's function or Greenian evaluated at $r=0$. Taking together $\mathcal{G}_0(\omega,r=0)$ and the single-particle potential term finally yields the T-matrix element, Eq. (19). $\mathbf{G}_{\mathbf{k}}(r=0)$ is real and self-adjoint, since the Greenian $\mathbf{G}_{\mathbf{k}}(\mathbf{r})$ is Hermitian (Kohn and Rostoker, 1954). Therefore the imaginary parts of the two terms in Eq. (75) cancel each other. The treatment of the singularities of the Green's function and the subsequent formulation of the T matrix have been discussed in Secs. II.C and III.A, respectively. Obviously, the singularities of $\mathcal{G}_0$ are also present in the reciprocal wave-vector representation. The sum in Eq. (74) contains divergent contributions, which can be treated in the same manner as before. We write

$$\sum_{\mathbf{K}}\ \frac{1}{(\omega/c)^2\mathcal{I}-|\mathbf{k}-\mathbf{K}|^2\boldsymbol{\Delta}_{\mathbf{k}-\mathbf{K}}}$$

$$=\sum_{\mathbf{K}}\ \left\{\frac{1}{(\omega/c)^2-|\mathbf{k}-\mathbf{K}|^2}\,\boldsymbol{\Delta}_{\mathbf{k}-\mathbf{K}}\right.$$

$$\left.+\frac{1}{(\omega/c)^2}\,(\widehat{\mathbf{k}-\mathbf{K}})\otimes(\widehat{\mathbf{k}-\mathbf{K}})\right),$$

$$= \sum_{\mathbf{K}} \left\{ \frac{1}{(\omega/c)^2 \mathcal{I} - |\mathbf{k}-\mathbf{K}|^2 \boldsymbol{\Delta}_{\mathbf{k}-\mathbf{K}}} + \frac{(1-\delta_{\mathbf{K},\mathbf{0}})}{K^2} \boldsymbol{\Delta}_{\mathbf{K}} - \frac{1}{(\omega/c)^2} \hat{\mathbf{K}} \otimes \hat{\mathbf{K}} \right\} - \sum_{\mathbf{K} \neq \mathbf{0}} \frac{1}{K^2} \boldsymbol{\Delta}_{\mathbf{K}} + \sum_{\mathbf{K}} \frac{1}{(\omega/c)^2} \hat{\mathbf{K}} \otimes \hat{\mathbf{K}}, \tag{77}$$

where the divergences have been identified and taken to be independent of $\mathbf{k}$. In accordance with the singularities of $\mathcal{G}_0(r=0)$ being proportional to the unit dyadic [see Eqs. (30) and (31)], we define

$$\frac{1}{\Omega} \sum_{\mathbf{K} \neq \mathbf{0}} \frac{1}{K^2} \boldsymbol{\Delta}_{\mathbf{K}} = \frac{1}{\Omega} \sum_{\mathbf{K} \neq \mathbf{0}} \frac{2}{3K^2} \mathcal{I} \equiv \frac{\Lambda_T}{6\pi} \mathcal{I}, \tag{78}$$

$$\frac{1}{\Omega} \sum_{\mathbf{K}} \hat{\mathbf{K}} \otimes \hat{\mathbf{K}} = \frac{1}{\Omega} \sum_{\mathbf{K}} \frac{1}{3} \mathcal{I} \equiv \frac{\Lambda_L^3}{6\pi} \mathcal{I}. \tag{79}$$

For cubic lattices these sums are indeed diagonal and isotropic in polarization space. For other lattice symmetries, the sums in Eqs. (78) and (79) may be approximated for large K by integrals giving (infinite) contributions proportional to the unit dyadic, while the summations over the smaller $\mathbf{K}$ vectors give rise to additional (finite) terms having a different structure in polarization space. From now on, we shall consider only lattices with cubic symmetry. Employing Eqs. (34) and (35), we find that condition (74) finally reduces to

$$\left\| \frac{1}{\Omega} \sum_{\mathbf{K}} \left\{ \frac{1}{(\omega/c)^2 \mathcal{I} - |\mathbf{k}-\mathbf{K}|^2 \boldsymbol{\Delta}_{\mathbf{k}-\mathbf{K}}} + \frac{2(1-\delta_{\mathbf{K},\mathbf{0}})}{3K^2} \mathcal{I} - \frac{1}{3(\omega/c)^2} \mathcal{I} \right\} - \gamma^{-1}(\omega) \mathcal{I} \right\| = 0, \tag{80}$$

where the "effective" interaction γ is defined according to

$$\gamma(\omega) \equiv -(\omega/c)^2 \tilde{\alpha}(\omega), \tag{81}$$

$$\tilde{\alpha}(\omega) \equiv \alpha(0) \times \frac{\omega_0^2}{\omega_0^2 - \omega^2}. \tag{82}$$

The interaction term γ resembles the T-matrix element (37) except that the imaginary part in the latter is now absent. Note that the third term in the sum of Eq. (80) is also present for $K=0$. The singularity of the longitudinal Green's function can also be thought of as originating from the δ function in Eq. (11) (see Sec. II.C). Using the identity $\Sigma_{\mathbf{R}} \delta(\mathbf{R}) = 1/\Omega \Sigma_{\mathbf{K}} 1$ one then immediately recognizes how to subtract the delta function of $\mathcal{G}_0^L$ from the Greenian of Eq. (76).[1] Equation (80) allows for a very efficient procedure for determining the dispersion law $\omega(\mathbf{k})$. Instead of numerically diagonalizing a $3N \times 3N$ matrix (where N is the number of $\mathbf{K}$ vectors taken into account), one needs to find the roots of an ω-dependent equation. Using Eq. (80) and its scalar version (Sprik *et al.*, 1996, van Coevorden *et al.*, 1996), one computes optical band structures of face-centered-cubic lattices of resonant point dipoles.

The dielectric constant for the lowest frequencies can be obtained analytically from Eq. (80). For the longest wavelengths the $K \neq 0$ transverse contributions are negligible, while the sum of longitudinal terms with $K \neq 0$ cancels against $\Sigma_{\mathbf{K} \neq \mathbf{0}} \mathcal{I}/[3(\omega/c)^2]$. The resulting expression, $[(\omega/c)^2 \mathcal{I} - k^2 \boldsymbol{\Delta}_{\mathbf{k}}]^{-1} - [3(\omega/c)^2]^{-1} \mathcal{I}$ equals the continuum Green's function (6) minus a factor that effectively removes the delta-function contribution in direct space. It then easily follows that the electric-field solutions $\mathbf{E}(\omega,\mathbf{k})$ are transverse and that

$$\varepsilon(\omega) \equiv \omega^2(\mathbf{k})/k^2 = 1 + \frac{\tilde{\alpha}(\omega)/\Omega}{1 - \tilde{\alpha}(\omega)/3\Omega}, \tag{83}$$

where $\tilde{\alpha}$ is given by Eq. (82). The dielectric constant is seen to satisfy the well-known LLR (Born and Wolf, 1980). Usually, the LLR refers to Eq. (83) when solved explicitly for the polarizability. Its zero-frequency version is often called the Clausius-Mossotti equation. The obtained Bloch wave $\mathbf{E}(\omega,\mathbf{k})$ is an exact solution with a real-valued $\omega(\mathbf{k})^2$ and therefore represents a state with an infinite radiative lifetime. Correspondingly, ε is real, since $\tilde{\alpha}$ is real. (If Eq. (83) were valid for all frequencies ε would not be a proper response function. Application of the Kramers-Kronig relations to Eq. (83) would give $\varepsilon(\omega^+) = 1 + \tilde{\alpha}(\omega^+)/[\Omega(1 - \tilde{\alpha}(\omega^+)/3\Omega)]$, which is complex only at the resonance frequency $\omega_{\mathrm{res}}^2 = \omega_0^2 - \tilde{\alpha}(0)/3\Omega$.) These results are consistent with those from Hopfield (1958), Lamb *et al.* (1980), Knoester and Mukamel (1989), Sözüer *et al.* (1992), and Juzeliūnas and Andrews (1994).

Sözüer *et al.* (1992) have studied the convergence problems that arise when diagonalizing the Maxwell-Helmholtz equation in reciprocal space for lattices of dielectric hard spheres. They show that care should be taken to obtain correct results. Here, Eq. (83) seems to be found using only the $K=0$ transverse term. It must be remembered that (infinitely many) $K \neq 0$ contributions, representing the singularities of $\mathcal{G}_0$, enter into the formulation of the polarizability $\tilde{\alpha}(\omega)$. Compared to the case of dielectric hard spheres (Sözüer *et al.*, 1992), it may then be expected that in our case convergence properties are considerably improved for the higher frequencies, where the $K \neq 0$ terms are important.

B. Disordered media

This subsection is based on recently published work done in collaboration with van Tiggelen and Nienhuis (Lagendijk *et al.*, 1997). The dielectric function of a configurationally disordered system originates from the col-

[1] This subtle point was overlooked in the paper by van Coevorden *et al.* (1996) leading to the incorrect result in the long-wavelength limit for cubic lattices that $\varepsilon(0) = 1 + \tilde{\alpha}(0)/\Omega$.

lective response of dipoles excited by the incoming field and the rescattered fields of all other dipoles. Finding an exact solution is very difficult, since it involves a genuine many-body problem. Within the framework of standard response theory the dielectric constant is given by

$$\varepsilon(\omega)=1+\rho\alpha(\omega), \tag{84}$$

in which ρ and α, respectively, represent the density and the (complex) polarizability of the microscopic constituents. By postulating the existence of a dynamic "local field" differing from the macroscopic field, Eq. (84) can be modified considerably, resulting in a very accurate description for gases and liquids (Böttcher, 1973). The connection between the local field and the macroscopic Maxwell field is given by the so-called Lorentz local-field factor (Born and Wolf, 1980). In its simplest form this factor is $(\varepsilon+2)/3$, yielding for the dielectric constant the LLR

$$\varepsilon(\omega)=1+\rho\alpha(\omega)\times\left(\frac{\varepsilon(\omega)+2}{3}\right)=1+\frac{\rho\alpha(\omega)}{1-\frac{1}{3}\rho\alpha(\omega)}. \tag{85}$$

The LLR apparently involves terms up to infinite order in the density. The local-field concept, however, is not expected to be exact and one would like to know which many-body contributions are included in the LLR and which are not. Many alternative and/or simplified derivations of the LLR rely on the concept of a local field and the application of macroscopic considerations based on Maxwell's equations, see, for example, van Kranendonk and Sipe (1977), Born and Wolf (1980), and Schnatterly and Tarrio (1992). The theoretical foundation of the LLR is therefore hard to assess and difficult to improve upon. In the conventional approaches it is generally assumed that the positions of the constituent dipoles can be replaced by a continuous dipole density, and one then applies arguments of the mean-field type. Some remnant of particle correlations are included by excluding a small sphere—the so-called Lorentz cavity—around some origin. A shortcoming of these conventional derivations can readily be pointed out: In multiple-scattering contributions, many-particle correlations have been taken into account only approximately.

In the scattering approach the exact Green's function $\mathcal{G}$, describing the dynamics of the dielectric medium, can be expanded into a series of scattering events that can be classified either as singly or multiply connected (Frisch, 1968). A singly connected event can, in contrast to a multiply connected event, be written as the product of lower-order events. Employing the Green's-function formalism proves to be very useful, since the dielectric constant is determined completely by the multiply connected scattering events. For liquids and gases $\mathcal{G}(\mathbf{r}_1,\mathbf{r}_2)$ is averaged over all particle positions: $\langle\mathcal{G}(\mathbf{r}_1,\mathbf{r}_2)\rangle\equiv\mathcal{G}(\mathbf{r}_1-\mathbf{r}_2)$ (Frisch, 1968). Its Fourier transform $\mathcal{G}(\mathbf{p})$ can then be written as

$$\mathcal{G}(\omega^+,\mathbf{p})=\frac{1}{\varepsilon(\omega^+,\mathbf{p})(\omega^+/c)^2\mathcal{I}-p^2\boldsymbol{\Delta}_{\mathbf{p}}}, \tag{86}$$

where the dielectric constant ε is connected to the self-energy (Frisch, 1968) of the averaged Green's function. The dispersion law given by the poles of $\mathcal{G}$ is generally complex valued, since plane or Bloch waves are not exact eigenstates of a disordered system. The use of point scatterers [see Eq. (16)], or Rayleigh hard-sphere particles considerably simplifies the computation of many-body contributions to the dielectric constant. For a single point scatterer, the scattering solution is exactly determined by the T matrix (20) and the T-matrix element (37). The corresponding polarizability is complex, since the T matrix satisfies the optical theorem. Therefore, contrary to the LLR given by Eq. (83) valid at low frequencies for cubic lattices, the above LLR is complex-valued.

A very common approximation involves scattering from as many particles as many times as possible, but never more than once from the same particle. In addition, particle correlations are neglected. This independent scattering approximation (ISA) amounts to considering only the events that are lowest order in the density and yields as a result Eq. (84), which also follows from response theory. Within the ISA, the scattering from particle i to particle j is counted as $\mathcal{T}_i\mathcal{G}_0\mathcal{T}_j$ in the Green's function $\mathcal{G}$ for all possible positions of particles i and j. In the following we fully account to all orders in the density for those configurations in coordinate space where point particles overlap, i.e., $\mathbf{R}_i=\mathbf{R}_j$, to be referred to as the forbidden region. It turns out that the LLR is obtained by adding to Eq. (84) contributions to all orders of the particle correlations in this region.

The probability distribution $g_m(1,\ldots,m)$ for observing m particles at positions $\mathbf{R}_1,\ldots,\mathbf{R}_m$, can be decomposed using the irreducible correlation functions $h_m(1,\ldots,m)$ according to

$$\begin{aligned}
&g_1(1)=h_1(1)=1,\\
&g_2(12)=h_1(1)h_1(2)+h_2(12),\\
&g_3(123)=1+h_1(1)h_2(23)+h_1(2)h_2(13)\\
&\qquad\qquad+h_1(3)h_2(12)+h_3(123),
\end{aligned} \tag{87}$$

and so on. The irreducible correlation function h_m contains that part of g_m that cannot be written as a linear combination of products of correlation functions h of lower order. In the forbidden region these functions are denoted by a union sign: $g_m^{\cup}$ and $h_m^{\cup}$. For classical particles clearly $g_m^{\cup}=0$ for $m>1$. Then it follows that $h_2^{\cup}=-1$, $h_3^{\cup}=+2$, and $h_4^{\cup}=-6$, and so on. The computation of high-order $h_m^{\cup}$ quickly becomes cumbersome. The correlation functions $\{h_m\}$ enter when the Green's function $\mathcal{G}$, expanded as a series of scattering events, is averaged over the particle positions. Singly and multiply connected events can then unambiguously be distinguished. For the dielectric constant only the latter should be considered.

For example, by considering the multiply connected two-particle contribution $h_2^{\cup}(ij)\mathcal{T}_i\mathcal{G}_0\mathcal{T}_j$ to ε, one is able automatically to take into account in $\mathcal{G}$ the singly connected three-particle events $h_2^{\cup}(ij)\mathcal{T}_i\mathcal{G}_0\mathcal{T}_j\mathcal{G}_0\mathcal{T}_k$ and

$h_2^{\cup}(jk)\mathcal{T}_i\mathcal{G}_0\mathcal{T}_j\mathcal{G}_0\mathcal{T}_k$ (note the order of the particles in h_m). Hence the remaining three-particle events, $h_2^{\cup}(ik)\mathcal{T}_i\mathcal{G}_0\mathcal{T}_j\mathcal{G}_0\mathcal{T}_k$ and $h_3^{\cup}(ijk)\mathcal{T}_i\mathcal{G}_0\mathcal{T}_j\mathcal{G}_0\mathcal{T}_k$, which are multiply connected, completely determine the third-order density contribution to the dielectric constant.

When averaging over the particle positions and taking into account only the forbidden region, one finds that the dominant contribution comes from the delta function in the Green's function (8) (Lagendijk and van Tiggelen, 1996), since for point scatterers the "effective" range of h_m is always smaller than the wavelength. It can then be shown that the dielectric constant ε to all orders in the density becomes

$$\varepsilon(\omega)=1+\rho\alpha(\omega)\sum_{m=0}^{\infty}H_{m+1}\left(-\frac{\rho\alpha(\omega)}{3}\right)^m, \tag{88}$$

where H_m denotes the sum of those products of $h_n^{\cup}$ ($n\leqslant m$) that enter in multiply connected scattering diagrams involving h, $\mathcal{T}$, and $\mathcal{G}_0$, e.g., $H_3\equiv h_1(j)h_2^{\cup}(ik)+h_3^{\cup}(ijk)=1$. It can be proven that

$$H_m=(-1)^{m+1}. \tag{89}$$

The latter result was found earlier by Felderhof *et al.* (1983), who followed an alternative approach for deriving the Clausius-Mossotti equation. Substituting Eq. (89) into Eq. (88) finally gives the LLR.

Microscopic derivations of the second-order term $\frac{1}{3}\rho^2\alpha^2$ of Eq. (85) employing point dipoles have already been obtained by Kuz'min *et al.* (1994) and Morice *et al.* (1995). The remarkable property that $H_{m+1}=H_{m-n}\times H_n$ means that uncontrolled approximations may turn out to give correct answers. Note that applying the Kirkwood superposition approximation (Hansen and McDonald, 1976), leading to entirely different expressions for the irreducible correlation functions h_m, would not reproduce the LLR in the above way.

Our approach can also be applied to AB mixtures, giving

$$\varepsilon_{AB}=1+\frac{\rho_A\alpha_A+\rho_B\alpha_B}{\left(1-\frac{1}{3}\rho_A\alpha_A-\frac{1}{3}\rho_B\alpha_B\right)}. \tag{90}$$

Transforming the densities into volume fractions, Eq. (90) essentially represents the well-known Maxwell-Garnett formula (Garnett, 1904).

VI. SUMMARY

Exact solutions describing the scattering of waves from one finite-size scatterer with or without an internal structure are generally too complicated and unmanageable to be useful in computations dealing with multiple-scattering effects. Going beyond the independent-scattering (Boltzmann) approximation one is basically faced with a complicated many-particle problem. A point scatterer representing a finite-size scatterer may then serve as an appropriate building block for this problem at appropriately chosen frequencies. Important information for adequately describing multiple-scattering phenomena can be contained in the exact scattering solution for one point scatterer: elastic scattering, polarization effects, tensorial polarizabilities, and internal (finite) resonance may all be taken into account. The point scatterer is equivalent to the (effective) two-level model system often used in atomic physics and quantum optics.

We have presented a closed scalar and dyadic Green's-function description of the scattering of classical electromagnetic waves from pointlike objects—pointlike in the sense that their structure cannot be resolved on the scale of the wavelength of light. Our approach has the following implications: The correct finite values of "global" scattering quantities such as the T matrix and the static or dynamic polarizability are ensured. Divergences in **r**-dependent quantities such as the local DOS appearing in the proximity of the scatterer have been removed. The singularities of Green's functions in coordinate space have been given a finite value in accordance with values for physical observables. The resulting regularized Green's functions are continuous functions in coordinate space. The nonuniqueness of the employed regularization procedures does not pose a problem, since the length scales $(1/\Lambda_{T,L})$ involved are much smaller than the wavelength. The parameters $1/\Lambda_T$ and $1/\Lambda_L$ can be shown to be smaller or of the order of the physical size of the finite-size object represented by the point scatterer, so a completely self-consistent description has been obtained. In multiple-scattering calculations one may straightforwardly consider higher-order scattering processes involving higher powers of $\tilde{\mathcal{G}}$ which would otherwise give divergent results.

We saw that in the case of scalar waves a single regularization parameter is required, whereas in the vector description two different ones are to be distinguished. One, the longitudinal parameter Λ_L, is associated with a static quantity, i.e., the size of the point scatterer. The parameter Λ_T is determined by dynamic parameters, i.e., the resonance frequency ω_0 and the quality factor Q of the resonance. The static parameter relates the bare polarizability α_B with the static polarizability $\alpha(0)$. Making the choice $\Lambda_T\approx\Lambda_L$ leads to the unphysical result $Q\leqslant 1$ [cf. Eq. (41)]. Moreover, at resonance one then has $\Lambda_T\leqslant\omega_0/c$, which would not be consistent with the point-scatterer approach.

The obtained T matrix for the point scatterer has been related to the behavior of several physical models in certain regimes. The usefulness of the regularized Green's functions has been shown by calculating the radiative local DOS in the presence of one point scatterer. We have also applied our approach to the description of the electromagnetic response of a collection of dipoles. The Lorentz-Lorenz relation (LLR), relating the polarizability and the dielectric constant, has been derived for cubic lattices and for liquids and gases.

We have discussed the advantages of employing the notion of point scatterers in multiple-scattering problems. Much theoretical progress has been achieved using point scatterers as a microscopic building block in very diverse fields of physics. These include weak localization

and diffusive transport of light [for reviews see Sheng (1995) and Lagendijk and van Tiggelen (1996)], photonic bandgap materials (Sprik *et al.*, 1996; van Coevorden *et al.*, 1996), Bose-condensed gases (Anderson *et al.*, 1995; Bradley *et al.*, 1995; Davies *et al.*, 1995), optical lattices (Birkl *et al.*, 1995; Tan *et al.*, 1995; Weidemüller *et al.*, 1995), and the optical analog of the Hall effect (van Tiggelen, 1995; van Tiggelen *et al.*, 1996). Undoubtedly, further developments in these fields are possible. For example, the study of theoretical refinements to the Lorentz-Lorenz relation for gases and liquids may be pursued further; see also Cichocki and Felderhof (1988a, 1988b, 1989) and van Tiggelen *et al.* (1990). Using a classical multiple-scattering formalism, one can consider possible Lorentz local-field corrections to stimulated emission of atoms in a dielectric environment. In this way, using Einstein's thermodynamic argument relating stimulated and spontaneous emissions, one can study the interesting problem of finding the correct local-field correction to the Einstein A coefficient, without recourse to quantum-mechanical calculations [see, for example, Knoester and Mukamel (1989) and Barnett *et al.* (1996)]. The velocity dependence of the free-space spontaneous emission of atoms (Wilkens, 1993) may also be investigated employing approaches described in this work.

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APPENDIX: COMPUTATION OF DYADIC GREEN'S FUNCTIONS

In the computation of $\mathcal{G}_0(\omega^+,\mathbf{r})$, $\mathcal{G}_0^T(\omega^+,\mathbf{r})$, $\mathcal{G}_0^L(\omega^+,\mathbf{r})$, and their regularized versions using the corresponding expressions in momentum space, one has to evaluate the angular integral $\int d\hat{\mathbf{p}}/(4\pi)\exp(i\mathbf{p}\cdot\mathbf{r})\hat{\mathbf{p}}\otimes\hat{\mathbf{p}}$. (Remember that $\nabla_{\mathbf{p}}=\mathcal{I}-\hat{\mathbf{p}}\otimes\hat{\mathbf{p}}$.) Employing $\exp(i\mathbf{p}\cdot\mathbf{r})\hat{\mathbf{p}}\otimes\hat{\mathbf{p}}=-(1/p^2)\nabla\otimes\nabla\ \exp(i\mathbf{p}\cdot\mathbf{r})$ one obtains

$$\begin{aligned}\int \frac{d\hat{\mathbf{p}}}{4\pi}\exp(i\mathbf{p}\cdot\mathbf{r})\hat{\mathbf{p}}\otimes\hat{\mathbf{p}} &= -\frac{1}{p^2}\nabla\otimes\nabla\int\frac{d\hat{\mathbf{p}}}{4\pi}\exp(i\mathbf{p}\cdot\mathbf{r}),\\ &= -\frac{1}{p^2}\nabla\otimes\nabla\frac{\sin pr}{pr},\\ &= \frac{j_1(pr)}{pr}\mathcal{I}-j_2(pr)\hat{\mathbf{r}}\otimes\hat{\mathbf{r}}, \qquad \text{(A1)}\end{aligned}$$

where the spherical Bessel functions j_1 and j_2 are given by $j_1(x)=\sin x/x^2-\cos x/x$ and $j_2(x)=(3/x^2-1)\sin x/x-3\cos x/x^2$. Integrals over p can be evaluated by performing contour integrations in the complex plane. The appearance of a delta-function contribution is discussed in Sec. II.A. Representation (7) of the solution $\mathcal{G}_0(\omega^+,\mathbf{r})$ simply follows from

$$\mathcal{G}_0(\omega^+,\mathbf{r})=\int\frac{d\mathbf{p}}{(2\pi)^3}\exp(i\mathbf{p}\cdot\mathbf{r})\left(\mathcal{I}-\frac{\mathbf{p}\otimes\mathbf{p}}{k^2}\right)\times\frac{1}{k^2-p^2+i\epsilon} \qquad \text{(A2)}$$

and from treating the factor $\exp(i\mathbf{p}\cdot\mathbf{r})\mathbf{p}\otimes\mathbf{p}$ as above.

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