PHYSICAL REVIEW A **70**, 062719 (2004)

Eigenchannel method for nonrelativistic scattering from zero-range potentials

Radosław Szmytkowski* and Marek Gruchowski
Atomic Physics Division, Department of Atomic Physics and Luminescence, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, PL 80-952 Gdańsk, Poland
(Received 16 June 2004; published 28 December 2004)

An eigenchannel method for nonrelativistic quantum scattering from an arbitrary system of zero-range potentials is presented. Eigenchannel vectors are defined as characteristic vectors of an auxiliary Hermitian matrix spectral problem with a positive semidefinite weight; real eigenvalues to this problem are the negative cotangents of eigenphase shifts. The eigenchannel vectors and the eigenphase shifts are used to construct particular solutions, called eigenchannels, of the pertinent Schrödinger equation. Analysis of the asymptotics of the eigenchannels in the far zone leads to a definition of eigenchannel harmonics, which for the problem at hand play the role analogous to that played by spherical harmonics for scattering in a central field. Representations of a far-field amplitude (for scattering of particles emitted from a point source) as well as a scattering amplitude, a scattering kernel, total, and total averaged cross sections (for scattering of a parallel beam of projectiles) in terms of the eigenphase shifts and the eigenchannel harmonics are derived. As an illustrative example, scattering of a plane wave from a system of four identical zero-range potentials, located in vertices of a regular tetrahedron, is worked out in detail.

DOI: 10.1103/PhysRevA.70.062719 PACS number(s): 03.65.Nk

I. INTRODUCTION

Since the very early days of quantum mechanics, a phase-shift method has been used for solving a problem of nonrelativistic potential scattering in a central field. In its original form, due to Faxén and Holtsmark [1], the method bases itself on the fact that the Schrödinger equation with a spherically symmetric potential is separable in spherical coordinates. This allows one to build a total scattering wave function as a superposition of elementary solutions (partial waves), being products of radial wave functions and angle-dependent spherical harmonics. Coefficients in this superposition depend on so-called phase shifts, which are energy-dependent and describe the influence of the potential on phases of radial functions in the asymptotic region. A scattering amplitude and a total cross section are superpositions of contributions due to individual partial waves; again, these contributions are expressible in terms of phase shifts and, in the case of the scattering amplitude, also in terms of products of spherical harmonics. An extension of the method to scattering of Dirac particles in a central field is also known and used [2].

The utility of the phase-shift method for scattering in spherically symmetric fields is so great that it is natural to ask whether this method may be extended to scattering in potential fields lacking the spherical symmetry? Within the framework of nonrelativistic quantum theory, Levitina and Brändas [3] have shown that such an extension is feasible provided a scattering potential is such that the corresponding Schrödinger equation is separable in general ellipsoidal coordinates. An alternative approach, of much wider applicability, has been recently developed by one of us in Ref. [4]. Following ideas exposed in works of Garbacz [5] and Harrington and Mautz [6] on so-called *characteristic modes* in electromagnetic scattering, we have formulated an *eigenchannel method*, which generalizes the phase-shift method to quantum scattering, both nonrelativistic and relativistic, from an *arbitrary* short-range (excluding, however, zero-range) potential. This method exploits a less common formulation of quantum mechanics in the language of integral equations. Solving a particular weighted integral eigenvalue problem, we have defined so-called *eigenphase shifts*, *eigenchannels*, and *eigenchannel harmonics*, generalizing phase shifts, partial waves, and spherical harmonics, respectively. Then, we have shown that a scattering amplitude and a total cross section may be expressed in terms of the eigenphase shifts and the eigenchannel harmonics in the way very much the same as in the case of scattering in a spherically symmetric field.

Zero-range potentials, widely used in model considerations in atomic physics [7–9], are not potentials in the common sense; rather, they are represented by limiting conditions imposed on a wave function at the points where they are located. Consequently, the mathematical formalism of Ref. [4] is not directly applicable to this type of interactions. It is the purpose of the present paper to extend the eigenchannel method to the model of zero-range potentials. Some results we present here, e.g., formulas for a scattering amplitude and cross sections, may be already found in earlier works of Demkov *et al.* [10]. Still, our presentation, which logically follows that from Ref. [4], is more exhaustive. Also, we mention that although our approach has points of contact with one adopted in a recent work of Li and Heller [11], there are technical differences between the two methods. They stem from the fact that while the auxiliary matrix eigensystem exploited in the present work is weighted and Hermitian, the one of Ref. [11] has the unit weight at the cost of being non-Hermitian.

The structure of the paper is as follows. Section II is of a preparatory character and presents these facts from the general theory of scattering from zero-range potentials, which

*Corresponding author. Email address: radek@mif.pg.gda.pl

constitute a basis for later considerations. In particular, we show that, on the mathematical side, the scattering problem may be reduced to a problem of solving an inhomogeneous algebraic system with a complex symmetric, but non-Hermitian, matrix. In Sec. III we consider an auxiliary generalized Hermitian matrix spectral problem with a positive semidefinite weight. Eigenvalues to this system serve to define *eigenphase shifts*, the former being the negative cotangents of the latter. A totality of eigensolutions to this eigensystem is used to define a set of particular solutions, called *eigenchannels*, of a Schrödinger equation for a particle in the presence of a system of zero-range potentials. Analyzing an asymptotic behavior of the eigenchannels at large distances from the target, we come across *eigenchannel harmonics*, which are shown to form an orthonormal set on the unit sphere. In Sec. IV we use eigensolutions to the auxiliary matrix eigensystem discussed in Sec. III to solve the inhomogeneous algebraic system from Sec. II. The resulting solution is then used to express various quantities characterizing the scattering process, such as far-field amplitudes, a scattering kernel, total, and total averaged cross sections, in terms of the eigenphase shifts and the eigenchannel harmonics. Also, we split the total wave function into two parts: one which undergoes scattering and a remainder, for which a target is transparent. In Sec. V we provide an analytical example, illustrating the utility of the method, and consider the particular problem of scattering of a parallel beam of projectiles from a system of four identical zero-range potentials located in vertices of a regular tetrahedron. Prospective applications and planned extensions of the formalism are mentioned in Sec. VI. The paper ends with three Appendixes.

II. NONRELATIVISTIC SCATTERING FROM ZERO-RANGE POTENTIALS

A. Neighboring source

Consider a system consisting of $N \geqslant 1$ spherically symmetric spin-less zero-range scatterers, located at points $\{\mathbf{r}_n\}$ $(1 \leqslant n \leqslant N)$ and of a monoenergetic, spherically symmetric, point source of particles, located at $\mathbf{r}_0$. The source intensity [i.e., number of particles emitted in the unit of time] is I_0; the energy of emitted particles is $E > 0$. Impinging on the scatterers, the particles diffract and run away to infinity. It is our first goal to find the angular distribution of the particles in the far zone.

Within the model of spherically symmetric zero-range potentials adopted here, everywhere except the points $\{\mathbf{r}_n\}$ the time-independent wave function $\Psi(E,\mathbf{r},\mathbf{r}_0)$ describing the particles satisfies the inhomogeneous Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - E\right]\Psi(E,\mathbf{r},\mathbf{r}_0) = \sqrt{\frac{\pi\hbar^3 I_0}{mk}}\,\delta^{(3)}(\mathbf{r}-\mathbf{r}_0)$$

$$(\mathbf{r} \neq \mathbf{r}_n; 1 \leqslant n \leqslant N) \tag{2.1}$$

and has the form

$$\Psi(E,\mathbf{r},\mathbf{r}_0) = \Phi(E,\mathbf{r},\mathbf{r}_0) + \sum_{n=1}^{N} a_n(E,\mathbf{r}_0)\Phi(E,\mathbf{r},\mathbf{r}_n), \tag{2.2}$$

where

$$\Phi(E,\mathbf{r},\mathbf{r}') = \sqrt{\frac{mI_0}{4\pi\hbar k}}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}, \tag{2.3}$$

with m denoting the particle mass and

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{2.4}$$

The interaction between the particles and the zero-range scatterers is modeled by imposing the following limiting conditions on $\Psi(E,\mathbf{r},\mathbf{r}_0)$ at the points $\{\mathbf{r}_n\}$, where the scatterers are located:

$$\lim_{\mathbf{r}\to\mathbf{r}_n}[1 + \kappa_n(E)|\mathbf{r}-\mathbf{r}_n| + (\mathbf{r}-\mathbf{r}_n)\cdot\boldsymbol{\nabla}]\Psi(E,\mathbf{r},\mathbf{r}_0) = 0$$

$$(1 \leqslant n \leqslant N). \tag{2.5}$$

Here $\kappa_n(E)$ is a real, in general energy-dependent, parameter characterizing the nth scatterer. Evidently, the wave function $\Psi(E,\mathbf{r},\mathbf{r}_0)$ is simply proportional to the outgoing Green function for the problem at hand.

Arranging the coefficients $\{a_n(E,\mathbf{r}_0)\}$, appearing in Eq. (2.2), into an N-component column vector $\mathsf{a}(E,\mathbf{r}_0)$, from Eqs. (2.2) and (2.5) we infer the inhomogeneous linear algebraic system

$$\mathsf{L}(E)\mathsf{a}(E,\mathbf{r}_0) = -\,\mathsf{b}(E,\mathbf{r}_0), \tag{2.6}$$

where $\mathsf{L}(E)$ is a square $N\times N$ complex symmetric matrix with elements

$$L_{nn'}(E) = [ik + \kappa_n(E)]\delta_{nn'} + \frac{e^{ik|\mathbf{r}_n-\mathbf{r}_{n'}|}}{|\mathbf{r}_n-\mathbf{r}_{n'}|}(1-\delta_{nn'}), \tag{2.7}$$

while $\mathsf{b}(E,\mathbf{r}_0)$ is an N-component vector with elements

$$b_n(E,\mathbf{r}_0) = \frac{e^{ik|\mathbf{r}_n-\mathbf{r}_0|}}{|\mathbf{r}_n-\mathbf{r}_0|}. \tag{2.8}$$

We shall present a particular method solving the system (2.6) in Sec. IV A.

Once the system (2.6) is solved and the coefficients $\{a_n(E,\mathbf{r}_0)\}$ are known, from the well-known asymptotic formula [with $\mathbf{r}'$ fixed]

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \overset{r\to\infty}{\sim} e^{-ik\mathbf{n}_r\cdot\mathbf{r}'}\frac{e^{ikr}}{r}, \tag{2.9}$$

where $\mathbf{n}_r = \mathbf{r}/r$, we have

$$\Psi(E,\mathbf{r},\mathbf{r}_0) \overset{r\to\infty}{\sim} \sqrt{\frac{mI_0}{\hbar k}}\mathcal{F}(E,\mathbf{n}_r,\mathbf{r}_0)\frac{e^{ikr}}{r}, \tag{2.10}$$

with

$$\mathcal{F}(E,\mathbf{n}_r,\mathbf{r}_0) = \frac{1}{\sqrt{4\pi}}\left[e^{-ik\mathbf{n}_r\cdot\mathbf{r}_0} + \sum_{n=1}^{N} a_n(E,\mathbf{r}_0)e^{-ik\mathbf{n}_r\cdot\mathbf{r}_n}\right]. \tag{2.11}$$

The angular distribution of the particles in the far zone is best characterized by their current through an infinitesimal surface of area $r^2 d^2\mathbf{n}_r$ (with $d^2\mathbf{n}_r$ denoting the infinitesimal solid angle in the direction $\mathbf{n}_r$) perpendicular to $\mathbf{n}_r$. This quantity is given by $I(E,\mathbf{n}_r,\mathbf{r}_0)d^2\mathbf{n}_r$, where

$$\begin{aligned} I(E,\mathbf{n}_r,\mathbf{r}_0) &= \lim_{r\to\infty} r^2 \frac{\hbar}{m}\mathrm{Im}[\Psi^*(E,\mathbf{r},\mathbf{r}_0)\mathbf{n}_r \cdot \boldsymbol{\nabla}\,\Psi(E,\mathbf{r},\mathbf{r}_0)] \\ &= I_0|\mathcal{F}(E,\mathbf{n}_r,\mathbf{r}_0)|^2. \end{aligned} \tag{2.12}$$

B. Source at infinity: Scattering of a parallel beam

Consider now the case when the source is moved far away from the scatterers, i.e., assume that $r_0\to\infty$. Defining $\psi(E,\mathbf{r},\mathbf{n}_0)$ and $c_n(E,\mathbf{n}_0)$, where $\mathbf{n}_0=\mathbf{r}_0/r_0$, through the asymptotic relations

$$\Psi(E,\mathbf{r},-\mathbf{r}_0) \overset{r_0\to\infty}{\sim} \sqrt{\frac{mI_0}{4\pi\hbar k}}\psi(E,\mathbf{r},\mathbf{n}_0)\frac{e^{ikr_0}}{r_0} \tag{2.13}$$

and

$$a_n(E,-\mathbf{r}_0) \overset{r_0\to\infty}{\sim} c_n(E,\mathbf{n}_0)\frac{e^{ikr_0}}{r_0}, \tag{2.14}$$

from Eqs. (2.2), (2.1), (2.5), (2.6), and (2.8) we deduce that the function $\psi(E,\mathbf{r},\mathbf{n}_0)$ is explicitly given by

$$\psi(E,\mathbf{r},\mathbf{n}_0) = e^{ik\mathbf{n}_0\cdot\mathbf{r}} + \sum_{n=1}^{N} c_n(E,\mathbf{n}_0)\frac{e^{ik|\mathbf{r}-\mathbf{r}_n|}}{|\mathbf{r}-\mathbf{r}_n|} \tag{2.15}$$

and satisfies

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - E\right]\psi(E,\mathbf{r},\mathbf{n}_0) = 0$$

$$(\mathbf{r}\neq\mathbf{r}_n; 1\leqslant n\leqslant N), \tag{2.16}$$

$$\lim_{\mathbf{r}\to\mathbf{r}_n}[1+\kappa_n(E)|\mathbf{r}-\mathbf{r}_n| + (\mathbf{r}-\mathbf{r}_n)\cdot\boldsymbol{\nabla}]\psi(E,\mathbf{r},\mathbf{n}_0) = 0$$

$$(1\leqslant n\leqslant N), \tag{2.17}$$

while the vector $\mathsf{c}(E,\mathbf{n}_0)$, composed of the coefficients $\{c_n(E,\mathbf{n}_0)\}$, solves the system

$$\mathsf{L}(E)\mathsf{c}(E,\mathbf{n}_0) = -\mathsf{d}(E,\mathbf{n}_0), \tag{2.18}$$

where the inhomogeneity $\mathsf{d}(E,\mathbf{n}_0)$ has components

$$d_n(E,\mathbf{n}_0) = e^{ik\mathbf{n}_0\cdot\mathbf{r}_n}. \tag{2.19}$$

The function (2.15) has an obvious physical meaning: it represents a parallel beam of monochromatic particles propagating initially in the direction $\mathbf{n}_0$ and diffracting then on the system of zero-range scatterers.

Asymptotically, the function (2.15) is of the form

$$\psi(E,\mathbf{r},\mathbf{n}_0) \overset{r\to\infty}{\sim} \operatorname*{asymp}_{r\to\infty} e^{ik\mathbf{n}_0\cdot\mathbf{r}} + F(E,\mathbf{n}_r,\mathbf{n}_0)\frac{e^{ikr}}{r}, \tag{2.20}$$

where

$$\operatorname*{asymp}_{r\to\infty} e^{ik\mathbf{n}_0\cdot\mathbf{r}} = \frac{2\pi i}{k}\left[\delta^{(2)}(\mathbf{n}_r+\mathbf{n}_0)\frac{e^{-ikr}}{r} - \delta^{(2)}(\mathbf{n}_r-\mathbf{n}_0)\frac{e^{ikr}}{r}\right], \tag{2.21}$$

while

$$F(E,\mathbf{n}_r,\mathbf{n}_0) = \sum_{n=1}^{N} c_n(E,\mathbf{n}_0)e^{-ik\mathbf{n}_r\cdot\mathbf{r}_n} \tag{2.22}$$

is the scattering amplitude. Equivalently, the asymptotic formula (2.20) may be rewritten as

$$\psi(E,\mathbf{r},\mathbf{n}_0) \overset{r\to\infty}{\sim} \frac{2\pi i}{k}\left[\delta^{(2)}(\mathbf{n}_r+\mathbf{n}_0)\frac{e^{-ikr}}{r} - S(E,\mathbf{n}_r,\mathbf{n}_0)\frac{e^{ikr}}{r}\right], \tag{2.23}$$

where

$$S(E,\mathbf{n}_r,\mathbf{n}_0) = \delta^{(2)}(\mathbf{n}_r-\mathbf{n}_0) + \frac{ik}{2\pi}F(E,\mathbf{n}_r,\mathbf{n}_0) \tag{2.24}$$

is a scattering kernel (i.e., a kernel of the scattering operator).

The angular distribution of scattered particles is usually characterized by a differential cross section defined as

$$\frac{d^2\sigma(E,\mathbf{n}_r,\mathbf{n}_0)}{d^2\mathbf{n}_r} = \lim_{r\to\infty} r^2\frac{j_{scat}(E,\mathbf{r},\mathbf{n}_0)}{j_{inc}(E,\mathbf{r},\mathbf{n}_0)}, \tag{2.25}$$

where

$$j_{scat}(E,\mathbf{r},\mathbf{n}_0) = \frac{\hbar}{m}\mathrm{Im}[\psi^*_{scat}(E,\mathbf{r},\mathbf{n}_0)\mathbf{n}_r\cdot\boldsymbol{\nabla}\,\psi_{scat}(E,\mathbf{r},\mathbf{n}_0)], \tag{2.26}$$

with

$$\psi_{scat}(E,\mathbf{r},\mathbf{n}_0) = \psi(E,\mathbf{r},\mathbf{n}_0) - e^{ik\mathbf{n}_0\cdot\mathbf{r}}, \tag{2.27}$$

is the radial current density in the scattered wave and

$$j_{inc}(E,\mathbf{r},\mathbf{n}_0) = \frac{\hbar}{m}\mathrm{Im}[e^{-ik\mathbf{n}_0\cdot\mathbf{r}}\mathbf{n}_0\cdot\boldsymbol{\nabla}\,e^{ik\mathbf{n}_0\cdot\mathbf{r}}] = \frac{\hbar k}{m} \tag{2.28}$$

is the current density in the incident plane wave. One finds

$$\frac{d^2\sigma(E,\mathbf{n}_r,\mathbf{n}_0)}{d^2\mathbf{n}_r} = |F(E,\mathbf{n}_r,\mathbf{n}_0)|^2. \tag{2.29}$$

Two global quantities characterizing scattering are in use. The first one is a total cross section for a fixed direction of incidence $\mathbf{n}_0$, defined as

$$\sigma(E,\mathbf{n}_0) = \oint_{4\pi} d^2\mathbf{n}_r\frac{d^2\sigma(E,\mathbf{n}_r,\mathbf{n}_0)}{d^2\mathbf{n}_r}, \tag{2.30}$$

while the second one is a total cross section averaged over all directions of incidence:

$$\langle\sigma(E)\rangle = \frac{1}{4\pi}\oint_{4\pi} d^2\mathbf{n}_0 \sigma(E,\mathbf{n}_0). \tag{2.31}$$

The cross section (2.30) may be evaluated with no difficulty. Indeed, exploiting Eqs. (2.22) and (2.29), one finds

$$\sigma(E,\mathbf{n}_0) = \sum_{n,n'=1}^{N} c_n^*(E,\mathbf{n}_0) c_{n'}(E,\mathbf{n}_0) \oint_{4\pi} d^2\mathbf{n}_r e^{ik\mathbf{n}_r\cdot(\mathbf{r}_n-\mathbf{r}_{n'})}. \tag{2.32}$$

The integral in Eq. (2.32) is

$$\oint_{4\pi} d^2\mathbf{n}_r e^{ik\mathbf{n}_r\cdot(\mathbf{r}_n-\mathbf{r}_{n'})} = \frac{4\pi}{k}[\mathsf{L}_A(E)]_{nn'}, \tag{2.33}$$

where

$$[\mathsf{L}_A(E)]_{nn'} = k\delta_{nn'} + \frac{\sin k|\mathbf{r}_n - \mathbf{r}_{n'}|}{|\mathbf{r}_n - \mathbf{r}_{n'}|}(1-\delta_{nn'}), \tag{2.34}$$

hence, it follows that

$$\sigma(E,\mathbf{n}_0) = \frac{4\pi}{k}\mathsf{c}^\dagger(E,\mathbf{n}_0)\mathsf{L}_A(E)\mathsf{c}(E,\mathbf{n}_0), \tag{2.35}$$

with $\mathsf{L}_A(E)$ denoting an $N\times N$ real symmetric (hence Hermitian) matrix with elements (2.34). Interestingly, the matrix $\mathsf{L}_A(E)$ is an anti-Hermitian part of the matrix $\mathsf{L}(E)$:

$$\mathsf{L}_A(E) = \frac{1}{2i}[\mathsf{L}(E) - \mathsf{L}^\dagger(E)]. \tag{2.36}$$

In Appendix B we prove that the matrix $\mathsf{L}_A(E)$ is at least positive semidefinite.

III. EIGENCHANNELS FOR ZERO-RANGE POTENTIALS

The key role throughout the rest of our considerations will be played by solutions to an auxiliary generalized (weighted) algebraic eigenproblem

$$\mathsf{L}_H(E)\mathsf{x}_\gamma(E) = \lambda_\gamma(E)\mathsf{L}_A(E)\mathsf{x}_\gamma(E), \tag{3.1}$$

in which the matrix

$$\mathsf{L}_H(E) = \frac{1}{2}[\mathsf{L}(E) + \mathsf{L}^\dagger(E)], \tag{3.2}$$

with elements

$$[\mathsf{L}_H(E)]_{nn'} = \kappa_n(E)\delta_{nn'} + \frac{\cos k|\mathbf{r}_n - \mathbf{r}_{n'}|}{|\mathbf{r}_n - \mathbf{r}_{n'}|}(1-\delta_{nn'}), \tag{3.3}$$

is a Hermitian part of $\mathsf{L}(E)$ [observe that $\mathsf{L}_H(E)$ is not only Hermitian, but, like $\mathsf{L}_A(E)$, even real symmetric], the weight matrix $\mathsf{L}_A(E)$ is an anti-Hermitian part of $\mathsf{L}(E)$ and has been defined in Eq. (2.36), $\lambda_\gamma(E)$ is an eigenvalue and $\mathsf{x}_\gamma(E)$, with elements $\{x_{n\gamma}(E)\}$, is an associated eigenvector. If $\mathsf{L}_A(E)$ is positive definite, the system (3.1) has exactly N pairs of eigensolutions. It is then an elementary exercise to show that all eigenvalues $\{\lambda_\gamma(E)\}$ are real and that eigenvectors associated with different eigenvalues satisfy the following weighted orthogonality relation:

$$\mathsf{x}_\gamma^\dagger(E)\mathsf{L}_A(E)\mathsf{x}_{\gamma'}(E) = 0 \quad [\lambda_\gamma(E) \neq \lambda_{\gamma'}(E)]. \tag{3.4}$$

In what follows, we shall be assuming that eigenvectors associated with degenerate eigenvalues (if there are any) have been also orthogonalized in the sense of Eq. (3.4) and that all eigenvectors have been normalized according to

$$\mathsf{x}_\gamma^\dagger(E)\mathsf{L}_A(E)\mathsf{x}_\gamma(E) = 1, \tag{3.5}$$

so that for two arbitrary eigenvectors the following orthonormality relation holds:

$$\mathsf{x}_\gamma^\dagger(E)\mathsf{L}_A(E)\mathsf{x}_{\gamma'}(E) = \delta_{\gamma\gamma'}. \tag{3.6}$$

Similarly, one has

$$\mathsf{x}_\gamma^\dagger(E)\mathsf{L}_H(E)\mathsf{x}_{\gamma'}(E) = \lambda_\gamma(E)\delta_{\gamma\gamma'}. \tag{3.7}$$

A weighted closure relation obeyed by the orthonormalized eigenvectors is

$$\sum_{\gamma=1}^{N}\mathsf{x}_\gamma(E)\mathsf{x}_\gamma^\dagger(E)\mathsf{L}_A(E) = \mathsf{L}_A(E)\sum_{\gamma=1}^{N}\mathsf{x}_\gamma(E)\mathsf{x}_\gamma^\dagger(E) = \mathsf{I}, \tag{3.8}$$

where I is the $N\times N$ unit matrix. The case of $\mathsf{L}_A(E)$ positive *semi*definite may be treated as a limit of the case of $\mathsf{L}_A(E)$ positive definite.

Once eigensolutions to the system (3.1) have been found, one may use them to construct N functions

$$X_\gamma(E,\mathbf{r}) = -\sqrt{\frac{m}{2\pi\hbar^2}}\sum_{n=1}^{N}\left[\frac{\cos k|\mathbf{r}-\mathbf{r}_n|}{|\mathbf{r}-\mathbf{r}_n|} - \lambda_\gamma(E)\frac{\sin k|\mathbf{r}-\mathbf{r}_n|}{|\mathbf{r}-\mathbf{r}_n|}\right]x_{n\gamma}(E), \tag{3.9}$$

termed *eigenchannels*. (The seemingly superfluous factor in front of the sum has been introduced for compatibility with the notation of Ref. [4].) It is easy to verify that everywhere except the points $\{\mathbf{r}_n\}$ the eigenchannels obey the source-free Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - E\right]X_\gamma(E,\mathbf{r}) = 0 \quad (\mathbf{r}\neq\mathbf{r}_n; 1\leqslant n\leqslant N), \tag{3.10}$$

and that at the points $\{\mathbf{r}_n\}$ they satisfy the limiting conditions

$$\lim_{\mathbf{r}\to\mathbf{r}_n}[1 + \kappa_n(E)|\mathbf{r}-\mathbf{r}_n| + (\mathbf{r}-\mathbf{r}_n)\cdot\boldsymbol{\nabla}]X_\gamma(E,\mathbf{r}) = 0 \quad (1\leqslant n\leqslant N), \tag{3.11}$$

identical with these in Eqs. (2.5) and (2.17).

At this stage, it is convenient to introduce so-called *eigenphase shifts* $\{\delta_\gamma(E)\}$, related to the eigenvalues $\{\lambda_\gamma(E)\}$ through

$$\lambda_\gamma(E) = -\cot\delta_\gamma(E). \tag{3.12}$$

It follows from the reality of $\{\lambda_\gamma(E)\}$ that the eigenphase shifts are also real. When at some energy E a particular eigenvalue $\lambda_\gamma(E)$ is infinite [this happens when $\mathsf{L}_A(E)$ is positive *semi*definite], a corresponding eigenphase shift is an integer multiple of π. With the aid of the eigenphase shifts, the definition (3.9) may be rewritten as

$$X_\gamma(E,\mathbf{r}) = -\sqrt{\frac{m}{2\pi\hbar^2}}\frac{1}{\sin\delta_\gamma(E)} \times\sum_{n=1}^{N}\frac{\sin[k|\mathbf{r}-\mathbf{r}_n| + \delta_\gamma(E)]}{|\mathbf{r}-\mathbf{r}_n|}x_{n\gamma}(E). \tag{3.13}$$

From Eq. (3.13) one deduces that asymptotically the eigenchannels have the form

$$X_\gamma(E,\mathbf{r}) \overset{r\to\infty}{\sim} \sqrt{\frac{m}{2\hbar^2 k}}\frac{1}{i\sin\delta_\gamma(E)}\left[\mathcal{Y}_\gamma(E,-\mathbf{n}_r)\frac{e^{-ikr-i\delta_\gamma(E)}}{r} - \mathcal{Y}_\gamma(E,\mathbf{n}_r)\frac{e^{ikr+i\delta_\gamma(E)}}{r}\right], \tag{3.14}$$

where the angular functions

$$\mathcal{Y}_\gamma(E,\mathbf{n}_r) = \sqrt{\frac{k}{4\pi}}\sum_{n=1}^{N}x_{n\gamma}(E)e^{-ik\mathbf{n}_r\cdot\mathbf{r}_n} \tag{3.15}$$

are energy-dependent *eigenchannel harmonics*. In Appendix C we prove that these harmonics form an orthonormal set on the unit sphere:

$$\oint_{4\pi} d^2\mathbf{n}_r \mathcal{Y}^*_\gamma(E,\mathbf{n}_r)\mathcal{Y}_{\gamma'}(E,\mathbf{n}_r) = \delta_{\gamma\gamma'}. \tag{3.16}$$

Since both matrices $\mathsf{L}_H(E)$ and $\mathsf{L}_A(E)$ are real and since the eigenvalues $\{\lambda_\gamma(E)\}$ are also real, it is possible (although not necessary) to choose the eigenvectors $\{\mathsf{x}_\gamma(E)\}$ to be real. If such a choice is made, this implies the reality of the eigenchannels (3.10). Moreover, in this case the eigenchannel harmonics (3.15) obey

$$\mathcal{Y}_\gamma(E,-\mathbf{n}_r) = \mathcal{Y}^*_\gamma(E,\mathbf{n}_r) \quad [\mathsf{x}_\gamma(E) \text{ real}] \tag{3.17}$$

and one has

$$X_\gamma(E,\mathbf{r}) \overset{r\to\infty}{\sim} -\sqrt{\frac{2m}{\hbar^2 k}}\frac{1}{\sin\delta_\gamma(E)}\frac{\sin[kr + \varphi_\gamma(E,\mathbf{n}_r) + \delta_\gamma(E)]}{r} \times|\mathcal{Y}_\gamma(E,\mathbf{n}_r)| \quad [\mathsf{x}_\gamma(E) \text{ real}], \tag{3.18}$$

where

$$\varphi_\gamma(E,\mathbf{n}_r) = \arg\mathcal{Y}_\gamma(E,\mathbf{n}_r). \tag{3.19}$$

Concluding this section, we emphasize that the eigenchannel vectors $\{\mathsf{x}_\gamma(E)\}$, the eigenphase shifts $\{\delta_\gamma(E)\}$, and the eigenchannels $\{X_\gamma(E,\mathbf{r})\}$ are inherent to the system of scatterers and are independent of any external sources.

IV. APPLICATIONS OF EIGENCHANNEL VECTORS, EIGENCHANNEL HARMONICS, AND EIGENCHANNELS IN SCATTERING PROBLEMS

In this section we shall show that, apart from being interesting for themselves, various objects defined in the preceding section appear to be useful for solving the scattering problems posed in Sec. II.

A. Neighboring source

We begin with the problem of scattering of particles emitted from the neighboring point source located at $\mathbf{r}_0$. We shall seek the solution to the linear system (2.6) in the form of a linear combination of the eigenchannel vectors $\{\mathsf{x}_\gamma(E)\}$:

$$\mathsf{a}(E,\mathbf{r}_0) = \sum_{\gamma'=1}^{N}\alpha_{\gamma'}(E,\mathbf{r}_0)\mathsf{x}_{\gamma'}(E). \tag{4.1}$$

To find the combination coefficients $\{\alpha_\gamma(E,\mathbf{r}_0)\}$, we substitute Eq. (4.1) into Eq. (2.6), decompose the system matrix $\mathsf{L}(E)$ according to

$$\mathsf{L}(E) = \mathsf{L}_H(E) + i\mathsf{L}_A(E), \tag{4.2}$$

and exploit the eigenvalue equation (3.1), obtaining

$$\sum_{\gamma'=1}^{N}\alpha_{\gamma'}(E,\mathbf{r}_0)[\lambda_{\gamma'}(E) + i]\mathsf{L}_A(E)\mathsf{x}_{\gamma'}(E) = -\mathsf{b}(E,\mathbf{r}_0). \tag{4.3}$$

Then, operating on Eq. (4.3) from the left with $\mathsf{x}^\dagger_\gamma(E)$ and invoking the orthonormality relation (3.6), we arrive at

$$\alpha_\gamma(E,\mathbf{r}_0) = -[\lambda_\gamma(E) + i]^{-1}\mathsf{x}^\dagger_\gamma(E)\mathsf{b}(E,\mathbf{r}_0). \tag{4.4}$$

Hence, it follows that the solution to the system (2.6) is

$$\mathsf{a}(E,\mathbf{r}_0) = -\sum_{\gamma=1}^{N}[\lambda_\gamma(E) + i]^{-1}\mathsf{x}_\gamma(E)\mathsf{x}^\dagger_\gamma(E)\mathsf{b}(E,\mathbf{r}_0). \tag{4.5}$$

Observe that Eqs. (2.6) and (4.5) imply that, in terms of eigensolutions to the system (3.1), the generalized spectral representation of the matrix $\mathsf{L}^{-1}(E)$ is

$$\mathsf{L}^{-1}(E) = \sum_{\gamma=1}^{N}[\lambda_\gamma(E) + i]^{-1}\mathsf{x}_\gamma(E)\mathsf{x}^\dagger_\gamma(E). \tag{4.6}$$

In terms of the eigenphase shifts, Eq. (4.5) reads

$$\mathsf{a}(E,\mathbf{r}_0) = \sum_{\gamma=1}^{N}e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathsf{x}_\gamma(E)\mathsf{x}^\dagger_\gamma(E)\mathsf{b}(E,\mathbf{r}_0). \tag{4.7}$$

Substituting this into Eq. (2.2) yields the particle's wave function

$$\Psi(E,\mathbf{r},\mathbf{r}_0) = \Phi(E,\mathbf{r},\mathbf{r}_0) + \sum_{\gamma=1}^{N}\Phi_\gamma(E,\mathbf{r},\mathbf{r}_0) \tag{4.8}$$

expressed in terms of the radiation eigenmodes

$$\Phi_\gamma(E,\mathbf{r},\mathbf{r}_0) = e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathsf{x}_\gamma^\dagger(E)\mathsf{b}(E,\mathbf{r}_0) \times\sum_{n=1}^{N} x_{n\gamma}(E)\Phi(E,\mathbf{r},\mathbf{r}_n). \tag{4.9}$$

Similarly, exploiting Eq. (4.7) in Eq. (2.11) leads to the following expression for the far-field amplitude:

$$\mathcal{F}(E,\mathbf{n}_r,\mathbf{r}_0) = \frac{1}{\sqrt{4\pi}}e^{-ik\mathbf{n}_r\cdot\mathbf{r}_0} + \sum_{\gamma=1}^{N}\mathcal{F}_\gamma(E,\mathbf{n}_r,\mathbf{r}_0), \tag{4.10}$$

with

$$\mathcal{F}_\gamma(E,\mathbf{n}_r,\mathbf{r}_0) = \frac{1}{\sqrt{k}}e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathsf{x}_\gamma^\dagger(E)\mathsf{b}(E,\mathbf{r}_0)\mathcal{Y}_\gamma(E,\mathbf{n}_r). \tag{4.11}$$

B. Source at infinity: Scattering of a parallel beam

Next we turn to the problem of scattering of a parallel beam of projectiles. Considerations analogous with these which have led us to Eq. (4.7), followed by the use of the definition (3.15), yield

$$\mathsf{c}(E,\mathbf{n}_0) = \sqrt{\frac{4\pi}{k}}\sum_{\gamma=1}^{N} e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma^*(E,\mathbf{n}_0)\mathsf{x}_\gamma(E). \tag{4.12}$$

Combining this with Eq. (2.15) leads to the following representation of the scattering wave function:

$$\psi(E,\mathbf{r},\mathbf{n}_0) = e^{ik\mathbf{n}_0\cdot\mathbf{r}} + \sqrt{\frac{4\pi}{k}}\sum_{\gamma=1}^{N} e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma^*(E,\mathbf{n}_0) \times\sum_{n=1}^{N} x_{n\gamma}(E)\frac{e^{ik|\mathbf{r}-\mathbf{r}_n|}}{|\mathbf{r}-\mathbf{r}_n|}. \tag{4.13}$$

Let us define

$$\psi_{nint}(E,\mathbf{r},\mathbf{n}_0) = \oint_{4\pi} d^2\mathbf{n}_r' P(E,\mathbf{n}_r',\mathbf{n}_0)e^{ik\mathbf{n}_r'\cdot\mathbf{r}}, \tag{4.14}$$

where the projecting kernel $P(E,\mathbf{n}_r,\mathbf{n}_0)$ is

$$P(E,\mathbf{n}_r,\mathbf{n}_0) = \delta^{(2)}(\mathbf{n}_r-\mathbf{n}_0) - \sum_{\gamma=1}^{N}\mathcal{Y}_\gamma(E,\mathbf{n}_r)\mathcal{Y}_\gamma^*(E,\mathbf{n}_0). \tag{4.15}$$

Exploiting the definition (3.15), after elementary operations one arrives at

$$\psi_{nint}(E,\mathbf{r},\mathbf{n}_0) = e^{ik\mathbf{n}_0\cdot\mathbf{r}} - \sqrt{\frac{4\pi}{k}}\sum_{\gamma=1}^{N}\mathcal{Y}_\gamma^*(E,\mathbf{n}_0) \times\sum_{n=1}^{N}\frac{\sin k|\mathbf{r}-\mathbf{r}_n|}{|\mathbf{r}-\mathbf{r}_n|}x_{n\gamma}(E). \tag{4.16}$$

Asymptotically, the function $\psi_{nint}(E,\mathbf{r},\mathbf{n}_0)$ is of the form

$$\psi_{nint}(E,\mathbf{r},\mathbf{n}_0) \overset{r\to\infty}{\sim} \frac{2\pi i}{k}\left[P(E,-\mathbf{n}_r,\mathbf{n}_0)\frac{e^{-ikr}}{r} - P(E,\mathbf{n}_r,\mathbf{n}_0)\frac{e^{ikr}}{r}\right]. \tag{4.17}$$

The reason for introducing the function $\psi_{nint}(E,\mathbf{r},\mathbf{n}_0)$ lies in the fact that it is possible to split the scattering wave function (4.13) according to

$$\psi(E,\mathbf{r},\mathbf{n}_0) = \psi_{nint}(E,\mathbf{r},\mathbf{n}_0) + \psi_{int}(E,\mathbf{r},\mathbf{n}_0), \tag{4.18}$$

where the second term on the right-hand side has the eigenchannel representation

$$\psi_{int}(E,\mathbf{r},\mathbf{n}_0) = -\sqrt{\frac{8\pi^2\hbar^2}{mk}}\sum_{\gamma=1}^{N} e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma^*(E,\mathbf{n}_0)X_\gamma(E,\mathbf{r}) \tag{4.19}$$

and asymptotically behaves as

$$\psi_{int}(E,\mathbf{r},\mathbf{n}_0) \overset{r\to\infty}{\sim} \frac{2\pi i}{k}\left\{[\delta^{(2)}(\mathbf{n}_r+\mathbf{n}_0) - P(E,-\mathbf{n}_r,\mathbf{n}_0)]\frac{e^{-ikr}}{r} - S_{red}(E,\mathbf{n}_r,\mathbf{n}_0)\frac{e^{ikr}}{r}\right\}, \tag{4.20}$$

with

$$S_{red}(E,\mathbf{n}_r,\mathbf{n}_0) = \sum_{\gamma=1}^{N} e^{2i\delta_\gamma(E)}\mathcal{Y}_\gamma(E,\mathbf{n}_r)\mathcal{Y}_\gamma^*(E,\mathbf{n}_0) \tag{4.21}$$

being the *reduced* scattering kernel. Evidently, the function (4.16) satisfies the free-particle Schrödinger equation *everywhere* in $\mathbb{R}^3$. In contrast, the function (4.19), being a linear combination of the eigenchannels $\{X_\gamma(E,\mathbf{r})\}$, satisfies the free-particle Schrödinger equation everywhere *except* the points $\{\mathbf{r}_n\}$, where it is subjected to the same limiting conditions (2.17) as the total scattering function $\psi(E,\mathbf{r},\mathbf{n}_0)$ [cf. Eqs. (3.10) and (3.11)]. Consequently, $\psi_{nint}(E,\mathbf{r},\mathbf{n}_0)$ is that part of $\psi(E,\mathbf{r},\mathbf{n}_0)$ for which the target is transparent, while $\psi_{int}(E,\mathbf{r},\mathbf{n}_0)$ essentially describes the scattering process.

With the aid of Eqs. (4.12) and (3.15), from Eq. (2.22) one deduces the following representation of the scattering amplitude in terms of the eigenphase shifts and the eigenchannel harmonics:

$$F(E,\mathbf{n}_r,\mathbf{n}_0) = \frac{4\pi}{k}\sum_{\gamma=1}^{N} e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma(E,\mathbf{n}_r)\mathcal{Y}_\gamma^*(E,\mathbf{n}_0). \tag{4.22}$$

Hence, after combining Eq. (4.22) with the relation (2.24), one obtains the scattering kernel in the form

$$S(E,\mathbf{n}_r,\mathbf{n}_0) = \delta^{(2)}(\mathbf{n}_r-\mathbf{n}_0) + \sum_{\gamma=1}^{N}[e^{2i\delta_\gamma(E)}-1] \times\mathcal{Y}_\gamma(E,\mathbf{n}_r)\mathcal{Y}_\gamma^*(E,\mathbf{n}_0) = P(E,\mathbf{n}_r,\mathbf{n}_0) + S_{red}(E,\mathbf{n}_r,\mathbf{n}_0). \tag{4.23}$$

It is evident from the representations (4.22) and (4.23) and from the orthonormality relation (3.16) that it holds:

$$\oint_{4\pi} d^2\mathbf{n}_0 F(E,\mathbf{n}_r,\mathbf{n}_0)\mathcal{Y}_\gamma(E,\mathbf{n}_0) = \frac{4\pi}{k} e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma(E,\mathbf{n}_r) \tag{4.24}$$

and

$$\oint_{4\pi} d^2\mathbf{n}_0 S(E,\mathbf{n}_r,\mathbf{n}_0)\mathcal{Y}_\gamma(E,\mathbf{n}_0) = e^{2i\delta_\gamma(E)}\mathcal{Y}_\gamma(E,\mathbf{n}_r), \tag{4.25}$$

i.e., the eigenchannel harmonics $\{\mathcal{Y}_\gamma(E,\mathbf{n}_0)\}$ are eigenfunctions of the integral operators represented by the kernels $F(E,\mathbf{n}_r,\mathbf{n}_0)$ and $S(E,\mathbf{n}_r,\mathbf{n}_0)$, with the eigenvalues $\{4\pi k^{-1}\exp[i\delta_\gamma(E)]\sin\delta_\gamma(E)\}$ and $\{\exp[2i\delta_\gamma(E)]\}$, respectively. The relation analogous to Eq. (4.25) holds also for the reduced scattering kernel (4.21).

Various properties of the scattering amplitude and the scattering kernel may be straightforwardly deduced from the representations (4.22) and (4.23). For instance, exploiting the fact that the eigenchannel harmonics *may* be chosen to satisfy the relation (3.17), one infers the time-reversal reciprocity relations

$$F(E,-\mathbf{n}_r,-\mathbf{n}_0) = F(E,\mathbf{n}_0,\mathbf{n}_r) \tag{4.26}$$

and

$$S(E,-\mathbf{n}_r,-\mathbf{n}_0) = S(E,\mathbf{n}_0,\mathbf{n}_r). \tag{4.27}$$

Also, with no difficulty one proves the generalized optical relations

$$\oint_{4\pi} d^2\mathbf{n}_r F^*(E,\mathbf{n}_r,\mathbf{n}_0)F(E,\mathbf{n}_r,\mathbf{n}_0') = \frac{2\pi i}{k}[F^*(E,\mathbf{n}_0',\mathbf{n}_0) - F(E,\mathbf{n}_0,\mathbf{n}_0')], \tag{4.28}$$

$$\oint_{4\pi} d^2\mathbf{n}_r F(E,\mathbf{n}_0,\mathbf{n}_r)F^*(E,\mathbf{n}_0',\mathbf{n}_r) = \frac{2\pi i}{k}[F^*(E,\mathbf{n}_0',\mathbf{n}_0) - F(E,\mathbf{n}_0,\mathbf{n}_0')], \tag{4.29}$$

and the unitarity relations

$$\oint_{4\pi} d^2\mathbf{n}_r S^*(E,\mathbf{n}_r,\mathbf{n}_0)S(E,\mathbf{n}_r,\mathbf{n}_0') = \delta^{(2)}(\mathbf{n}_0 - \mathbf{n}_0'), \tag{4.30}$$

$$\oint_{4\pi} d^2\mathbf{n}_r S(E,\mathbf{n}_0,\mathbf{n}_r)S^*(E,\mathbf{n}_0',\mathbf{n}_r) = \delta^{(2)}(\mathbf{n}_0 - \mathbf{n}_0'). \tag{4.31}$$

It remains to consider cross sections. Combining Eqs. (2.30) and (2.29) with the expansion (4.22), and making use of the orthonormality relation (3.16), yields the total cross section in the form

$$\sigma(E,\mathbf{n}_0) = \frac{16\pi^2}{k^2}\sum_{\gamma=1}^{N}\sin^2\delta_\gamma(E)|\mathcal{Y}_\gamma(E,\mathbf{n}_0)|^2. \tag{4.32}$$

From this and from Eq. (4.22) one infers the optical relation

$$\sigma(E,\mathbf{n}_0) = \frac{4\pi}{k}\mathrm{Im}\ F(E,\mathbf{n}_0,\mathbf{n}_0), \tag{4.33}$$

which follows also from Eqs. (2.30) and (2.29) and from either of Eqs. (4.28) or (4.29) considered at $\mathbf{n}_0'=\mathbf{n}_0$. Finally, averaging the total cross section (4.32) over all directions of incidence $\mathbf{n}_0$, we obtain, again with the aid of Eq. (3.16):

$$\langle\sigma(E)\rangle = \frac{4\pi}{k^2}\sum_{\gamma=1}^{N}\sin^2\delta_\gamma(E). \tag{4.34}$$

V. EXAMPLE: PARALLEL BEAM SCATTERING FROM AN X_4 STRUCTURE WITH TETRAEDRIC SYMMETRY

As an analytical example illustrating the general theory presented above, we shall consider scattering of a parallel beam from a system of four identical zero-range potentials located at the points

$$\mathbf{r}_1 = \frac{\rho}{2\sqrt{2}}(\mathbf{n}_x + \mathbf{n}_y + \mathbf{n}_z), \tag{5.1a}$$

$$\mathbf{r}_2 = \frac{\rho}{2\sqrt{2}}(-\mathbf{n}_x - \mathbf{n}_y + \mathbf{n}_z), \tag{5.1b}$$

$$\mathbf{r}_3 = \frac{\rho}{2\sqrt{2}}(\mathbf{n}_x - \mathbf{n}_y - \mathbf{n}_z), \tag{5.1c}$$

$$\mathbf{r}_4 = \frac{\rho}{2\sqrt{2}}(-\mathbf{n}_x + \mathbf{n}_y - \mathbf{n}_z) \tag{5.1d}$$

($\mathbf{n}_x$ is the unit vector along the OX axis of the Cartesian coordinate system; $\mathbf{n}_y$ and $\mathbf{n}_z$ are defined analogously), i.e., in vertices of a regular tetrahedron of edge length ρ. The symmetry of the resulting X_4 structure is that of the T-group [13].

In the problem at hand, the matrices $\mathsf{L}_H(E)$ and $\mathsf{L}_A(E)$ have elements

$$[\mathsf{L}_H(E)]_{nn'} = \kappa(E)\delta_{nn'} + \frac{\cos k\rho}{\rho}(1-\delta_{nn'}) \tag{5.2}$$

and

$$[\mathsf{L}_A(E)]_{nn'} = k\delta_{nn'} + \frac{\sin k\rho}{\rho}(1-\delta_{nn'}), \tag{5.3}$$

respectively. With no difficulty, one finds that the generalized eigenproblem (3.1) has only two distinct eigenvalues: a nondegenerate eigenvalue

$$\lambda_a(E) \equiv -\cot\delta_a(E) = \frac{\kappa(E)\rho + 3\cos k\rho}{k\rho + 3\sin k\rho} \tag{5.4}$$

and a triply degenerate eigenvalue

$$\lambda_t(E) \equiv -\cot\delta_t(E) = \frac{\kappa(E)\rho - \cos k\rho}{k\rho - \sin k\rho} \tag{5.5}$$

(the meaning of the indices will become clear shortly). An eigenvector associated with the eigenvalue (5.4), normalized according to Eq. (3.5), is

$$\mathsf{x}_a(E) = \frac{1}{\sqrt{4k[1+3(\sin k\rho)/k\rho]}}(+1+1+1+1)^{\mathrm{T}}. \tag{5.6}$$

Since the eigenvalue (5.5) is degenerate, there is some freedom in choosing linearly independent eigenvectors in its associated eigenspace. A convenient choice, preserving the orthonormality constraint (3.6) and adopted hereafter, is

$$\mathsf{x}_{t,x}(E) = \frac{i}{\sqrt{4k[1-(\sin k\rho)/k\rho]}}(+1-1+1-1)^{\mathrm{T}}, \tag{5.7a}$$

$$\mathsf{x}_{t,y}(E) = \frac{i}{\sqrt{4k[1-(\sin k\rho)/k\rho]}}(+1-1-1+1)^{\mathrm{T}}, \tag{5.7b}$$

$$\mathsf{x}_{t,z}(E) = \frac{i}{\sqrt{4k[1-(\sin k\rho)/k\rho]}}(+1+1-1-1)^{\mathrm{T}}. \tag{5.7c}$$

Once the orthonormal [in the sense of Eq. (3.6)] eigenvectors have been found, from the definition (3.15) one obtains the corresponding eigenchannel harmonics

$$\mathcal{Y}_a(E,\mathbf{n}_r) = \frac{1}{\sqrt{16\pi[1+3(\sin k\rho)/k\rho]}}[e^{-ik\mathbf{n}_r\cdot\mathbf{r}_1} + e^{-ik\mathbf{n}_r\cdot\mathbf{r}_2} + e^{-ik\mathbf{n}_r\cdot\mathbf{r}_3} + e^{-ik\mathbf{n}_r\cdot\mathbf{r}_4}], \tag{5.8}$$

$$\mathcal{Y}_{t,x}(E,\mathbf{n}_r) = \frac{i}{\sqrt{16\pi[1-(\sin k\rho)/k\rho]}}[e^{-ik\mathbf{n}_r\cdot\mathbf{r}_1} - e^{-ik\mathbf{n}_r\cdot\mathbf{r}_2} + e^{-ik\mathbf{n}_r\cdot\mathbf{r}_3} - e^{-ik\mathbf{n}_r\cdot\mathbf{r}_4}], \tag{5.9a}$$

$$\mathcal{Y}_{t,y}(E,\mathbf{n}_r) = \frac{i}{\sqrt{16\pi[1-(\sin k\rho)/k\rho]}}[e^{-ik\mathbf{n}_r\cdot\mathbf{r}_1} - e^{-ik\mathbf{n}_r\cdot\mathbf{r}_2} - e^{-ik\mathbf{n}_r\cdot\mathbf{r}_3} + e^{-ik\mathbf{n}_r\cdot\mathbf{r}_4}], \tag{5.9b}$$

$$\mathcal{Y}_{t,z}(E,\mathbf{n}_r) = \frac{i}{\sqrt{16\pi[1-(\sin k\rho)/k\rho]}}[e^{-ik\mathbf{n}_r\cdot\mathbf{r}_1} + e^{-ik\mathbf{n}_r\cdot\mathbf{r}_2} - e^{-ik\mathbf{n}_r\cdot\mathbf{r}_3} - e^{-ik\mathbf{n}_r\cdot\mathbf{r}_4}], \tag{5.9c}$$

orthonormal in the sense of Eq. (3.16). The harmonic (5.8) forms a basis for a one-dimensional irreducible representation a of the T symmetry group, while the harmonics (5.9a), (5.9b), and (5.9c) form a basis for a three-dimensional representation t of this group. In the limit $k\rho \to 0$, approached either at low energies or for closely grouped scatterers, the a harmonic tends to the $l=0$ spherical harmonic:

$$\mathcal{Y}_a(E,\mathbf{n}_r) \overset{k\rho\to 0}{\longrightarrow} \frac{1}{\sqrt{4\pi}} = Y_{0,0}(\mathbf{n}_r), \tag{5.10}$$

while the three t harmonics go over into particular linear combinations of the three $l=1$ spherical harmonics:

$$\mathcal{Y}_{t,x}(E,\mathbf{n}_r) \overset{k\rho\to 0}{\longrightarrow} \sqrt{\frac{3}{4\pi}}\mathbf{n}_x\cdot\mathbf{n}_r = -\frac{1}{\sqrt{2}}Y_{1,+1}(\mathbf{n}_r) + \frac{1}{\sqrt{2}}Y_{1,-1}(\mathbf{n}_r), \tag{5.11a}$$

$$\mathcal{Y}_{t,y}(E,\mathbf{n}_r) \overset{k\rho\to 0}{\longrightarrow} \sqrt{\frac{3}{4\pi}}\mathbf{n}_y\cdot\mathbf{n}_r = \frac{i}{\sqrt{2}}Y_{1,+1}(\mathbf{n}_r) + \frac{i}{\sqrt{2}}Y_{1,-1}(\mathbf{n}_r), \tag{5.11b}$$

$$\mathcal{Y}_{t,z}(E,\mathbf{n}_r) \overset{k\rho\to 0}{\longrightarrow} \sqrt{\frac{3}{4\pi}}\mathbf{n}_z\cdot\mathbf{n}_r = Y_{1,0}(\mathbf{n}_r) \tag{5.11c}$$

[the reason for choosing the three t eigenvectors (5.7a), (5.7b), and (5.7c) purely imaginary has been to enforce that in the limit $k\rho\to 0$ the corresponding eigenchannel harmonics become real].

From Eqs. (4.34), (5.4), and (5.5) we obtain the total averaged cross section in the form

$$\langle\sigma(E)\rangle = \langle\sigma_a(E)\rangle + 3\langle\sigma_t(E)\rangle, \tag{5.12}$$

with the partial contributions

$$\langle\sigma_a(E)\rangle \equiv \frac{4\pi}{k^2}\sin^2\delta_a(E) = \frac{4\pi}{k^2}\frac{[k\rho + 3\sin k\rho]^2}{[\kappa(E)\rho + 3\cos k\rho]^2 + [k\rho + 3\sin k\rho]^2}, \tag{5.13}$$

$$\langle\sigma_t(E)\rangle \equiv \frac{4\pi}{k^2}\sin^2\delta_t(E) = \frac{4\pi}{k^2}\frac{[k\rho - \sin k\rho]^2}{[\kappa(E)\rho - \cos k\rho]^2 + [k\rho - \sin k\rho]^2}. \tag{5.14}$$

The results presented above coincide with those of Ref. [14], where a different approach has been used.

VI. CONCLUDING REMARKS

There are several directions in which we plan to continue this work in the nearest future. First, it is certainly worth to extend the formalism to elastic scattering of Dirac particles. We are currently working on this problem (which is by no means trivial and has required from us a prior formulation of the method of zero-range potentials for the Dirac equation) and we expect to present our results very soon. Second, it would be interesting to apply the eigenchannel method, both for the Schrödinger and Dirac equations, to scattering from complex absorbing zero-range potentials, as well as from zero-range targets with an internal energetic structure. Finally, we shall look for practical applications of the formalism in actual problems of atomic physics.

Concluding, we point out that although in this paper we have constrained ourselves to the context of quantum scattering, the applicability of the formalism presented above is much broader. Indeed, it should be evident that after redefining the meaning of constants, the method is immediately applicable, as it stands, to scattering of *any* time-harmonic scalar Helmholtz wave from a system of isotropic point targets. We shall exploit this fact and in a separate publication we shall present an application of the method to a specific problem in theoretical acoustics.

ACKNOWLEDGMENT

Discussions with R. Augusiak are acknowledged.

APPENDIX A: EQUIVALENCE OF THE MODEL OF REF. [11] WITH THE MODEL OF ZERO-RANGE POTENTIALS

Li and Heller [11] adopted Foldy's model [12], in which a wave function describing scattering of a monochromatic plane wave from a system of N point-like targets, located at $\{\mathbf{r}_n\}$, is

$$\psi_{LH}(E,\mathbf{r},\mathbf{n}_0) = e^{ik\mathbf{n}_0\cdot\mathbf{r}} + \sum_{n=1}^{N} \phi_n(E,\mathbf{n}_0) f_n(E) \frac{e^{ik|\mathbf{r}-\mathbf{r}_n|}}{|\mathbf{r}-\mathbf{r}_n|}, \quad \text{(A1)}$$

where the coefficients $\{\phi_n(E,\mathbf{n}_0)\}$ are solutions to the algebraic system

$$\phi_n(E,\mathbf{n}_0) = e^{ik\mathbf{n}_0\cdot\mathbf{r}_n} + \sum_{\substack{n'=1 \\ (n'\neq n)}}^{N} \phi_{n'}(E,\mathbf{n}_0) f_{n'}(E) \frac{e^{ik|\mathbf{r}_n-\mathbf{r}_{n'}|}}{|\mathbf{r}_n-\mathbf{r}_{n'}|}$$

$$(1 \leqslant n \leqslant N). \quad \text{(A2)}$$

The known coefficients $\{f_n(E)\}$ characterize individually the targets and are expressible in terms of real, in general energy-dependent, parameters $\{\eta_n(E)\}$ according to

$$f_n(E) = \frac{1}{k} \frac{1}{\cot \eta_n(E) - i}. \quad \text{(A3)}$$

If we define

$$c_n(E,\mathbf{n}_0) = \phi_n(E,\mathbf{n}_0) f_n(E) \quad \text{(A4)}$$

and

$$\kappa_n(E) = -k \cot \eta_n(E), \quad \text{(A5)}$$

it becomes evident that the system (A2) is identical with the system (2.18) and the wave function (A1) is identical with the wave function in Eq. (2.15). Thus, Foldy's model is completely equivalent with the model of zero-range potentials.

A matrix eigenvalue system underlying the reasoning presented in Ref. [11] is, in our notation,

$$[-\mathsf{L}_A^{-1}(E)\mathsf{L}_H(E) - i\mathsf{I}]^{-1}\mathsf{x}_\gamma(E) = -[\lambda_\gamma(E) + i]^{-1}\mathsf{x}_\gamma(E) \quad \text{(A6)}$$

or, equivalently,

$$[-\mathsf{L}_A^{-1}(E)\mathsf{L}_H(E) - i\mathsf{I}]^{-1}\mathsf{x}_\gamma(E) = e^{i\delta_\gamma(E)}\sin\delta_\gamma(E)\mathsf{x}_\gamma(E). \quad \text{(A7)}$$

The system matrix in Eq. (A6) is evidently non-Hermitian. Consequently, unless the system (A6) is transformed to the Hermitian form (3.1) (and this has *not* been done in Ref. [11]), it is difficult to infer that $\{\lambda_\gamma(E)\}$, hence also $\{\delta_\gamma(E)\}$, are real and that the eigenvectors $\{\mathsf{x}_\gamma(E)\}$ are orthogonal in the sense of Eq. (3.4).

APPENDIX B: POSITIVE SEMIDEFINITENESS OF THE MATRIX $\mathsf{L}_A(E)$

Let z be an arbitrary N-component vector with elements $\{z_n\}$. Consider the expression $\mathsf{z}^\dagger\mathsf{L}_A(E)\mathsf{z}$. Invoking Eq. (2.33), one has

$$\mathsf{z}^\dagger\mathsf{L}_A(E)\mathsf{z} = \frac{k}{4\pi}\sum_{n,n'=1}^{N} z_n^* z_{n'} \oint_{4\pi} d^2\mathbf{n}_r e^{ik\mathbf{n}_r\cdot(\mathbf{r}_n-\mathbf{r}_{n'})}. \quad \text{(B1)}$$

After elementary manipulations, Eq. (B1) may be rewritten as

$$\mathsf{z}^\dagger\mathsf{L}_A(E)\mathsf{z} = \frac{k}{4\pi}\oint_{4\pi} d^2\mathbf{n}_r \left| \sum_{n=1}^{N} z_n e^{-ik\mathbf{n}_r\cdot\mathbf{r}_n} \right|^2 \geqslant 0. \quad \text{(B2)}$$

Hence, it follows that the matrix $\mathsf{L}_A(E)$ is at least positive semidefinite.

APPENDIX C: ORTHONORMALITY OF EIGENCHANNEL HARMONICS

Consider the integral

$$I_{\gamma\gamma'}(E) = \oint_{4\pi} d^2\mathbf{n}_r \mathcal{Y}_\gamma^*(E,\mathbf{n}_r)\mathcal{Y}_{\gamma'}(E,\mathbf{n}_r). \quad \text{(C1)}$$

Exploiting the definition (3.15) transforms Eq. (C1) into

$$I_{\gamma\gamma'}(E) = \frac{k}{4\pi}\sum_{n,n'=1}^{N} x_{n\gamma}^*(E) x_{n'\gamma'}(E) \oint_{4\pi} d^2\mathbf{n}_r e^{ik\mathbf{n}_r\cdot(\mathbf{r}_n-\mathbf{r}_{n'})}. \quad \text{(C2)}$$

Next, application of Eq. (2.33) leads to

$$I_{\gamma\gamma'}(E) = \mathsf{x}_\gamma^\dagger(E)\mathsf{L}_A(E)\mathsf{x}_{\gamma'}(E). \quad \text{(C3)}$$

Comparison of Eq. (C3) with Eq. (3.6) yields

$$I_{\gamma\gamma'}(E) = \delta_{\gamma\gamma'}, \quad \text{(C4)}$$

i.e., the eigenchannel harmonics form an orthonormal set on the unit sphere.

[1] H. Faxén and J. Holtsmark, Z. Phys. **45**, 307 (1927); J. Holtsmark, *ibid.* **55**, 437 (1929).
[2] A. I. Akhiezer and V. B. Berestetsky, *Quantum Electrodynamics*, 2nd ed. (Fizmatgiz, Moscow, 1959), Sec. 14 (in Russian); N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions*, 3rd ed. (Oxford University Press, Oxford, 1965), Sec. IX.4.
[3] T. Levitina and E. J. Brändas, Int. J. Quantum Chem., Quantum Chem. Symp. **30**, 5 (1996); Int. J. Quantum Chem. **65**, 601 (1997); **70**, 1017 (1998); Comput. Phys. Commun. **126**, 107 (2000); T. V. Levitina and E. J. Brändas, Comput. Biol. Chem. **27**, 445 (2003).
[4] R. Szmytkowski, Ann. Phys. (N.Y.) **311**, 503 (2004).
[5] R. J. Garbacz, Proc. IEEE **53**, 856 (1965); Ph.D. thesis, Ohio State University, 1968.
[6] R. F. Harrington and J. R. Mautz, IEEE Trans. Antennas Propag. **19**, 622 (1971); **20**, 194 (1972); R. F. Harrington, in *Numerical and Asymptotic Techniques in Electromagnetics*, edited by R. Mittra (Springer, Berlin, 1975), p. 51.
[7] Yu. N. Demkov and V. N. Ostrovskii, *Method of Zero-Range Potentials in Atomic Physics* (Leningrad University Press, Leningrad, 1975) (in Russian); English translation: *Zero-Range Potentials and Their Applications in Atomic Physics* (Plenum, New York, 1988).
[8] G. Drukarev, Adv. Quantum Chem. **11**, 251 (1978).
[9] For recent applications and generalizations of the zero-range potentials model, cf., e.g., A. S. Baltenkov, Phys. Lett. A **268**, 92 (2000); A. S. Baltenkov, V. K. Dolmatov, and S. T. Manson, Phys. Rev. A **64**, 062707 (2001); G. Gasaneo and J. H. Macek, J. Phys. B **35**, 2239 (2002); J. H. Macek, Few-Body Syst. **31**, 241 (2002); S. B. Leble and S. Yalunin, Phys. Lett. A **306**, 35 (2002); Radiat. Phys. Chem. **68**, 181 (2003).
[10] Yu. N. Demkov and V. S. Rudakov, Zh. Eksp. Teor. Fiz. **59**, 2035 (1970), particularly Sec. V; Ref. [7], Chap. IV, particularly Sec. IV.4. See also T. G. Andreeva and V. S. Rudakov, Vestn. Leningr. Univ., Ser. 4: Fiz., Khim. **4**, 12 (1977); V. S. Rudakov, *ibid.* **3**, 88 (1987); L. M. Grigorian, A. V. Malev, and V. S. Rudakov, *ibid.* **4**, 94 (1989); L. M. Grigorian and V. S. Rudakov, *ibid.* **1**, 97 (1990).
[11] S. Li and E. J. Heller, Phys. Rev. A **67**, 032712 (2003).
[12] L. L. Foldy, Phys. Rev. **67**, 107 (1945); L. S. Rodberg and R. M. Thaler, *Introduction to the Quantum Theory of Scattering* (Academic, New York, 1967), pp. 361–363.
[13] Actually, the X_4 structure considered in Sec. V has a symmetry higher than T, namely that of the T_d group. However, this fact has no implications for the example discussed.
[14] R. Szmytkowski and Cz. Szmytkowski, J. Math. Chem. **26**, 243 (1999).