Transfer matrix of a spherical scatterer

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We derive the off-shell scattering matrix for a spherical scatterer. The result obtained generalizes the off-on-shell matrix commonly used in the theory of scalar waves propagation in random media. [S0163-1829(96)02141-8]

I. INTRODUCTION

It was recently recognized that the internal structure of scatterers can significantly alter the picture of wave propagation and localization in random media.[1,2] When the size of scatterers cannot be neglected, scattering is anisotropic and a ''dwell time'' for waves appears in addition to the time of flight between scattering.[2,3] This substantially modifies such parameters describing wave propagation as the diffusion coefficient,[2,4–11] transport mean free path,[10,11] and transport velocity.[12–14] The microscopic approach to the problem of the renormalization of the diffusion coefficient is based on the Bethe-Salpeter equation for the field-field correlation function. This equation and the solution obtained involve the transfer matrix for a single scatterer, $t_{\mathbf{k}\mathbf{k}'}^{\omega}$, where $\mathbf{k},\mathbf{k}'$ are outgoing and incident momenta, respectively, and ω is the frequency.[15] This matrix contains all information relating to a scatterer's structure, its influence on the anisotropy of scattering, and on internal resonances. A great deal of this information is ignored in the commonly used *on-shell* approximation for the transfer matrix where both momenta $\mathbf{k}$ and $\mathbf{k}'$ are taken on the ''mass shell,'' $k^2=\omega^2$. The *off-shell* transfer matrix, originally arising in the Bethe-Salpeter equation, is not restricted by this condition. This matrix resolves the structure of a scattered field at any distance away from a scatterer, while the on-shell matrix gives the far-zone asymptote of a field only. The on-shell approximation formally enters the theory of wave transport in random media via the commonly accepted δ-function approximation for the imaginary part of the Green function, $\mathrm{Im}G_{k,\omega}\propto\delta(\omega^2-c_p^2k^2)$. The δ approximation confines all transfer matrices in the expression of the diffusion coefficient on the mass shell. However, the presence of derivatives of $t_{\mathbf{k}\mathbf{k}'}^{\omega}$ does not allow one to set $\omega=k$ automatically. Even within the on-shell approximation, one has to first calculate the derivatives and then to allow $k\to\omega$. Neglecting this fact can lead to unexpected results. For instance, numerical calculations of the influence of weak absorption within the on-shell approximation show that the diffusion coefficient becomes larger than its value in the medium without microstructure.[16] This effect disappears if the off-shell matrix is used.[10,11]

The *off-on-shell* matrix for a scatterer with an infinite permittivity was first used in Ref. 1. Such a matrix gives a far-zone asymptote of a scattered field when the source is located at a finite distance from a scatterer. This destroys the symmetry between the incident and scattered momenta

which exists due to the reciprocal principal for the Green function. Analysis of the renormalization of the diffusion coefficient employing the off-on-shell transfer matrix of a scatterer with a finite permittivity[10,11] has shown a strong enhancement of the previously obtained[2,7] corrections to D and qualitatively agrees with experimental data.[17] Numerical agreement can be attained with the use of an exact off-shell matrix. In this paper we derive the transfer matrix of a dielectric sphere and analyze some of its general properties.

II. TRANSFER MATRIX OF A DIELECTRIC SPHERE

The transfer matrix of a single scatterer is originally introduced via the Green function of the wave equation

$$\{\omega^2[1+\varepsilon(\mathbf{r})]+\triangle\}G_{\mathbf{r},\mathbf{r}'}=-\delta_{\mathbf{r}-\mathbf{r}'}, \qquad (1)$$

where $\mathbf{r},\mathbf{r}'$ are location vectors of the point of observation and the source, respectively; $\varepsilon(r)$ has a constant value, ε, inside the scatterer and vanishes outside, the wave speed in this equation and below is equal to unity. Equation (1) must be solved under conditions that $G_{\mathbf{r},\mathbf{r}'}$ and its derivatives $\partial G_{\mathbf{r},\mathbf{r}'}/\partial\mathbf{r}$ are continuous in the entire space outside the source.[18] For a spherical scatterer, one can obtain $G_{\mathbf{r},\mathbf{r}'}$ by utilizing separation of the spherical coordinates and using proper boundary conditions at the surface of the scatterer

$$G_{\mathbf{r},\mathbf{r}'}=\frac{e^{i\omega R}}{4\pi R}+i/4\sum_{l=0}^{\infty}\frac{(l+1/2)P(\hat{\mathbf{r}}\hat{\mathbf{r}}')H_{\omega r}H_{\omega r'}}{\sqrt{rr'}}A_l$$

when $r,r'\geq a$,

$$\qquad (2)$$

$$G_{\mathbf{r},\mathbf{r}'}=i/4\sum_{l=0}^{\infty}\frac{(l+1/2)P(\hat{\mathbf{r}}\hat{\mathbf{r}}')J_{\Omega r}H_{\omega r'}}{\sqrt{rr'}}B_l$$

when $r\leq a,r'\geq a$,

$$G_{\mathbf{r},\mathbf{r}'}=i/4\sum_{l=0}^{\infty}\frac{(l+1/2)P(\hat{\mathbf{r}}\hat{\mathbf{r}}')H_{\omega r}J_{\Omega r'}}{\sqrt{rr'}}B_l$$

when $r\geq a,r'\leq a$,

$$G_{\mathbf{r},\mathbf{r}'} = \frac{e^{i\Omega R}}{4\pi R} + i/4 \sum_{l=0}^{\infty} \frac{(l+1/2)P(\hat{\mathbf{r}}\hat{\mathbf{r}}')J_{\Omega r}J_{\Omega r'}}{\sqrt{rr'}} C_l$$

$$\text{when } r,r' \leq a,$$

where a is the radius of the scatterer, $R = |\mathbf{r} - \mathbf{r}'|$ is the distance between the point of observation and the source, and $\Omega^2 = \omega^2(1+\varepsilon)$. In these equations and below we omit the index l denoting $P(x) = P_l(x)$, $J_x = J_{l+1/2}(x)$ and $H_x = H_{l+1/2}^+(x)$, where $P_l(x)$ are the Legendre polynomials, $J_{l+1/2}(x)$ are the Bessel functions, and $H_{l+1/2}^+(x)$ are the Hankel functions of the first kind. The coefficients of these expansions, obtained by boundary matching, have the form

$$A_l = -\frac{|J_{\omega a}J_{\Omega a}|}{|H_{\omega a}J_{\Omega a}|}, \quad C_l = -\frac{|H_{\omega a}H_{\Omega a}|}{|H_{\omega a}J_{\Omega a}|},$$

$$B_l = -\frac{2i/\pi a}{|H_{\omega a}J_{\Omega a}|}. \tag{3}$$

Here we use a short notation of the following determinant based on any pair of cylindrical functions $U_\nu(x)$ and $V_\nu(x)$:

$$|U_{\alpha x}V_{\beta x}| = \begin{vmatrix} U_\nu(\alpha x) & V_\nu(\beta x) \\ \alpha U_{\nu+1}(\alpha x) & \beta V_{\nu+1}(\beta x) \end{vmatrix}. \tag{4}$$

By definition, the transfer matrix and the Green function are related by equation, $G_{\mathbf{kk}'} = \delta_{\mathbf{kk}'}D_k^\omega + t_{\mathbf{kk}'}^\omega D_k^\omega D_{k'}^\omega$, where $D_k^\omega = [k^2 - \omega^2]^{-1}$ is the wave propagator in empty space. Calculating the Fourier transform of the Green function, $\int_{\mathbf{r}}\int_{\mathbf{r}'}(2\pi)^{-3}G_{\mathbf{r},\mathbf{r}'}\exp(-i\mathbf{kr}+i\mathbf{k}'\mathbf{r}')$, and using expansions of the spherical and plane waves over the spherical functions, Y_{lm}, one can obtain

$$t_{\mathbf{kk}'}^\omega D_k^\omega D_{k'}^\omega = \sum_{l=0}^{\infty} \frac{i(l+1/2)P(\hat{\mathbf{k}}\hat{\mathbf{k}}')}{4\sqrt{kk'}} \left[\int_0^\infty (D_q^\Omega - D_q^\omega)\frac{dq^2}{i\pi} \right.$$

$$\times \int_0^a rJ_{kr}J_{qr}dr \int_0^a r'J_{k'r'}J_{qr'}dr'$$

$$+ \int_a^\infty rJ_{kr}H_{\omega r}dr \int_0^a r'J_{k'r'}J_{\omega r'}dr'$$

$$+ \int_0^a rJ_{kr}J_{\omega r}dr \int_a^\infty r'J_{k'r'}H_{\omega r'}dr'$$

$$+ \left(\int_a^\infty rJ_{kr}H_{\omega r}dr; \int_0^a rJ_{kr}J_{\Omega r}dr \right) \begin{pmatrix} A_l & B_l \\ B_l & C_l \end{pmatrix}$$

$$\times \left. \begin{pmatrix} \int_a^\infty r'J_{k'r'}H_{\omega r'}dr' \\ \int_0^a r'J_{k'r'}J_{\Omega r'}dr' \end{pmatrix} \right]. \tag{5}$$

The integrals of the Bessel functions arising in Eq. (5) can be found in Ref. 19

$$\int_0^a xJ_{\alpha x}J_{\beta x}dx = \frac{a}{\beta^2 - \alpha^2}|J_{\alpha a}J_{\beta a}|. \tag{6}$$

The integrals containing Hankel functions diverge on the upper limit. However, since we deal with the retarded Green function, the frequency is shifted in the upper half-plane, $\omega \to \omega + i0$. This gives an exponentially decaying factor in $H_{\omega r}$ when $r \to \infty$ and provides convergence of the integrals. Using recurrence relations between cylindrical functions one can show

$$\int_a^\infty xJ_{\alpha x}H_{\beta x}dx = \frac{a}{\alpha^2 - \beta^2}|J_{\alpha a}H_{\beta a}|. \tag{7}$$

Using Eqs. (3), (6), and (7) one can represent the *off-shell* transfer matrix of a dielectric sphere in the form

$$t_{\mathbf{kk}'}^\omega = \sum_{l=0}^{\infty} \frac{ia^2(l+1/2)P(\hat{\mathbf{k}}\hat{\mathbf{k}}')}{4\sqrt{kk'}} \left[L_k^\omega L_{k'}^\omega \right.$$

$$\times \int_0^\infty \frac{i\varepsilon\omega^2 dq^2 |J_{ka}J_{qa}||J_{k'a}J_{qa}|}{\pi(q^2-k^2)(q^2-k'^2)(q^2-\omega^2)(q^2-\Omega^2)}$$

$$+ |J_{ka}H_{\omega a}||J_{k'a}J_{\omega a}| + |J_{ka}J_{\omega a}||J_{k'a}H_{\omega a}|$$

$$- \frac{1}{|H_{\omega a}J_{\Omega a}|}(-|J_{ka}H_{\omega a}|; L_k^\omega D_k^\Omega |J_{ka}J_{\Omega a}|)$$

$$\times \left. \begin{pmatrix} |J_{\omega a}J_{\Omega a}| & 2i/\pi a \\ 2i/\pi a & |H_{\omega a}H_{\Omega a}| \end{pmatrix} \begin{pmatrix} -|J_{k'a}H_{\omega a}| \\ L_{k'}^\omega D_{k'}^\Omega |J_{k'a}J_{\Omega a}| \end{pmatrix} \right], \tag{8}$$

where $L_k^\omega = k^2 - \omega^2$ is the inverse wave propagator in empty space. This expression has an explicit symmetry, $t_{\mathbf{kk}'} = t_{\mathbf{k}'\mathbf{k}}$, as it must for a spherical scatterer. Equation (8) cannot be simplified any more in a general situation.

The *off-on-shell* matrix can be obtained from Eq. (8) by taking the outgoing momentum to the mass shell, $\mathbf{k} = \omega\hat{\mathbf{k}}$, and using the facts that $|J_{\omega a}J_{\omega a}| = L_\omega^\omega = 0$ and $|J_{\omega a}H_{\omega a}| = -2i/\pi a$

$$t_{\omega\hat{\mathbf{k}}\mathbf{k}'}^\omega = \sum_{l=0}^{\infty} \frac{a(l+1/2)P(\hat{\mathbf{k}}\hat{\mathbf{k}}')}{2\pi\sqrt{\omega k'}} \left[|J_{k'a}J_{\omega a}| \right.$$

$$+ \left. \frac{1}{|H_{\omega a}J_{\Omega a}|}(|J_{\omega a}J_{\Omega a}|; 2i/\pi a)\begin{pmatrix} -|J_{k'a}H_{\omega a}| \\ L_{k'}^\omega D_{k'}^\Omega |J_{k'a}J_{\Omega a}| \end{pmatrix} \right]. \tag{9}$$

The transfer matrix given by Eq. (9) coincides with the result of Refs. 10 and 11. In the limit $\varepsilon \to \infty$ ($\Omega \to \infty$) it reproduces the result of Ref. 1. This transfer matrix defines the far-zone asymptote of the scattered field in the case that the point source is located at a finite distance from the scatterer. That destroys the symmetry between the incident and scattered momenta.

For a source at an infinite distance we have to take the incident momentum, $\mathbf{k}'$, in Eq. (9) to the mass shell. This results in the well-known expression for the *on-shell* transfer matrix of a spherical dielectric scatterer[20]

$$t_{\hat{\mathbf{k}}\hat{k}'}^{\omega} = \sum_{l=0}^{\infty} \frac{i(l+1/2)P(\hat{\mathbf{k}}\hat{\mathbf{k}}')|J_{\omega a}J_{\Omega a}|}{\pi^2 \omega |H_{\omega a}J_{\Omega a}|}. \qquad (10)$$

III. RAYLEIGH LIMIT

All expressions given by Eqs. (8)–(10) can be substantially simplified in the Rayleigh limit when the scatterer size is the smallest linear scale in a problem. Taking into account conditions $\omega a, \Omega a, ka, k'a \ll 1$ and using the asymptotes for cylindrical functions one can show that

$$|J_{\alpha a}J_{\beta a}| \approx \frac{a(\beta^2 - \alpha^2)(\alpha\beta a^2/4)^{l+1/2}}{2\Gamma(l+3/2)\Gamma(l+5/3)},$$

$$|H_{\alpha a}J_{\beta a}| \approx \frac{-2}{ai\pi}\left(\frac{\beta}{\alpha}\right)^{l+1/2},$$

$$|H_{\alpha a}H_{\beta a}| \approx \frac{a(\beta^2 - \alpha^2)\Gamma^2(l+1/2)\left(\dfrac{\alpha\beta a^2}{4}\right)^{-(l+1/2)}}{2\pi^2(l-1/2)}.$$

Substitution of these equations into Eq. (8) yields the transfer matrix for long waves

$$t_{\mathbf{k}\mathbf{k}'}^{\omega} \approx \sum_{l=0}^{\infty} \frac{a^2(l+1/2)P(\hat{\mathbf{k}}\hat{\mathbf{k}}')(kk'a^2/4)^{l+1/2}}{4\pi\sqrt{kk'}\Gamma(l+3/2)\Gamma(l+5/2)}\left[2(L_k^{\omega}+L_{k'}^{\omega}) + \varepsilon\omega^2\left(1 + \frac{a^2 L_k^{\omega}L_{k'}^{\omega}}{4(l+1/2)^2[(l+1/2)^2-1]}\right)\right.$$

$$\left. + \varepsilon\omega^2 L_k^{\omega}L_{k'}^{\omega}\int_0^{\infty} \frac{q^2(2l+3)/2J_{l+3/2}^2(qa) - qa(k^2+k'^2)/2J_{l+1/2}(qa)J_{l+3/2}(qa) + (kk'a')^2/2(2l+3)J_{l+1/2}^2(qa)}{(q^2-k^2)(q^2-k'^2)(q^2-\omega^2)(q^2-\Omega^2)}dq^2\right]. \tag{11}$$

Due to the presence of two factorial functions in the denominator of Eq. (11), the main term in the sum is the term with $l=0$. This shows that in the Rayleigh limit an isotropic S term dominates in the scattered field even at distances of the order of the wavelength from the scatterer. Calculating the isotropic term of the transfer matrix at the mass shell we reproduce the well-known Rayleigh scattering amplitude, $t(\omega) = \varepsilon\omega^2 a^3/6\pi^2$.

Equation (11) contains three types of terms with different behavior at the mass shell. The first type of term remains finite when $k, k' \to \omega$, the second type vanishes as L_k^{ω}, and the third type vanishes as $(L_k^{\omega})^2$. The third type of term were usually missed in calculations, since the off-on-shell transfer matrix was used instead of the off-shell matrix. This leads to incorrect values of the partial derivatives $\partial t_{\mathbf{k}\mathbf{k}}^{\omega}/\partial\omega^2|_{k=\omega}$ and $\partial t_{\mathbf{k}\mathbf{k}}^{\omega}/\partial k^2|_{k=\omega}$ in the expression for the diffusion coefficient. Using Eqs. (8),(11) enables one to obtain correct results for these derivatives. Below we obtain some general relations for $\partial t_{\mathbf{k}\mathbf{k}}^{\omega}/\partial\omega^2$ and $\partial t_{\mathbf{k}\mathbf{k}}^{\omega}/\partial\mathbf{k}$ which allow one to avoid lengthy straightforward calculations.

IV. DERIVATIVES OF THE t MATRIX

Calculating the derivative of the operator equation $G = D + DtD$ with respect to ω^2 and using the fact that $\partial D/\partial\omega^2 = D^2$ one can obtain

$$\frac{\partial G}{\partial\omega^2} = D^2 + D^2 tD + DtD^2 + D\frac{\partial t}{\partial\omega^2}D. \tag{12}$$

On the other hand, differentiation of Eq. (1) yields

$$\frac{\partial G}{\partial\omega^2} = G(1+\mathcal{E})G = (D+DtD)(1+\mathcal{E})(D+DtD). \tag{13}$$

Here the operators D and $\mathcal{E}$ are diagonal in the momentum and coordinate representations, respectively, $\langle\mathbf{k}|D|\mathbf{k}'\rangle = \delta_{\mathbf{k}\mathbf{k}'}(k^2-\omega^2)^{-1}$, $\langle\mathbf{x}|\mathcal{E}|\mathbf{x}'\rangle = \varepsilon(\mathbf{x})\delta_{\mathbf{x}\mathbf{x}'}$. From the perturbation series expansion of the scattering operator, $t = \omega^2\mathcal{E} + \omega^4\mathcal{E}D\mathcal{E} + \cdots$, it follows that $\mathcal{E}Dt = tD\mathcal{E} = t/\omega^2 - \mathcal{E}$. Using this relation to eliminate $\mathcal{E}$ from Eq. (13) and comparing the result with Eq. (12), we obtain the operator equation

$$\frac{\partial t}{\partial\omega^2} = \frac{t}{\omega^2} + t\left(D^2 + \frac{D}{\omega^2}\right)t. \tag{14}$$

Using the explicit form for matrix elements of all operators in Eq. (14), we obtain an expression for the derivative $\partial t_{\mathbf{k}\mathbf{k}'}^{\omega}/\partial\omega^2$

$$\frac{\partial t_{\mathbf{k}\mathbf{k}'}^{\omega}}{\partial\omega^2} = \frac{t_{\mathbf{k}\mathbf{k}'}^{\omega}}{\omega^2} + \int t_{\mathbf{k}\mathbf{q}}^{\omega} t_{\mathbf{q}\mathbf{k}'}^{\omega}\frac{q^2 d\mathbf{q}}{\omega^2(q^2-\omega^2)^2}. \tag{15}$$

A similar formula for derivatives of $t_{\mathbf{k}\mathbf{k}'}^{\omega}$ with respect to wave vectors or their combinations can be obtained by differentiating the momentum representation for the perturbation expansion of the scattering operator,

$$t^{\omega}_{\mathbf{kk'}} = \omega^2 \mathcal{E}_{\mathbf{kk'}} + \omega^4 \int_{\mathbf{q}} \mathcal{E}_{\mathbf{kq}} D_{\mathbf{q}} \mathcal{E}_{\mathbf{qk'}}$$

$$+ \omega^6 \int_{\mathbf{q}} \int_{\mathbf{q'}} \mathcal{E}_{\mathbf{kq}} D_{\mathbf{q}} \mathcal{E}_{\mathbf{qq'}} D_{\mathbf{q'}} \mathcal{E}_{\mathbf{q'k'}} \dots \quad .$$

As a result we have

$$\frac{\partial t^{\omega}_{\mathbf{kk'}}}{\partial \mathbf{k}} = \omega^2 \frac{\partial \mathcal{E}_{\mathbf{kk'}}}{\partial \mathbf{k}} + \omega^2 \int \frac{d\mathbf{q}}{(q^2 - \omega^2)} \frac{\partial \mathcal{E}_{\mathbf{kq}}}{\partial \mathbf{k}} t^{\omega}_{\mathbf{qk'}} . \quad (16)$$

Here $\mathcal{E}_{\mathbf{kk'}} = \mathcal{E}(\mathbf{k} - \mathbf{k'})$ is the Fourier transform of the dielectric function of a scatterer, $\varepsilon(\mathbf{x})$. In the case of a spherical scatterer with the constant permittivity $\mathcal{E}(\mathbf{k})$ has the form that is easy to differentiate $\mathcal{E}(\mathbf{q}) = (\sin qa - qa \cos qa) 4\pi\varepsilon/q^3$.

Equations (15) and (16) are particularly convenient when both momenta $\mathbf{k}$ and $\mathbf{k'}$ are taken on the mass shell. In this case on-shell and off-on-shell matrices only appear in the expressions for the derivatives and one does not have to differentiate the cumbersome Eq. (8) and then calculate the limit of $k \to \omega$.

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