Available online at www.sciencedirect.com
SCIENCE DIRECT®

Annals of Physics 311 (2004) 503–540

ANNALS of PHYSICS

www.elsevier.com/locate/aop

Eigenchannel method in quantum potential scattering

Radosław Szmytkowski*

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 22 November 2003

Abstract

The eigenchannel method, generalizing the familiar phaseshift method, is formulated for scattering from a Hermitian short range potential. Scattering eigenchannels are defined as eigenstates of some generalized (weighted) operator spectral problem. Eigenvalues of that problem define eigenphaseshifts, the former being the negative of cotangents of the latter. Eigenchannel representations of generalized scattering states, transition operators, and Green operators are constructed. A variational approach to the method is also presented. The general theory is illustrated by applications to scattering of Schrödinger and Dirac particles.

PACS: 03.65.Nk

1. Introduction

The idea to generalize the well-known phaseshift method [1–10] to quantum scattering from arbitrary potentials may be traced back to a work of Lippmann and Schwinger [11]. These authors observed that scattering cross-sections might be conveniently expressed in terms of eigenvectors of a scattering matrix and so-called eigenphaseshifts δ_γ, related to eigenvalues s_γ of the scattering matrix through $s_\gamma = \exp(2i\delta_\gamma)$. The matter was pursued further by Biedenharn and co-workers [12–14] (cf. also more recent works by Newton [15–18]). However, the results of

* Fax: +48583472821.
E-mail address: radek@mif.pg.gda.pl.

0003-4916/$ - see front matter © 2003 Elsevier Inc. All rights reserved.
doi:10.1016/j.aop.2003.12.006

[11–14] were perceived as an interesting theoretical detail and did not find applications until Danos and Greiner [19] proposed a practical approach enabling one to find eigenvectors of the scattering matrix and eigenphaseshifts, hence also cross-sections, without prior knowledge of the scattering matrix. This approach, termed *the eigenchannel method*, was subsequently used in nuclear physics [20–28] and, usually in conjunction with the quantum defect theory, in atomic and molecular physics [29–37].

The purpose of this paper is to present a consistent, self-contained, formulation of the eigenchannel method for quantum scattering from a Hermitian short range potential. Our approach, which is technically different from that proposed by Danos and Greiner [19], has been inspired by ideas contained in works of Garbacz [38,39] and Harrington and Mautz [40–42] on so-called characteristic modes in the electromagnetic theory (cf. also works of Katsenelenbaum et al. [43–47] on the classical diffraction theory). Some of the results presented in this paper have been anticipated by results which may be found in works of Demkov et al. [48,49] on the quantum scattering theory and Ziesche et al. [50–54] on the quantum solid state theory.

The arrangement of the paper is as follows. Section 2 contains definitions and summarizes basic properties of principal mathematical objects (Green operators, generalized scattering states, and transition operators) used in later considerations. In Section 3 we define so-called eigenchannels as eigenstates to an abstract generalized spectral problem and investigate some of their properties. Next we use the eigenchannels as an expansion basis, constructing series representations of the generalized scattering states, generalized transition operators, and Green operators. In Section 4 we introduce eigenphaseshifts. Rather than defining them through their relationship to eigenvalues of the scattering matrix, we relate them to eigenvalues of the spectral problem introduced in Section 3. In Section 5 the variational approach to the eigenchannel method is discussed. Sections 6 and 7 illustrate the utility of the general theory exposed in the preceding sections and present its applications to spatial coordinate descriptions of scattering processes involving Schrödinger and Dirac particles, respectively. Section 8 contains concluding remarks. The paper ends with three appendices.

2. Preliminaries

2.1. Free-particle Green operators

Let $\hat{H}_0$ denote a free-particle Hamiltonian and let $E \in \mathbb{R}$ be a number from a (continuous) spectrum of $\hat{H}_0$. We define the related outgoing ($\hat{G}_0^{(+)}(E)$) and ingoing ($\hat{G}_0^{(-)}(E)$) Green operators as

$$\hat{G}_0^{(\pm)}(E) = [\hat{H}_0 - E \mp \mathrm{i}\epsilon]^{-1}. \tag{2.1}$$

Here and throughout the rest of the paper, it is understood that $\epsilon \in \mathbb{R}_+$ and $\epsilon \downarrow 0$. The two Green operators are mutually Hermitian adjoint:

$$\hat{G}_0^{(\pm)\dagger}(E) = \hat{G}_0^{(\mp)}(E). \tag{2.2}$$

A general Green operator $\hat{G}_0^{(\eta)}(E)$ for the Hamiltonian $\hat{H}_0$ is defined as the following linear combination of the outgoing and ingoing Green operators:

$$\hat{G}_0^{(\eta)}(E) = \frac{1}{2}(1+\eta)\hat{G}_0^{(+)}(E) + \frac{1}{2}(1-\eta)\hat{G}_0^{(-)}(E), \tag{2.3}$$

where $\eta \in \mathbb{C}$. From Eqs. (2.2) and (2.3) it follows that:

$$\hat{G}_0^{(\eta)\dagger}(E) = \hat{G}_0^{(-\eta^*)}(E), \tag{2.4}$$

where the asterisk denotes the complex conjugation. Evidently, the going Green operators $\hat{G}_0^{(\pm)}(E)$ are particular cases of $\hat{G}_0^{(\eta)}(E)$, corresponding to the choices $\eta = \pm 1$:

$$\hat{G}_0^{(\pm)}(E) = \hat{G}_0^{(\pm 1)}(E). \tag{2.5}$$

Still another choice, $\eta = 0$, results in the Hermitian standing (or Principal Value) Green operator

$$\hat{G}_0^{(0)}(E) = \frac{1}{2}[\hat{G}_0^{(+)}(E) + \hat{G}_0^{(-)}(E)] = \mathrm{PV}[\hat{H}_0 - E]^{-1}. \tag{2.6}$$

The Green operator $\hat{G}_0^{(\eta)}(E)$ may be decomposed as follows:

$$\hat{G}_0^{(\eta)}(E) = \hat{G}_0^{(0)}(E) + \mathrm{i}\eta\hat{D}_0(E), \tag{2.7}$$

$$\hat{G}_0^{(\eta)}(E) = \hat{G}_0^{(\pm)}(E) \mp \mathrm{i}(1 \mp \eta)\hat{D}_0(E), \tag{2.8}$$

with the Hermitian operator

$$\hat{D}_0(E) = \frac{1}{2\mathrm{i}}[\hat{G}_0^{(+)}(E) - \hat{G}_0^{(-)}(E)] = \frac{\epsilon}{[\hat{H}_0 - E]^2 + \epsilon^2}. \tag{2.9}$$

Evidently, eigenstates of $\hat{D}_0(E)$ coincide with those of $\hat{H}_0$. If E' is in the spectrum of $\hat{H}_0$ then $\epsilon/[(E'-E)^2 + \epsilon^2] > 0$ is in the spectrum of $\hat{D}_0(E)$. Since eigenvalues of $\hat{D}_0(E)$ are positive, this operator is positive definite.

In virtue of the definitions (2.9), (2.6), and (2.1), the operator $\hat{D}_0(E)$ obeys

$$[\hat{H}_0 - E]\hat{D}_0(E) = \epsilon\hat{G}_0^{(0)}(E). \tag{2.10}$$

From Eq. (2.7) one deduces

$$\hat{G}_0^{(0)}(E) = \frac{1}{2}[\hat{G}_0^{(\eta)}(E) + \hat{G}_0^{(-\eta)}(E)] \tag{2.11}$$

and

$$\hat{D}_0(E) = \frac{1}{2\mathrm{i}\eta}[\hat{G}_0^{(\eta)}(E) - \hat{G}_0^{(-\eta)}(E)], \tag{2.12}$$

which generalize Eqs. (2.6) and (2.9), respectively. Finally, operating on Eq. (2.8) from the left with $\hat{H}_0 - E \mp \mathrm{i}\epsilon$, with the aid of the definition (2.1) and the relation (2.10), we find that $\hat{G}_0^{(\eta)}(E)$ is a solution to the inhomogeneous operator equation

$$[\hat{H}_0 - E \mp \mathrm{i}\epsilon]\hat{G}_0^{(\eta)}(E) = \hat{I} \mp \mathrm{i}\epsilon(1 \mp \eta)\hat{G}_0^{(\mp)}(E), \tag{2.13}$$

where $\hat{I}$ is the identity operator.

2.2. Generalized scattering states and transition operators

Let the state $|\Phi(E)\rangle$ be a solution to the stationary free-particle Schrödinger equation

$$[\hat{H}_0 - E]|\Phi(E)\rangle = 0 \tag{2.14}$$

and let $\hat{V}$ be a short range Hermitian potential operator such that $E \in \mathbb{R}$ is in the continuous spectrum of the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}. \tag{2.15}$$

For the Hamiltonian (2.15) and energy E, a generalized scattering state $|\Psi^{(\eta)}(E)\rangle$, induced by the state $|\Phi(E)\rangle$ and associated with the free-particle Green operator $\hat{G}_0^{(\eta)}(E)$, is defined as a solution to the Lippmann–Schwinger equation

$$|\Psi^{(\eta)}(E)\rangle = |\Phi(E)\rangle - \hat{G}_0^{(\eta)}(E)\hat{V}|\Psi^{(\eta)}(E)\rangle. \tag{2.16}$$

Operating on Eq. (2.16) from the left with $\hat{H}_0 - E \mp \mathrm{i}\epsilon$ and exploiting Eq. (2.13), we arrive at the following Schrödinger equations equivalent to Eq. (2.16):

$$[\hat{H} - E \mp \mathrm{i}\epsilon \mp \mathrm{i}\epsilon(1 \mp \eta)\hat{G}_0^{(\mp)}(E)\hat{V}]|\Psi^{(\eta)}(E)\rangle = \mp\mathrm{i}\epsilon|\Phi(E)\rangle. \tag{2.17}$$

The generalized transition operator $\hat{T}^{(\eta)}(E)$, defined through the relationship

$$\hat{T}^{(\eta)}(E)|\Phi(E)\rangle = \hat{V}|\Psi^{(\eta)}(E)\rangle, \tag{2.18}$$

obeys the operator equation

$$\hat{T}^{(\eta)}(E) = \hat{V} - \hat{V}\hat{G}_0^{(\eta)}(E)\hat{T}^{(\eta)}(E) \tag{2.19}$$

and is formally given by

$$\hat{T}^{(\eta)}(E) = \hat{V}\left[\hat{I} + \hat{G}_0^{(\eta)}(E)\hat{V}\right]^{-1} = \left[\hat{I} + \hat{V}\hat{G}_0^{(\eta)}(E)\right]^{-1}\hat{V}. \tag{2.20}$$

In terms of $\hat{T}^{(\eta)}(E)$, the Lippmann–Schwinger equation (2.16) is

$$|\Psi^{(\eta)}(E)\rangle = |\Phi(E)\rangle - \hat{G}_0^{(\eta)}(E)\hat{T}^{(\eta)}(E)|\Phi(E)\rangle. \tag{2.21}$$

In virtue of Eqs. (2.20) and (2.4), and the Hermiticity of $\hat{V}$, the operators $\hat{T}^{(\eta)}(E)$ and $\hat{T}^{(-\eta^*)}(E)$ obey

$$\hat{T}^{(\eta)\dagger}(E) = \hat{T}^{(-\eta^*)}(E). \tag{2.22}$$

Moreover, from Eq. (2.20) we have

$$\hat{T}^{(\eta)}(E) - \hat{T}^{(\eta')}(E) = \hat{T}^{(\eta)}(E)\left[\hat{G}_0^{(\eta')}(E) - \hat{G}_0^{(\eta)}(E)\right]\hat{T}^{(\eta')}(E) \tag{2.23}$$

or equivalently, after exploiting Eq. (2.12),

$$\hat{T}^{(\eta)}(E) - \hat{T}^{(\eta')}(E) = \mathrm{i}(\eta' - \eta)\hat{T}^{(\eta)}(E)\hat{D}_0(E)\hat{T}^{(\eta')}(E). \tag{2.24}$$

Equation (2.24) expresses the generalized optical theorem.

The parameter η may be arbitrary complex. However, three special cases, namely $\eta = \pm 1$ and $\eta = 0$, are of particular importance and need a brief discussion here. The states $|\Psi^{(\pm 1)}(E)\rangle$ are identical with the standard going states $|\Psi^{(\pm)}(E)\rangle$ obeying

$$|\Psi^{(\pm)}(E)\rangle = |\Phi(E)\rangle - \hat{G}_0^{(\pm)}(E)\hat{V}|\Psi^{(\pm)}(E)\rangle, \tag{2.25}$$

while $|\Psi^{(0)}(E)\rangle$ is the standard standing state and obeys

$$|\Psi^{(0)}(E)\rangle = |\Phi(E)\rangle - \hat{G}_0^{(0)}(E)\hat{V}|\Psi^{(0)}(E)\rangle. \tag{2.26}$$

Similarly, the operator

$$\hat{T}^{(+)}(E) \equiv \hat{T}^{(+1)}(E) \tag{2.27}$$

is the standard transition operator $\hat{T}(E)$ from the potential scattering theory, the operator

$$\hat{T}^{(-)}(E) \equiv \hat{T}^{(-1)}(E) \tag{2.28}$$

is its Hermitian adjoint (cf. Eq. (2.22)), while the Hermitian (cf. again Eq. (2.22)) operator $\hat{T}^{(0)}(E)$ is related to the standard reactance operator $\hat{K}(E)$ through

$$\hat{T}^{(0)}(E) = -\hat{K}(E). \tag{2.29}$$

For $\eta = \pm 1$, $\eta' = \mp 1$, Eq. (2.24) reduces to the standard optical theorem

$$\hat{T}(E) - \hat{T}^{\dagger}(E) = -2\mathrm{i}\hat{T}(E)\hat{D}_0(E)\hat{T}^{\dagger}(E), \tag{2.30}$$

$$\hat{T}(E) - \hat{T}^{\dagger}(E) = -2\mathrm{i}\hat{T}^{\dagger}(E)\hat{D}_0(E)\hat{T}(E), \tag{2.31}$$

while for $\eta = 1$, $\eta' = 0$ and for $\eta = 0$, $\eta' = 1$ it yields the Heitler equations

$$\hat{T}(E) = -\hat{K}(E) + \mathrm{i}\hat{T}(E)\hat{D}_0(E)\hat{K}(E), \tag{2.32}$$

$$\hat{T}(E) = -\hat{K}(E) + \mathrm{i}\hat{K}(E)\hat{D}_0(E)\hat{T}(E). \tag{2.33}$$

2.3. Green operators

The Green operator $\hat{G}^{(\eta)}(E)$ is defined as a solution to the equation

$$\hat{G}^{(\eta)}(E) = \hat{G}_0^{(\eta)}(E) - \hat{G}_0^{(\eta)}(E)\hat{V}\hat{G}^{(\eta)}(E). \tag{2.34}$$

From Eqs. (2.34) and (2.20) it follows that:

$$\hat{G}^{(\eta)}(E) = \hat{G}_0^{(\eta)}(E) - \hat{G}_0^{(\eta)}(E)\hat{T}^{(\eta)}(E)\hat{G}_0^{(\eta)}(E). \tag{2.35}$$

The equation

$$\left[\hat{H} - E \mp \mathrm{i}\epsilon \mp \mathrm{i}\epsilon(1 \mp \eta)\hat{G}_0^{(\mp)}(E)\hat{V}\right]\hat{G}^{(\eta)}(E) = \hat{I} \mp \mathrm{i}\epsilon(1 \mp \eta)\hat{G}_0^{(\mp)}(E), \tag{2.36}$$

equivalent to Eq. (2.34), is obtained after operating on the latter from the left with $\hat{H}_0 - E \mp \mathrm{i}\epsilon$ and exploiting Eq. (2.13). From either of Eqs. (2.34) or (2.36), for the operators

$$\hat{G}^{(\pm)}(E) = \hat{G}^{(\pm 1)}(E) \tag{2.37}$$

we have

$$\hat{G}^{(\pm)}(E) = [\hat{H} - E \mp \mathrm{i}\epsilon]^{-1}. \tag{2.38}$$

3. Eigenchannels

3.1. Definition and basic properties

We define eigenchannels $\{|X_\gamma(E)\rangle\}$ as eigenstates of the spectral problem

$$\left[\hat{I} + \hat{G}_0^{(0)}(E)\hat{V}\right]|X_\gamma(E)\rangle = \lambda_\gamma(E)\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle, \tag{3.1}$$

in which $E \in \mathbb{R}$ is from the continuous spectra of both $\hat{H}_0$ and $\hat{H}$ and is fixed, while $\lambda_\gamma(E)$ is an eigenvalue. It should be emphasized that the eigenproblem (3.1) belongs to the category of weighted (generalized) eigenproblems. Throughout the rest of this work, we shall be assuming that, in addition to what has been said about the potential operator $\hat{V}$ at the beginning of Section 2.2, $\hat{V}$ is also such that a spectrum to the eigenproblem (3.1) is nonempty and purely discrete.

For the sake of later applications, it is convenient to rewrite Eq. (3.1), with the aid of Eq. (2.7), in the form

$$\left[\hat{I} + \hat{G}_0^{(\eta)}(E)\hat{V}\right]|X_\gamma(E)\rangle = [\lambda_\gamma(E) + \mathrm{i}\eta]\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle. \tag{3.2}$$

Moreover, making use of Eqs. (2.11) and (2.12), it is possible to express Eq. (3.1) in terms of $\hat{G}_0^{(\pm\eta)}(E)$ as

$$|X_\gamma(E)\rangle = \frac{1}{2\mathrm{i}\eta}\left[[\lambda_\gamma(E) - \mathrm{i}\eta]\hat{G}_0^{(\eta)}(E) - [\lambda_\gamma(E) + \mathrm{i}\eta]\hat{G}_0^{(-\eta)}(E)\right]\hat{V}|X_\gamma(E)\rangle \tag{3.3}$$

or equivalently as

$$[\lambda_\gamma(E) - \mathrm{i}\eta]\left[\hat{I} + \hat{G}_0^{(\eta)}(E)\hat{V}\right]|X_\gamma(E)\rangle = [\lambda_\gamma(E) + \mathrm{i}\eta]\left[\hat{I} + \hat{G}_0^{(-\eta)}(E)\hat{V}\right]|X_\gamma(E)\rangle. \tag{3.4}$$

Finally, after operating on Eq. (3.1) from the left with $\hat{H}_0 - E \mp \mathrm{i}\epsilon$, one finds

$$[\hat{H} - E \mp \mathrm{i}\epsilon]|X_\gamma(E)\rangle = \epsilon[\lambda_\gamma(E) \pm \mathrm{i}]\hat{G}_0^{(\mp)}(E)\hat{V}|X_\gamma(E)\rangle, \tag{3.5}$$

which shows that the eigenstates $\{|X_\gamma(E)\rangle\}$ satisfy the Schrödinger equation at the energy E. We shall make use of Eqs. (3.2)–(3.5) in later considerations.

Evidently, the eigenproblem (3.1) is non-Hermitian. By acting on Eq. (3.1) from the left with the potential operator $\hat{V}$, we arrive at an eigenproblem

$$\left[\hat{V} + \hat{V}\hat{G}_0^{(0)}(E)\hat{V}\right]|X_\gamma(E)\rangle = \lambda_\gamma(E)\hat{V}\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle \tag{3.6}$$

possessing the same eigensolutions as the eigenproblem (3.1). However, as opposed to the latter, the eigenproblem (3.6) is manifestly Hermitian. Moreover, since the operator $\hat{D}_0(E)$ is positive definite (cf. the remark following Eq. (2.9)), the weight operator $\hat{V}\hat{D}_0(E)\hat{V}$ is also positive definite, i.e., it holds

$$\langle X_\gamma(E)|\hat{V}\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle > 0. \tag{3.7}$$

Hence, in the standard manner one may show that the eigenvalues $\{\lambda_\gamma(E)\}$ are real:

$$\lambda_\gamma^*(E) = \lambda_\gamma(E), \tag{3.8}$$

and that eigenchannels associated with different eigenvalues satisfy the weighted orthogonality relation

$$\langle X_\gamma(E)|\hat{V}\hat{D}_0(E)\hat{V}|X_{\gamma'}(E)\rangle = 0 \qquad (\lambda_\gamma(E) \neq \lambda_{\gamma'}(E)). \tag{3.9}$$

Normalizing the eigenchannels to unity according to

$$\langle X_\gamma(E)|\hat{V}\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle = 1 \tag{3.10}$$

from Eqs. (3.6) and (3.10) we have

$$\lambda_\gamma(E) = \langle X_\gamma(E)|\hat{V} + \hat{V}\hat{G}_0^{(0)}(E)\hat{V}|X_\gamma(E)\rangle. \tag{3.11}$$

If eigenchannels associated with degenerate eigenvalues (if there are any) have also been orthogonalized in the sense of Eq. (3.9), from the latter equation and from Eq. (3.10) we have the orthonormality relation

$$\langle X_\gamma(E)|\hat{V}\hat{D}_0(E)\hat{V}|X_{\gamma'}(E)\rangle = \delta_{\gamma\gamma'}. \tag{3.12}$$

Throughout the rest of the paper, the relation (3.12) will be assumed to hold.

The explicit form of the generalized Hermitian eigenproblem (3.6) suggests that the eigenchannels may obey the following closure relations:

$$\sum_\gamma \hat{V}\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V} = \hat{V}, \tag{3.13}$$

$$\sum_\gamma \hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}\hat{D}_0(E)\hat{V} = \hat{V}, \tag{3.14}$$

and in fact the considerations of Section 3.2 rely on the assumption that these relations do hold. However, it should be clearly stated here that at the present stage these relations are conjectures which remain to be proved.

3.2. Expansions in eigenchannels and applications

Although the eigenchannels are interesting for themselves, their importance lies primarily in the fact that they are useful for solving scattering problems. Below we shall illustrate this by finding eigenchannel representations of the generalized scattering state $|\Psi^{(\eta)}(E)\rangle$, the generalized transition operator $\hat{T}^{(\eta)}(E)$, and the Green operator $\hat{G}^{(\eta)}(E)$.

To find the eigenchannel representation of $|\Psi^{(\eta)}(E)\rangle$, consider the equation

$$\left[\hat{V} + \hat{V}\hat{G}_0^{(\eta)}(E)\hat{V}\right]|\Psi^{(\eta)}(E)\rangle = \hat{V}|\Phi(E)\rangle \tag{3.15}$$

resulting from Eq. (2.16) after acting on the latter from the left with $\hat{V}$. Since $\hat{V}$ has been assumed to be of the short range character, one should solve Eq. (3.15) for $\hat{V}|\Psi^{(\eta)}(E)\rangle$ rather than for $|\Psi^{(\eta)}(E)\rangle$. We shall seek $\hat{V}|\Psi^{(\eta)}(E)\rangle$ in the form of the following series:

$$\hat{V}|\Psi^{(\eta)}(E)\rangle = \sum_{\gamma} a_{\gamma}^{(\eta)}(E)\hat{V}|X_{\gamma}(E)\rangle, \tag{3.16}$$

where $\{a_{\gamma}^{(\eta)}(E)\}$ are coefficients to be determined. On substituting this series into Eq. (3.15) and making use of Eq. (3.2), we find

$$\sum_{\gamma} a_{\gamma}^{(\eta)}(E)[\lambda_{\gamma}(E) + \mathrm{i}\eta]\hat{V}\hat{D}_0(E)\hat{V}|X_{\gamma}(E)\rangle = \hat{V}|\Phi(E)\rangle. \tag{3.17}$$

Then, after projecting Eq. (3.17) onto the eigenchannels and making use of the orthonormality relation (3.12), we deduce

$$a_{\gamma}^{(\eta)}(E) = \frac{1}{\lambda_{\gamma}(E) + \mathrm{i}\eta}\langle X_{\gamma}(E)|\hat{V}|\Phi(E)\rangle, \tag{3.18}$$

and next, after substituting this result into the expansion (3.16), we arrive at

$$\hat{V}|\Psi^{(\eta)}(E)\rangle = \sum_{\gamma} \frac{1}{\lambda_{\gamma}(E) + \mathrm{i}\eta}\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V}|\Phi(E)\rangle. \tag{3.19}$$

Finally, after substitution of the expansion (3.19) into the second term on the right-hand side of Eq. (2.16), we obtain

$$|\Psi^{(\eta)}(E)\rangle = |\Phi(E)\rangle - \sum_{\gamma} \frac{1}{\lambda_{\gamma}(E) + \mathrm{i}\eta}\hat{G}_0^{(\eta)}(E)\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V}|\Phi(E)\rangle, \tag{3.20}$$

which is the sought representation of the generalized scattering state $|\Psi^{(\eta)}(E)\rangle$ in terms of eigenchannels.

As a by-product, the above considerations yield the eigenchannel representation of the generalized transition operator $\hat{T}^{(\eta)}(E)$. Indeed, on comparing Eqs. (3.19) and (2.18), we find

$$\hat{T}^{(\eta)}(E) = \sum_{\gamma} \frac{1}{\lambda_{\gamma}(E) + \mathrm{i}\eta}\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V}. \tag{3.21}$$

The eigenchannel representation of the Green operator $\hat{G}^{(\eta)}(E)$:

$$\hat{G}^{(\eta)}(E) = \hat{G}_0^{(\eta)}(E) - \sum_{\gamma} \frac{1}{\lambda_{\gamma}(E) + \mathrm{i}\eta}\hat{G}_0^{(\eta)}(E)\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V}\hat{G}_0^{(\eta)}(E) \tag{3.22}$$

follows directly from Eqs. (3.21) and (2.35). It may be instructive, however, to derive this representation without referring to Eq. (2.35). To this end, consider the equation for $\hat{V}\hat{G}^{(\eta)}(E)$:

$$\left[\hat{V} + \hat{V}\hat{G}_0^{(\eta)}(E)\hat{V}\right]\hat{G}^{(\eta)}(E) = \hat{V}\hat{G}_0^{(\eta)}(E) \tag{3.23}$$

stemming from Eq. (2.34). We shall seek its solution in the form

$$\hat{V}\hat{G}^{(\eta)}(E) = \sum_{\gamma} \hat{V}|X_{\gamma}(E)\rangle\langle A_{\gamma}^{(\eta)}(E)|, \tag{3.24}$$

where the bras $\{\langle A_{\gamma}^{(\eta)}(E)|\}$ are expansion coefficients. After substituting the expansion (3.24) into Eq. (3.23), making use of Eq. (3.2), and projecting the resulting equation

$$\sum_{\gamma}[\lambda_{\gamma}(E) + \mathrm{i}\eta]\hat{V}\hat{D}_0(E)\hat{V}|X_{\gamma}(E)\rangle\langle A_{\gamma}^{(\eta)}(E)| = \hat{V}\hat{G}_0^{(\eta)}(E) \tag{3.25}$$

from the left onto the eigenchannels, we find

$$\langle A_{\gamma}^{(\eta)}(E)| = \frac{1}{\lambda_{\gamma}(E) + \mathrm{i}\eta}\langle X_{\gamma}(E)|\hat{V}\hat{G}_0^{(\eta)}(E), \tag{3.26}$$

hence

$$\hat{V}\hat{G}^{(\eta)}(E) = \sum_{\gamma} \frac{1}{\lambda_{\gamma}(E) + \mathrm{i}\eta}\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V}\hat{G}_0^{(\eta)}(E). \tag{3.27}$$

Substitution of this result into the second term on the right-hand side of Eq. (2.34) leads to the representation (3.22).

The eigenchannel representation (3.21) may be considered as a definition of the generalized transition operator $\hat{T}^{(\eta)}(E)$, alternative to that provided in Eq. (2.20). Therefore, one expects it should be possible to prove various properties of $\hat{T}^{(\eta)}(E)$ using only Eq. (3.21) and relevant properties of the eigenchannels. This is indeed the case. For instance, on performing the Hermitian conjugation of Eq. (3.21), in virtue of reality of the eigenvalues $\{\lambda_{\gamma}(E)\}$, we obtain

$$\hat{T}^{(\eta)\dagger}(E) = \sum_{\gamma} \frac{1}{\lambda_{\gamma}(E) - \mathrm{i}\eta^{*}}\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V} = \hat{T}^{(-\eta^{*})}(E), \tag{3.28}$$

i.e., the property (2.22). Similarly, from Eq. (3.21) we have

$$\hat{T}^{(\eta)}(E) - \hat{T}^{(\eta')}(E) = \mathrm{i}(\eta' - \eta)\sum_{\gamma} \frac{1}{[\lambda_{\gamma}(E) + \mathrm{i}\eta][\lambda_{\gamma}(E) + \mathrm{i}\eta']}\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V} \tag{3.29}$$

and, after exploiting the orthonormality relation (3.12),

$$\hat{T}^{(\eta)}(E)\hat{D}_0(E)\hat{T}^{(\eta')}(E) = \sum_{\gamma} \frac{1}{[\lambda_{\gamma}(E) + \mathrm{i}\eta][\lambda_{\gamma}(E) + \mathrm{i}\eta']}\hat{V}|X_{\gamma}(E)\rangle\langle X_{\gamma}(E)|\hat{V}, \tag{3.30}$$

hence, the generalized optical theorem (2.24) follows immediately.

Before concluding this section, a remark concerning the meaning of the expansion (3.21) is in order: this expansion is *not* a spectral expansion of $\hat{T}^{(\eta)}(E)$. The reason for this is that the kets $\{\hat{V}|X_{\gamma}(E)\rangle\}$ are eigenstates of neither $\hat{T}^{(\eta)}(E)$ nor $\hat{T}^{(\eta)\dagger}(E)$. However, let us define a modified generalized transition operator

$$\hat{\mathscr{T}}^{(\eta)}(E) = \hat{T}^{(\eta)}(E)\hat{D}_0(E). \tag{3.31}$$

From Eqs. (3.31), (3.21), and (3.12) one infers the eigenequation

$$\hat{\mathscr{T}}^{(\eta)}(E)\hat{V}|X_\gamma(E)\rangle = \frac{1}{\lambda_\gamma(E)+\mathrm{i}\eta}\hat{V}|X_\gamma(E)\rangle \tag{3.32}$$

(Eq. (3.32) follows also from the definitions (2.20) and (3.31) and from the eigenequation (3.2)). Consequently, $\{\hat{V}|X_\gamma(E)\rangle\}$ are eigenstates of $\hat{\mathscr{T}}^{(\eta)}(E)$ and $\{[\lambda_\gamma(E)+\mathrm{i}\eta]^{-1}\}$ are associated eigenvalues. From Eqs. (3.31) and (2.22) we find that the Hermitian adjoint of $\hat{\mathscr{T}}^{(\eta)}(E)$ is

$$\hat{\mathscr{T}}^{(\eta)\dagger}(E) = \hat{D}_0(E)\hat{T}^{(-\eta^*)}(E) \tag{3.33}$$

and from Eqs. (3.33), (3.28), and (3.12) one deduces the eigenequation

$$\hat{\mathscr{T}}^{(\eta)\dagger}(E)\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle = \frac{1}{\lambda_\gamma(E)-\mathrm{i}\eta^*}\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle. \tag{3.34}$$

It is seen that $\{\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle\}$ are eigenstates of $\hat{\mathscr{T}}^{(\eta)\dagger}(E)$ and $\{[\lambda_\gamma(E)-\mathrm{i}\eta^*]^{-1}\}$ are associated eigenvalues. From the eigensolutions to Eqs. (3.32) and (3.34), keeping in mind the orthonormality relation (3.12), one constructs the spectral expansions of $\hat{\mathscr{T}}^{(\eta)}(E)$ and $\hat{\mathscr{T}}^{(\eta)\dagger}(E)$:

$$\hat{\mathscr{T}}^{(\eta)}(E) = \sum_\gamma \frac{1}{\lambda_\gamma(E)+\mathrm{i}\eta}\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}\hat{D}_0(E), \tag{3.35}$$

$$\hat{\mathscr{T}}^{(\eta)\dagger}(E) = \sum_\gamma \frac{1}{\lambda_\gamma(E)-\mathrm{i}\eta^*}\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}. \tag{3.36}$$

4. Eigenphases

When $\eta = 0$ or $\eta = \pm 1$, instead of working with the eigenvalues $\{\lambda_\gamma(E)\}$, as we have been doing in Section 3, it is convenient to introduce so-called eigenphases (eigenphaseshifts) $\{\delta_\gamma(E)\}$, related to the eigenvalues $\{\lambda_\gamma(E)\}$ through

$$\lambda_\gamma(E) = -\cot\delta_\gamma(E). \tag{4.1}$$

We have already argued in Section 3 that the eigenvalues $\{\lambda_\gamma(E)\}$ are real. Consequently, from the definition (4.1) it follows that the eigenphases are also real:

$$\delta_\gamma^*(E) = \delta_\gamma(E). \tag{4.2}$$

In terms of the eigenphases, the defining eigenequation (3.1) becomes

$$\left[\hat{I} + \hat{G}_0^{(0)}(E)\hat{V}\right]|X_\gamma(E)\rangle = -\cot\delta_\gamma(E)\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle, \tag{4.3}$$

while Eqs. (3.2)–(3.4), specialized to the cases $\eta = \pm 1$, read

$$\left[\hat{I} + \hat{G}_0^{(\pm)}(E)\hat{V}\right]|X_\gamma(E)\rangle = -\frac{\mathrm{e}^{\mp\mathrm{i}\delta_\gamma(E)}}{\sin\delta_\gamma(E)}\hat{D}_0(E)\hat{V}|X_\gamma(E)\rangle, \tag{4.4}$$

$$|X_\gamma(E)\rangle = \frac{1}{2\mathrm{i}\sin\delta_\gamma(E)}\left[\mathrm{e}^{-\mathrm{i}\delta_\gamma(E)}\hat{G}_0^{(-)}(E) - \mathrm{e}^{\mathrm{i}\delta_\gamma(E)}\hat{G}_0^{(+)}(E)\right]\hat{V}|X_\gamma(E)\rangle, \tag{4.5}$$

$$\mathrm{e}^{\mathrm{i}\delta_\gamma(E)}\left[\hat{I} + \hat{G}_0^{(+)}(E)\hat{V}\right]|X_\gamma(E)\rangle = \mathrm{e}^{-\mathrm{i}\delta_\gamma(E)}\left[\hat{I} + \hat{G}_0^{(-)}(E)\hat{V}\right]|X_\gamma(E)\rangle. \tag{4.6}$$

Further, for $\eta = 0$, from Eqs. (3.20), (3.22), (2.29), and (3.21), we infer

$$|\Psi^{(0)}(E)\rangle = |\Phi(E)\rangle + \sum_\gamma \tan\delta_\gamma(E)\hat{G}_0^{(0)}(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}|\Phi(E)\rangle, \tag{4.7}$$

$$\hat{G}^{(0)}(E) = \hat{G}_0^{(0)}(E) + \sum_\gamma \tan\delta_\gamma(E)\hat{G}_0^{(0)}(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}\hat{G}_0^{(0)}(E), \tag{4.8}$$

$$\hat{K}(E) \equiv -\hat{T}^{(0)}(E) = \sum_\gamma \tan\delta_\gamma(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}. \tag{4.9}$$

Similarly, for $\eta = \pm 1$, from Eqs. (3.20), (3.22), and (3.21), we find

$$|\Psi^{(\pm)}(E)\rangle = |\Phi(E)\rangle + \sum_\gamma \mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)\hat{G}_0^{(\pm)}(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}|\Phi(E)\rangle, \tag{4.10}$$

$$\hat{G}^{(\pm)}(E) = \hat{G}_0^{(\pm)}(E) + \sum_\gamma \mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)\hat{G}_0^{(\pm)}(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}\hat{G}_0^{(\pm)}(E), \tag{4.11}$$

$$\hat{T}^{(\pm)}(E) = -\sum_\gamma \mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)\hat{V}|X_\gamma(E)\rangle\langle X_\gamma(E)|\hat{V}. \tag{4.12}$$

5. Variational approach

In actual applications of the general theory presented above the potential operator $\hat{V}$ may be such that exact solutions to the spectral problem (3.1) will not be available. In such cases one may resort to the variational approach which we shall discuss in this section at some length.

Three variational principles appear to be particularly useful for the present purposes. The first principle, constructed in Appendix B, is the one for eigenvalues to the spectral system (3.1) (for brevity, throughout the rest of this section we shall omit labels at eigensolutions):

$$\delta\mathscr{F}_1[|X(E)\rangle, \langle X(E)|] = 0, \tag{5.1}$$

$$\lambda(E) = \mathscr{F}_1[|X(E)\rangle, \langle X(E)|], \tag{5.2}$$

with the functional

$$\mathscr{F}_1\left[|\overline{X}\rangle, \langle\overline{X}|\right] = \frac{\langle\overline{X}|\hat{V} + \hat{V}\hat{G}_0^{(0)}(E)\hat{V}|\overline{X}\rangle}{\langle\overline{X}|\hat{V}\hat{D}_0(E)\hat{V}|\overline{X}\rangle}. \tag{5.3}$$

Here $|\overline{X}\rangle$ is some estimate of $|X(E)\rangle$ and $\langle\overline{X}|$ is its Hermitian adjoint. Next, let $|\Phi_\alpha(E)\rangle$ and $|\Phi_\beta(E)\rangle$ be two solutions to the free-particle Schrödinger equation (2.14), both corresponding to the same energy E and otherwise arbitrary, and let

$$T^{(\eta)}_{\beta\alpha}(E) = \langle\Phi_\beta(E)|\hat{T}^{(\eta)}(E)|\Phi_\alpha(E)\rangle. \tag{5.4}$$

The second variational principle we consider is the Schwinger principle [55]

$$\delta\mathscr{F}_2[|\Psi^{(\eta)}_\alpha(E)\rangle, \langle\Psi^{(-\eta^*)}_\beta(E)|] = 0, \tag{5.5}$$

$$T^{(\eta)}_{\beta\alpha}(E) = \mathscr{F}_2[|\Psi^{(\eta)}_\alpha(E)\rangle, \langle\Psi^{(-\eta^*)}_\beta(E)|], \tag{5.6}$$

with the linear functional

$$\begin{aligned}\mathscr{F}_2[|\overline{\Psi}^{(\eta)}_\alpha\rangle, \langle\overline{\Psi}^{(-\eta^*)}_\beta|] = {}& \langle\Phi_\beta(E)|\hat{V}|\overline{\Psi}^{(\eta)}_\alpha\rangle + \langle\overline{\Psi}^{(-\eta^*)}_\beta|\hat{V}|\Phi_\alpha(E)\rangle \\ & - \langle\overline{\Psi}^{(-\eta^*)}_\beta|\hat{V} + \hat{V}\hat{G}^{(\eta)}_0(E)\hat{V}|\overline{\Psi}^{(\eta)}_\alpha\rangle.\end{aligned} \tag{5.7}$$

The third principle is the Schwinger principle [55]

$$\delta\mathscr{F}_3[|\Psi^{(\eta)}_\alpha(E)\rangle, \langle\Psi^{(-\eta^*)}_\beta(E)|] = 0, \tag{5.8}$$

$$T^{(\eta)}_{\beta\alpha}(E) = \mathscr{F}_3[|\Psi^{(\eta)}_\alpha(E)\rangle, \langle\Psi^{(-\eta^*)}_\beta(E)|], \tag{5.9}$$

with the fractional functional

$$\mathscr{F}_3[|\overline{\Psi}^{(\eta)}_\alpha\rangle, \langle\overline{\Psi}^{(-\eta^*)}_\beta|] = \frac{\langle\Phi_\beta(E)|\hat{V}|\overline{\Psi}^{(\eta)}_\alpha\rangle\langle\overline{\Psi}^{(-\eta^*)}_\beta|\hat{V}|\Phi_\alpha(E)\rangle}{\langle\overline{\Psi}^{(-\eta^*)}_\beta|\hat{V} + \hat{V}\hat{G}^{(\eta)}_0(E)\hat{V}|\overline{\Psi}^{(\eta)}_\alpha\rangle}. \tag{5.10}$$

In the functionals (5.7) and (5.10), $|\overline{\Psi}^{(\eta)}_\alpha\rangle$ and $\langle\overline{\Psi}^{(-\eta^*)}_\beta|$ are estimates of $|\Psi^{(\eta)}_\alpha(E)\rangle$ and $\langle\Psi^{(-\eta^*)}_\beta(E)|$, respectively, where the state $|\Psi^{(\eta)}_\alpha(E)\rangle$ is a solution to the Lippmann–Schwinger equation (2.16) with $|\Phi(E)\rangle = |\Phi_\alpha(E)\rangle$ and $\langle\Psi^{(-\eta^*)}_\beta(E)|$ is a Hermitian adjoint to $|\Psi^{(-\eta^*)}_\beta(E)\rangle$, the latter being defined analogously to $|\Psi^{(\eta)}_\alpha(E)\rangle$. It is worth noticing that, since the functional (5.10) has the property that for arbitrary $\mu_\alpha, \mu_\beta \in \mathbb{C} \setminus \{0\}$ it holds

$$\mathscr{F}_3[\mu_\alpha|\overline{\Psi}^{(\eta)}_\alpha\rangle, \mu_\beta\langle\overline{\Psi}^{(-\eta^*)}_\beta|] = \mathscr{F}_3[|\overline{\Psi}^{(\eta)}_\alpha\rangle, \langle\overline{\Psi}^{(-\eta^*)}_\beta|], \tag{5.11}$$

the principle (5.8) and (5.9) may be replaced by the following more general one:

$$\delta\mathscr{F}_3[\mu_\alpha|\Psi^{(\eta)}_\alpha(E)\rangle, \mu_\beta\langle\Psi^{(-\eta^*)}_\beta(E)|] = 0, \tag{5.12}$$

$$T^{(\eta)}_{\beta\alpha}(E) = \mathscr{F}_3[\mu_\alpha|\Psi^{(\eta)}_\alpha(E)\rangle, \mu_\beta\langle\Psi^{(-\eta^*)}_\beta(E)|]. \tag{5.13}$$

To see how the variational method works in practice, let us approximate $|X(E)\rangle$ as a linear combination of n linearly independent (but not necessarily orthogonal) vectors $\{|\chi_i\rangle\}$:

$$|\overline{X}\rangle = \sum_{i=1}^{n} \overline{c}_i|\chi_i\rangle, \tag{5.14}$$

where $\{\bar{c}_i\}$ are yet unknown coefficients which remain to be optimized. Substitution of this estimate, and its adjoint, into the functional (5.3) yields

$$\mathscr{F}_1\left[\bar{\mathsf{c}}^\dagger, \bar{\mathsf{c}}\right] = \frac{\bar{\mathsf{c}}^\dagger \mathsf{A}(E)\bar{\mathsf{c}}}{\bar{\mathsf{c}}^\dagger \mathsf{B}(E)\bar{\mathsf{c}}}, \tag{5.15}$$

where $\bar{\mathsf{c}}$ is an n-component column matrix with elements $\{\bar{c}_i\}$, $\bar{\mathsf{c}}^\dagger$ is an n-component row matrix with elements $\{\bar{c}_i^*\}$, while $\mathsf{A}(E)$ and $\mathsf{B}(E)$ are $n \times n$ Hermitian matrices with elements

$$A_{ij}(E) = \langle \chi_i | \hat{V} + \hat{V}\hat{G}_0^{(0)}(E)\hat{V} | \chi_j \rangle \tag{5.16}$$

and

$$B_{ij}(E) = \langle \chi_i | \hat{V}\hat{D}_0(E)\hat{V} | \chi_j \rangle, \tag{5.17}$$

respectively. We shall denote by $\tilde{\mathsf{c}}(E)$ and $\tilde{\mathsf{c}}^\dagger(E)$ these vectors $\bar{\mathsf{c}}$ and $\bar{\mathsf{c}}^\dagger$ for which the functional (5.15) is stationary with respect to variations in their components, i.e.,

$$\delta\mathscr{F}_1[\tilde{\mathsf{c}}^\dagger(E), \tilde{\mathsf{c}}(E)] = 0, \tag{5.18}$$

and define

$$\tilde{\lambda}(E) = \mathscr{F}_1\left[\tilde{\mathsf{c}}^\dagger(E), \tilde{\mathsf{c}}(E)\right]. \tag{5.19}$$

Eqs. (5.15), (5.18), and (5.19) lead to the generalized matrix eigensystem

$$\mathsf{A}(E)\tilde{\mathsf{c}}(E) = \tilde{\lambda}(E)\mathsf{B}(E)\tilde{\mathsf{c}}(E) \tag{5.20}$$

and to its Hermitian adjoint. In general, the eigensystem (5.20) will have $v \leqslant n$ eigenvalues $\{\tilde{\lambda}_\gamma(E)\}$ and associated eigenvectors $\{\tilde{\mathsf{c}}_\gamma(E)\}$ (the index γ serves to distinguish between *eigenvectors*, i.e., in the case of degeneracy some eigenvalues with different indices will coincide). Since both the matrices $\mathsf{A}(E)$ and $\mathsf{B}(E)$ are Hermitian and B is positive definite, the eigenvalues to the system (5.20) possess the desired property of being real:

$$\tilde{\lambda}_\gamma^*(E) = \tilde{\lambda}_\gamma(E), \tag{5.21}$$

while eigenvectors belonging to different eigenvalues are orthogonal in the sense of

$$\tilde{\mathsf{c}}_\gamma^\dagger(E)\mathsf{B}(E)\tilde{\mathsf{c}}_{\gamma'}(E) = 0 \qquad \left(\tilde{\lambda}_\gamma(E) \neq \tilde{\lambda}_{\gamma'}(E)\right). \tag{5.22}$$

In what follows, we shall be assuming that eigenvectors belonging to degenerate eigenvalues (if there are any) have been also orthogonalized in the sense analogous to Eq. (5.22) and that all eigenvectors have been normalized so that it holds

$$\tilde{\mathsf{c}}_\gamma^\dagger(E)\mathsf{B}(E)\tilde{\mathsf{c}}_{\gamma'}(E) = \delta_{\gamma\gamma'}. \tag{5.23}$$

With this assumption, from Eq. (5.20) we infer

$$\tilde{\mathsf{c}}_\gamma^\dagger(E)\mathsf{A}(E)\tilde{\mathsf{c}}_{\gamma'}(E) = \tilde{\lambda}_\gamma(E)\delta_{\gamma\gamma'}. \tag{5.24}$$

The eigenvalues $\{\tilde{\lambda}_\gamma(E)\}$ are variational estimates of the eigenvalues $\{\lambda_\gamma(E)\}$ and the vectors

$$|\tilde{X}_\gamma(E)\rangle = \sum_{i=1}^{n} \tilde{c}_{i\gamma}(E)|\chi_i\rangle, \tag{5.25}$$

where $\{\tilde{c}_{i\gamma}(E)\}$ are components of $\tilde{\mathsf{c}}_\gamma(E)$, are the best estimates of the associated eigenvectors $\{|X_\gamma(E)\rangle\}$ obtainable within the class (5.14). With the aid of Eqs. (5.17) and (5.23), it is easily verifiable that the states (5.25) are orthonormal in the sense of

$$\langle\tilde{X}_\gamma(E)|\hat{V}\hat{D}_0(E)\hat{V}|\tilde{X}_{\gamma'}(E)\rangle = \delta_{\gamma\gamma'} \tag{5.26}$$

(cf. the orthonormality relation (3.12)). Moreover, from Eqs. (5.25), (5.16), and (5.24) one infers

$$\langle\tilde{X}_\gamma(E)|\hat{V} + \hat{V}\hat{G}_0^{(0)}(E)\hat{V}|\tilde{X}_{\gamma'}(E)\rangle = \tilde{\lambda}_\gamma(E)\delta_{\gamma\gamma'}. \tag{5.27}$$

Hence, on combining the relations (5.26) and (5.27) with the definition (2.7), one also obtains

$$\langle\tilde{X}_\gamma(E)|\hat{V} + \hat{V}\hat{G}_0^{(\eta)}(E)\hat{V}|\tilde{X}_{\gamma'}(E)\rangle = [\tilde{\lambda}_\gamma(E) + \mathrm{i}\eta]\delta_{\gamma\gamma'}. \tag{5.28}$$

From elements of the sets $\{\tilde{\lambda}_\gamma(E)\}$, $\{|\tilde{X}_\gamma(E)\rangle\}$, and $\{\langle\tilde{X}_\gamma(E)|\}$ one may directly construct the following operator:

$$\hat{\tilde{T}}^{(\eta)}(E) = \sum_{\gamma=1}^{v} \frac{1}{\tilde{\lambda}_\gamma(E) + \mathrm{i}\eta} \hat{V}|\tilde{X}_\gamma(E)\rangle\langle\tilde{X}_\gamma(E)|\hat{V} \tag{5.29}$$

approximating $\hat{T}^{(\eta)}(E)$ (cf. Eq. (3.21)). Below we shall show that the operator (5.29) is optimal in the sense that it is a variational approximation to $\hat{T}^{(\eta)}(E)$. To this end, consider the functional (5.7) with

$$\hat{V}|\overline{\Psi}_\alpha^{(\eta)}\rangle = \sum_{\gamma=1}^{v} \overline{a}_{\gamma\alpha}^{(\eta)} \hat{V}|\tilde{X}_\gamma(E)\rangle, \tag{5.30}$$

$$\langle\overline{\Psi}_\beta^{(-\eta^*)}|\hat{V} = \sum_{\gamma=1}^{v} \overline{a}_{\gamma\beta}^{(-\eta^*)*} \langle\tilde{X}_\gamma(E)|\hat{V}, \tag{5.31}$$

where $\{\overline{a}_{\gamma\alpha}^{(\eta)}\}$ and $\{\overline{a}_{\gamma\beta}^{(-\eta^*)*}\}$ are as yet undetermined constants. After making use of Eq. (5.28), we have

$$\mathscr{F}_2\left[\overline{\mathsf{a}}_\alpha^{(\eta)}, \overline{\mathsf{a}}_\beta^{(-\eta^*)\dagger}\right] = \tilde{\mathsf{V}}_\beta^\dagger(E)\overline{\mathsf{a}}_\alpha^{(\eta)} + \overline{\mathsf{a}}_\beta^{(-\eta^*)\dagger}\tilde{\mathsf{V}}_\alpha(E) - \overline{\mathsf{a}}_\beta^{(-\eta^*)\dagger}[\tilde{\Lambda}(E) + \mathrm{i}\eta\mathsf{I}]\overline{\mathsf{a}}_\alpha^{(\eta)}. \tag{5.32}$$

Here $\tilde{\Lambda}(E)$ is a $v \times v$ diagonal matrix with elements $\{\tilde{\lambda}_\gamma(E)\delta_{\gamma\gamma'}\}$, I is the $v \times v$ unit matrix, $\overline{\mathsf{a}}_\alpha^{(\eta)}$ and $\tilde{\mathsf{V}}_\alpha(E)$ are, respectively, v-element column matrices with elements $\{\overline{a}_{\gamma\alpha}^{(\eta)}\}$ and $\{\tilde{V}_{\gamma\alpha}(E)\}$, where

$$\tilde{V}_{\gamma\alpha}(E) = \langle\tilde{X}_\gamma(E)|\hat{V}|\Phi_\alpha(E)\rangle, \tag{5.33}$$

while $\overline{\mathsf{a}}_\beta^{(-\eta^*)\dagger}$ and $\tilde{\mathsf{V}}_\beta^\dagger(E)$ are v-element row matrices with elements $\{\overline{a}_{\gamma\beta}^{(-\eta^*)*}\}$ and $\{\tilde{V}_{\gamma\beta}^*(E)\}$, respectively. In what follows, we shall denote by $\tilde{\mathsf{a}}_\alpha^{(\eta)}(E)$ and $\tilde{\mathsf{a}}_\beta^{(-\eta^*)\dagger}(E)$ these vectors $\overline{\mathsf{a}}_\alpha^{(\eta)}$ and $\overline{\mathsf{a}}_\beta^{(-\eta^*)\dagger}$ which make the functional (5.32) stationary with respect to variations in their components, i.e.,

$$\delta\mathscr{F}_2\left[\tilde{\mathsf{a}}_\alpha^{(\eta)}(E), \tilde{\mathsf{a}}_\beta^{(-\eta^*)\dagger}(E)\right] = 0, \tag{5.34}$$

and define

$$\tilde{T}_{\beta\alpha}^{(\eta)}(E) = \mathscr{F}_2\left[\tilde{\mathsf{a}}_\alpha^{(\eta)}(E), \tilde{\mathsf{a}}_\beta^{(-\eta^*)\dagger}(E)\right]. \tag{5.35}$$

The stationarity condition (5.34) leads to the following algebraic systems for $\tilde{\mathsf{a}}_\alpha^{(\eta)}(E)$ and $\tilde{\mathsf{a}}_\beta^{(-\eta^*)\dagger}(E)$:

$$[\tilde{\Lambda}(E) + \mathrm{i}\eta\mathsf{I}]\tilde{\mathsf{a}}_\alpha^{(\eta)}(E) = \tilde{\mathsf{V}}_\alpha(E), \tag{5.36}$$

$$\tilde{\mathsf{a}}_\beta^{(-\eta^*)\dagger}(E)[\tilde{\Lambda}(E) + \mathrm{i}\eta\mathsf{I}] = \tilde{\mathsf{V}}_\beta^\dagger(E), \tag{5.37}$$

with solutions

$$\tilde{\mathsf{a}}_\alpha^{(\eta)}(E) = [\tilde{\Lambda}(E) + \mathrm{i}\eta\mathsf{I}]^{-1}\tilde{\mathsf{V}}_\alpha(E) \tag{5.38}$$

and

$$\tilde{\mathsf{a}}_\beta^{(-\eta^*)\dagger}(E) = \tilde{\mathsf{V}}_\beta^\dagger(E)[\tilde{\Lambda}(E) + \mathrm{i}\eta\mathsf{I}]^{-1}, \tag{5.39}$$

respectively. Invoking the definition (5.32) and substituting the results (5.38) and (5.39) into Eq. (5.35) gives

$$\tilde{T}_{\beta\alpha}^{(\eta)}(E) = \tilde{\mathsf{V}}_\beta^\dagger(E)[\tilde{\Lambda}(E) + \mathrm{i}\eta\mathsf{I}]^{-1}\tilde{\mathsf{V}}_\alpha(E) \tag{5.40}$$

or equivalently

$$\tilde{T}_{\beta\alpha}^{(\eta)}(E) = \sum_{\gamma=1}^{v} \frac{1}{\tilde{\lambda}_\gamma(E) + \mathrm{i}\eta} \langle \Phi_\beta(E)|\hat{V}|\tilde{X}_\gamma(E)\rangle\langle\tilde{X}_\gamma(E)|\hat{V}|\Phi_\alpha(E)\rangle. \tag{5.41}$$

Eq. (5.41) provides a variational estimate of the matrix element (5.4). However, Eq. (5.41) may also be rewritten in the form

$$\tilde{T}_{\beta\alpha}^{(\eta)}(E) = \langle \Phi_\beta(E)|\hat{\tilde{T}}^{(\eta)}(E)|\Phi_\alpha(E)\rangle, \tag{5.42}$$

where $\hat{\tilde{T}}^{(\eta)}(E)$ is the operator defined in Eq. (5.29). Since $|\Phi_\alpha(E)\rangle$ and $\langle\Phi_\beta(E)|$ are arbitrary (cf. the remark preceding Eq. (5.4)), the operator (5.29) may be considered to be a variational approximation to $\hat{T}^{(\eta)}(E)$.

It is interesting that considerations analogous to those presented above but with the functional (5.7) replaced by the fractional functional (5.10) also yield the operator (5.29) as a variational approximation to $\hat{T}^{(\eta)}(E)$.

6. Application to Schrödinger particles

6.1. Eigenchannel wave functions and eigenchannel harmonics

Consider a Schrödinger particle in three spatial dimensions. The free-particle Green functions

$$G_0^{(\pm)}(E,\mathbf{r},\mathbf{r}') \equiv \langle \mathbf{r}|\hat{G}_0^{(\pm)}(E)|\mathbf{r}'\rangle \tag{6.1}$$

are those solutions to the inhomogeneous Schrödinger equation ($E > 0$, $\mathbf{r}'$ fixed)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - E\right] G_0^{(\pm)}(E,\mathbf{r},\mathbf{r}') = \delta^3(\mathbf{r}-\mathbf{r}'), \tag{6.2}$$

which asymptotically obey the Sommerfeld conditions

$$r\left(\frac{\partial}{\partial r} \mp \mathrm{i}k\right) G_0^{(\pm)}(E,\mathbf{r},\mathbf{r}') \overset{r\to\infty}{\longrightarrow} 0 \tag{6.3}$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{6.4}$$

The functions $G_0^{(\pm)}(E,\mathbf{r},\mathbf{r}')$ are explicitly given by

$$G_0^{(\pm)}(E,\mathbf{r},\mathbf{r}') = \frac{m}{2\pi\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}k|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \tag{6.5}$$

and may be rewritten as

$$G_0^{(\pm)}(E,\mathbf{r},\mathbf{r}') = G_0^{(0)}(E,\mathbf{r},\mathbf{r}') \pm \mathrm{i}D_0(E,\mathbf{r},\mathbf{r}'), \tag{6.6}$$

where

$$G_0^{(0)}(E,\mathbf{r},\mathbf{r}') \equiv \langle \mathbf{r}|\hat{G}_0^{(0)}(E)|\mathbf{r}'\rangle = \frac{m}{2\pi\hbar^2}\frac{\cos(k|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} \tag{6.7}$$

and

$$D_0(E,\mathbf{r},\mathbf{r}') \equiv \langle \mathbf{r}|\hat{D}_0(E)|\mathbf{r}'\rangle = \frac{m}{2\pi\hbar^2}\frac{\sin(k|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}. \tag{6.8}$$

Let $\hat{V}$ be a potential operator with a short range Hermitian kernel $V(\mathbf{r},\mathbf{r}')$. Following Eqs. (3.1) and (4.1), the spatial representations of the eigenchannels,

$$X_\gamma(E,\mathbf{r}) \equiv \langle \mathbf{r}|X_\gamma(E)\rangle, \tag{6.9}$$

hereafter called eigenchannel wave functions, are defined as eigenfunctions of the integral equation

$$X_\gamma(E,\mathbf{r}) = -\int_{\mathbb{R}^3} \mathrm{d}^3\mathbf{r}' \left[G_0^{(0)}(E,\mathbf{r},\mathbf{r}') + \cot\delta_\gamma(E) D_0(E,\mathbf{r},\mathbf{r}')\right] \hat{V} X_\gamma(E,\mathbf{r}'), \tag{6.10}$$

where $-\cot\delta_\gamma\,(E)$ is an eigenparameter. Equivalently, in terms of the Green functions $G_0^{(\pm)}(E,\mathbf{r},\mathbf{r}')$ the eigenequation (6.10) reads

$$X_\gamma(E,\mathbf{r}) = \frac{1}{2\mathrm{i}\sin\delta_\gamma(E)} \times \int_{\mathbb{R}^3} \mathrm{d}^3\mathbf{r}' \left[\mathrm{e}^{-\mathrm{i}\delta_\gamma(E)} G_0^{(-)}(E,\mathbf{r},\mathbf{r}') - \mathrm{e}^{\mathrm{i}\delta_\gamma(E)} G_0^{(+)}(E,\mathbf{r},\mathbf{r}')\right] \hat{V} X_\gamma(E,\mathbf{r}'). \tag{6.11}$$

Still another form of Eq. (6.10), resulting from employing Eqs. (6.7) and (6.8), is

$$X_\gamma(E,\boldsymbol{r}) = -\frac{m}{2\pi\hbar^2}\frac{1}{\sin\delta_\gamma(E)}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\,\frac{\sin[k|\boldsymbol{r}-\boldsymbol{r}'|+\delta_\gamma(E)]}{|\boldsymbol{r}-\boldsymbol{r}'|}\hat{V}X_\gamma(E,\boldsymbol{r}'). \tag{6.12}$$

From Eqs. (6.11) and (6.2) it follows that the eigenchannel wave functions are solutions to the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+\hat{V}-E\right]X_\gamma(E,\boldsymbol{r}) = 0. \tag{6.13}$$

In accordance with Eq. (3.12), hereafter we shall be assuming that the eigenchannel wave functions are orthonormal in the sense of

$$\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\,X_\gamma^*(E,\boldsymbol{r})\hat{V}D_0(E,\boldsymbol{r},\boldsymbol{r}')\hat{V}X_{\gamma'}(E,\boldsymbol{r}') = \delta_{\gamma\gamma'}. \tag{6.14}$$

If Eq. (6.14) holds, from Eq. (6.10) one has

$$\cot\delta_\gamma(E) = -\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\,X_\gamma^*(E,\boldsymbol{r})\hat{V}X_\gamma(E,\boldsymbol{r}) - \int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\,X_\gamma^*(E,\boldsymbol{r})\hat{V}G_0^{(0)}(E,\boldsymbol{r},\boldsymbol{r}')\hat{V}X_\gamma(E,\boldsymbol{r}'). \tag{6.15}$$

From Eq. (6.11) and from the asymptotic relations

$$G_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \overset{r\to\infty}{\longrightarrow} \frac{m}{2\pi\hbar^2}\Phi^*(E,\pm\boldsymbol{n},\boldsymbol{r}')\frac{\mathrm{e}^{\pm\mathrm{i}kr}}{r}, \tag{6.16}$$

where

$$\Phi(E,\boldsymbol{n},\boldsymbol{r}') \equiv \langle\boldsymbol{r}'|\Phi(E,\boldsymbol{n})\rangle = \mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot\boldsymbol{r}'}, \tag{6.17}$$

with $\boldsymbol{n} = \boldsymbol{r}/r$, one deduces that asymptotically

$$X_\gamma(E,\boldsymbol{r}) \overset{r\to\infty}{\longrightarrow} \sqrt{\frac{m}{2\hbar^2 k}}\frac{1}{\mathrm{i}\sin\delta_\gamma(E)}\left[\frac{\mathrm{e}^{-\mathrm{i}kr-\mathrm{i}\delta_\gamma(E)}}{r}Y_\gamma(E,-\boldsymbol{n}) - \frac{\mathrm{e}^{\mathrm{i}kr+\mathrm{i}\delta_\gamma(E)}}{r}Y_\gamma(E,\boldsymbol{n})\right]. \tag{6.18}$$

In Appendix C.1 we show that the angular functions

$$Y_\gamma(E,\boldsymbol{n}) = \sqrt{\frac{mk}{8\pi^2\hbar^2}}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\,\Phi^*(E,\boldsymbol{n},\boldsymbol{r}')\hat{V}X_\gamma(E,\boldsymbol{r}'), \tag{6.19}$$

hereafter termed the eigenchannel harmonics, form an orthonormal set on the unit sphere:

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}\,Y_\gamma^*(E,\boldsymbol{n})Y_{\gamma'}(E,\boldsymbol{n}) = \delta_{\gamma\gamma'}. \tag{6.20}$$

6.2. Eigenchannel expansions of wave functions and Green functions

The wave functions

$$\Psi^{(\pm)}(E,\boldsymbol{n}_0,\boldsymbol{r}) \equiv \langle\boldsymbol{r}|\Psi^{(\pm)}(E,\boldsymbol{n}_0)\rangle \tag{6.21}$$

are solutions to the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V} - E\right]\Psi^{(\pm)}(E,\boldsymbol{n}_0,\boldsymbol{r}) = 0 \tag{6.22}$$

with the asymptotic forms

$$\Psi^{(\pm)}(E,\boldsymbol{n}_0,\boldsymbol{r}) \overset{r\to\infty}{\longrightarrow} \lim_{r\to\infty} \Phi(E,\boldsymbol{n}_0,\boldsymbol{r}) + A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)\frac{\mathrm{e}^{\pm \mathrm{i}kr}}{r}, \tag{6.23}$$

where the far-field amplitudes $A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)$ are to be determined. The functions (6.21) obey also the Lippmann–Schwinger equations

$$\Psi^{(\pm)}(E,\boldsymbol{n}_0,\boldsymbol{r}) = \Phi(E,\boldsymbol{n}_0,\boldsymbol{r}) - \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, G_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}')\hat{V}\Psi^{(\pm)}(E,\boldsymbol{n}_0,\boldsymbol{r}'). \tag{6.24}$$

In view of Eqs. (4.10), (6.1), (6.9), (6.17), and (6.21), the representations of $\Psi^{(\pm)}(E,\boldsymbol{n}_0,\boldsymbol{r})$ in terms of the eigenchannel wave functions and eigenchannel harmonics are

$$\Psi^{(\pm)}(E,\boldsymbol{n}_0,\boldsymbol{r}) = \Phi(E,\boldsymbol{n}_0,\boldsymbol{r}) + \sqrt{\frac{8\pi^2\hbar^2}{mk}}\sum_\gamma \mathrm{e}^{\pm \mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)Y_\gamma^*(E,\boldsymbol{n}_0) \times \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, G_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}')\hat{V}X_\gamma(E,\boldsymbol{r}'). \tag{6.25}$$

The Green functions

$$G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \equiv \langle\boldsymbol{r}|\hat{G}^{(\pm)}(E)|\boldsymbol{r}'\rangle \tag{6.26}$$

are solutions to the inhomogeneous Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V} - E\right]G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') = \delta^3(\boldsymbol{r}-\boldsymbol{r}') \tag{6.27}$$

satisfying

$$r\left(\frac{\partial}{\partial r} \mp \mathrm{i}k\right)G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \overset{r\to\infty}{\longrightarrow} 0; \tag{6.28}$$

they obey also the integral equations

$$G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') = G_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') - \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}''\, G_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}'')\hat{V}G^{(\pm)}(E,\boldsymbol{r}'',\boldsymbol{r}). \tag{6.29}$$

In view of Eqs. (4.11), (6.1), (6.9), and (6.29), $G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}')$ may be represented as

$$G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') = G_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') + \sum_\gamma \mathrm{e}^{\pm \mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E) \times \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}''\, G_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}'')\hat{V}X_\gamma(E,\boldsymbol{r}'') \times \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'''\, X_\gamma^*(E,\boldsymbol{r}''')\hat{V}G_0^{(\pm)}(E,\boldsymbol{r}''',\boldsymbol{r}'). \tag{6.30}$$

From Eq. (6.30) and from the property (cf. Eq. (6.5))

$$G_0^{(\pm)*}(E,\boldsymbol{r},\boldsymbol{r}') = G_0^{(\mp)}(E,\boldsymbol{r}',\boldsymbol{r}) \tag{6.31}$$

it follows immediately that also

$$G^{(\pm)*}(E,\boldsymbol{r},\boldsymbol{r}') = G^{(\mp)}(E,\boldsymbol{r}',\boldsymbol{r}). \tag{6.32}$$

Moreover, from Eqs. (6.30), (6.16), (6.19), (6.25), and from the relation

$$\Phi^{*}(E,\pm\boldsymbol{n},\boldsymbol{r}') = \Phi(E,\mp\boldsymbol{n},\boldsymbol{r}') \tag{6.33}$$

one infers that

$$G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \overset{r\to\infty}{\longrightarrow} \frac{m}{2\pi\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}kr}}{r}\Psi^{(\mp)*}(E,\pm\boldsymbol{n},\boldsymbol{r}') \tag{6.34}$$

and

$$G^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \overset{r'\to\infty}{\longrightarrow} \frac{m}{2\pi\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}kr'}}{r'}\Psi^{(\pm)}(E,\mp\boldsymbol{n}',\boldsymbol{r}). \tag{6.35}$$

6.3. Far-field amplitudes

On passing in Eq. (6.25) to the limit $r \to \infty$, employing Eqs. (6.16) and (6.19), and making comparison of the result with Eq. (6.23), we arrive at the following representations of the far-field amplitudes in terms of the eigenchannel harmonics and the eigenphases:

$$A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0) = \frac{4\pi}{k}\sum_{\gamma}\mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)Y_\gamma(E,\pm\boldsymbol{n})Y_\gamma^{*}(E,\boldsymbol{n}_0). \tag{6.36}$$

It is worth observing that, in virtue of the orthonormality relation (6.20), one has

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}_0\,A^{(\pm)}(E,\pm\boldsymbol{n},\boldsymbol{n}_0)Y_\gamma(E,\boldsymbol{n}_0) = \frac{4\pi}{k}\mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)Y_\gamma(E,\boldsymbol{n}), \tag{6.37}$$

i.e., if the amplitudes $A^{(\pm)}(E,\pm\boldsymbol{n},\boldsymbol{n}_0)$ are considered as integral kernels, the eigenchannel harmonics $\{Y_\gamma(E,\boldsymbol{n})\}$ are their orthonormal eigenfunctions associated with the eigenvalues $\{(4\pi/k)\exp[\pm\mathrm{i}\delta_\gamma(E)]\sin\delta_\gamma(E)\}$. Consequently, after replacing $\boldsymbol{n}$ with $\pm\boldsymbol{n}$, Eq. (6.36) provides the spectral expansions of $A^{(\pm)}(E,\pm\boldsymbol{n},\boldsymbol{n}_0)$.

The expansions (6.36) may be used to deduce, in an elementary way, various properties of $A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)$. Examples are: the reciprocity relationships

$$A^{(\pm)*}(E,\boldsymbol{n},\boldsymbol{n}_0) = A^{(\mp)}(E,\mp\boldsymbol{n}_0,\pm\boldsymbol{n}), \tag{6.38}$$

and the optical relations

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}'\,A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}')A^{(\pm)*}(E,\boldsymbol{n}_0,\boldsymbol{n}') = \pm\frac{2\pi}{\mathrm{i}k}\left[A^{(\pm)}(E,\boldsymbol{n},\pm\boldsymbol{n}_0) - A^{(\pm)*}(E,\boldsymbol{n}_0,\pm\boldsymbol{n})\right], \tag{6.39}$$

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}'\,A^{(\pm)*}(E,\boldsymbol{n}',\boldsymbol{n})A^{(\pm)}(E,\boldsymbol{n}',\boldsymbol{n}_0) = \pm\frac{2\pi}{\mathrm{i}k}\left[A^{(\pm)}(E,\pm\boldsymbol{n},\boldsymbol{n}_0) - A^{(\pm)*}(E,\pm\boldsymbol{n}_0,\boldsymbol{n})\right], \tag{6.40}$$

which in the particular case $\boldsymbol{n} = \boldsymbol{n}_0$ reduce to

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}' \, |A^{(\pm)}(E, \boldsymbol{n}_0, \boldsymbol{n}')|^2 = \pm\frac{4\pi}{k} \mathrm{Im}A^{(\pm)}(E, \boldsymbol{n}_0, \pm\boldsymbol{n}_0) \tag{6.41}$$

and

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}' \, |A^{(\pm)}(E, \boldsymbol{n}', \boldsymbol{n}_0)|^2 = \pm\frac{4\pi}{k} \mathrm{Im}A^{(\pm)}(E, \pm\boldsymbol{n}_0, \boldsymbol{n}_0), \tag{6.42}$$

respectively. We leave derivations of Eqs. (6.38)–(6.40) from Eqs. (6.36) and (6.20) to the reader.

Concluding this section, we note that Eqs. (4.12), (6.19), and (6.36) imply that

$$A^{(\pm)}(E, \boldsymbol{n}, \boldsymbol{n}_0) = -\frac{m}{2\pi\hbar^2} \langle \Phi(E, \pm\boldsymbol{n}) | \hat{T}^{(\pm)}(E) | \Phi(E, \boldsymbol{n}_0) \rangle. \tag{6.43}$$

6.4. Scattering kernel

Let $\Psi(E, \boldsymbol{r})$ be an arbitrary regular solution to the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + \hat{V} - E \right] \Psi(E, \boldsymbol{r}) = 0. \tag{6.44}$$

Asymptotically, $\Psi(E, \boldsymbol{r})$ is of the form

$$\Psi(E, \boldsymbol{r}) \overset{r\to\infty}{\longrightarrow} F_-(E, \boldsymbol{n}) \frac{\mathrm{e}^{-\mathrm{i}kr}}{r} - F_+(E, \boldsymbol{n}) \frac{\mathrm{e}^{\mathrm{i}kr}}{r}. \tag{6.45}$$

The scattering kernel $S(E, \boldsymbol{n}, \boldsymbol{n}')$ is defined so that

$$F_+(E, \boldsymbol{n}) = \oint_{4\pi} \mathrm{d}^2\boldsymbol{n}' \, S(E, \boldsymbol{n}, -\boldsymbol{n}') F_-(E, \boldsymbol{n}'). \tag{6.46}$$

Let us make the following particular choice:

$$\Psi(E, \boldsymbol{r}) = \Psi^{(+)}(E, \boldsymbol{n}', \boldsymbol{r}). \tag{6.47}$$

Employing Eq. (6.23) and making use of the fact that

$$\Phi(E, \boldsymbol{n}', \boldsymbol{r}) \overset{r\to\infty}{\longrightarrow} \frac{2\pi\mathrm{i}}{k} \delta^2(\boldsymbol{n} + \boldsymbol{n}') \frac{\mathrm{e}^{-\mathrm{i}kr}}{r} - \frac{2\pi\mathrm{i}}{k} \delta^2(\boldsymbol{n} - \boldsymbol{n}') \frac{\mathrm{e}^{\mathrm{i}kr}}{r}, \tag{6.48}$$

we have

$$\Psi^{(+)}(E, \boldsymbol{n}', \boldsymbol{r}) \overset{r\to\infty}{\longrightarrow} \frac{2\pi\mathrm{i}}{k} \delta^2(\boldsymbol{n} + \boldsymbol{n}') \frac{\mathrm{e}^{-\mathrm{i}kr}}{r} - \frac{2\pi\mathrm{i}}{k} \left[\delta^2(\boldsymbol{n} - \boldsymbol{n}') + \frac{\mathrm{i}k}{2\pi} A^{(+)}(E, \boldsymbol{n}, \boldsymbol{n}') \right] \frac{\mathrm{e}^{\mathrm{i}kr}}{r}, \tag{6.49}$$

hence, on combining Eqs. (6.45)–(6.47) and (6.49), we obtain

$$S(E, \boldsymbol{n}, \boldsymbol{n}') = \delta^2(\boldsymbol{n} - \boldsymbol{n}') + \frac{\mathrm{i}k}{2\pi} A^{(+)}(E, \boldsymbol{n}, \boldsymbol{n}'). \tag{6.50}$$

Then, utilizing the expansion (6.36), we find the following representation of $S(E, \boldsymbol{n}, \boldsymbol{n}')$ in terms of the eigenchannel harmonics:

$$S(E, \boldsymbol{n}, \boldsymbol{n}') = \delta^2(\boldsymbol{n} - \boldsymbol{n}') + \sum_{\gamma} [\mathrm{e}^{2\mathrm{i}\delta_\gamma(E)} - 1] Y_\gamma(E, \boldsymbol{n}) Y_\gamma^*(E, \boldsymbol{n}'). \tag{6.51}$$

With the aid of this representation, one easily proves that

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}' \, S(E, \boldsymbol{n}, \boldsymbol{n}') Y_\gamma(E, \boldsymbol{n}') = \mathrm{e}^{2\mathrm{i}\delta_\gamma(E)} Y_\gamma(E, \boldsymbol{n}), \tag{6.52}$$

i.e., that the eigenchannel harmonics $\{Y_\gamma(E, \boldsymbol{n})\}$ are eigenfunctions of the scattering kernel associated with the eigenvalues $\{\exp[2\mathrm{i}\delta_\gamma(E)]\}$, and that

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}'' \, S(E, \boldsymbol{n}, \boldsymbol{n}'') S^*(E, \boldsymbol{n}', \boldsymbol{n}'') = \delta^2(\boldsymbol{n} - \boldsymbol{n}'), \tag{6.53}$$

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}'' \, S^*(E, \boldsymbol{n}'', \boldsymbol{n}) S(E, \boldsymbol{n}'', \boldsymbol{n}') = \delta^2(\boldsymbol{n} - \boldsymbol{n}'), \tag{6.54}$$

which means that the scattering kernel is unitary. Finally, we observe that if the potential $\hat{V}$ is such that the eigenchannel harmonics form a complete set on the unit sphere (which is *not* the case for finite-rank separable potentials!):

$$\sum_{\gamma} Y_\gamma(E, \boldsymbol{n}) Y_\gamma^*(E, \boldsymbol{n}') = \delta^2(\boldsymbol{n} - \boldsymbol{n}'), \tag{6.55}$$

Eq. (6.51) becomes

$$S(E, \boldsymbol{n}, \boldsymbol{n}') = \sum_{\gamma} \mathrm{e}^{2\mathrm{i}\delta_\gamma(E)} Y_\gamma(E, \boldsymbol{n}) Y_\gamma^*(E, \boldsymbol{n}'). \tag{6.56}$$

6.5. Scattering cross-sections

The function $\Psi^{(+)}(E, \boldsymbol{n}_0, \boldsymbol{r})$ is the physical scattering function induced by the monochromatic plane wave $\Phi(E, \boldsymbol{n}_0, \boldsymbol{r})$ and $A^{(+)}(E, \boldsymbol{n}, \boldsymbol{n}_0)$ is the corresponding scattering amplitude. Accordingly, the differential cross-section for scattering from the direction $\boldsymbol{n}_0$ into the direction $\boldsymbol{n}$ is

$$\frac{\mathrm{d}^2 Q(E, \boldsymbol{n}, \boldsymbol{n}_0)}{\mathrm{d}^2\boldsymbol{n}} = |A^{(+)}(E, \boldsymbol{n}, \boldsymbol{n}_0)|^2. \tag{6.57}$$

It follows from Eqs. (6.57), (6.36), and (6.20) that the total cross-section

$$Q(E, \boldsymbol{n}_0) = \oint_{4\pi} \mathrm{d}^2\boldsymbol{n} \, \frac{\mathrm{d}^2 Q(E, \boldsymbol{n}, \boldsymbol{n}_0)}{\mathrm{d}^2\boldsymbol{n}} \tag{6.58}$$

may be expressed in terms of the eigenchannel harmonics and the eigenphases in the following way:

$$Q(E, \boldsymbol{n}_0) = \frac{16\pi^2}{k^2} \sum_{\gamma} \sin^2 \delta_\gamma(E) |Y_\gamma(E, \boldsymbol{n}_0)|^2. \tag{6.59}$$

Averaging $Q(E, \boldsymbol{n}_0)$ over all directions of incidence $\boldsymbol{n}_0$ yields the average total cross-section

$$Q(E) = \frac{1}{4\pi} \oint_{4\pi} d^2\boldsymbol{n}_0 \, Q(E, \boldsymbol{n}_0), \tag{6.60}$$

for which, from Eqs. (6.59) and (6.20), one finds

$$Q(E) = \frac{4\pi}{k^2} \sum_{\gamma} \sin^2 \delta_\gamma(E). \tag{6.61}$$

6.6. Potential with a real symmetric kernel

Thus far, we have been assuming only that the potential $\hat{V}$ is of the short range nature and that its kernel $V(\boldsymbol{r}, \boldsymbol{r}')$ is Hermitian. Below we shall investigate briefly consequences of making an additional assumption that $V(\boldsymbol{r}, \boldsymbol{r}')$ is also real (hence, in virtue of the Hermiticity, symmetric).

It is seen from Eq. (6.10) that in the case considered here the complex conjugate of any eigenchannel wave function is also an eigenchannel wave function, both being associated with the same real eigenvalue. This implies that the eigenchannel wave functions may be chosen to be real:

$$X_\gamma^*(E, \boldsymbol{r}) = X_\gamma(E, \boldsymbol{r}), \tag{6.62}$$

and throughout the rest of this subsection we shall be assuming that Eq. (6.62) holds. With this assumption, from Eqs. (6.19) and (6.33) one finds that the eigenchannel harmonics obey

$$Y_\gamma^*(E, \boldsymbol{n}) = Y_\gamma(E, -\boldsymbol{n}). \tag{6.63}$$

Then

$$Y_\gamma(E, \pm\boldsymbol{n}) = |Y_\gamma(E, \boldsymbol{n})| e^{\pm i\varphi_\gamma(E)}, \tag{6.64}$$

where $\varphi_\gamma(E)$ is a real phase, and it follows from Eqs. (6.18) and (6.64) that asymptotically the eigenchannels are of the form

$$X_\gamma(E, \boldsymbol{r}) \overset{r\to\infty}{\longrightarrow} -\sqrt{\frac{2m}{\hbar^2 k}} \frac{\sin[kr + \varphi_\gamma(E) + \delta_\gamma(E)]}{\sin \delta_\gamma(E)} |Y_\gamma(E, \boldsymbol{n})|. \tag{6.65}$$

In the case considered here, in addition to the reciprocity relations (6.38), the far-field amplitudes obey also the reciprocity relations

$$A^{(\pm)}(E, \mp\boldsymbol{n}_0, \mp\boldsymbol{n}) = A^{(\pm)}(E, \boldsymbol{n}, \boldsymbol{n}_0). \tag{6.66}$$

Indeed, from the expansion (6.36) one has

$$A^{(\pm)}(E, \mp\boldsymbol{n}_0, \mp\boldsymbol{n}) = \frac{4\pi}{k} \sum_{\gamma} e^{\pm i\delta_\gamma(E)} \sin \delta_\gamma(E) Y_\gamma^*(E, \mp\boldsymbol{n}) Y_\gamma(E, -\boldsymbol{n}_0). \tag{6.67}$$

After employing the property (6.63), one sees that the right-hand side of Eq. (6.67) is identical with the right-hand side of Eq. (6.36), hence the relations (6.66) follow.

With the aid of Eqs. (6.31), (6.33), (6.62), (6.63), and the symmetry relations

$$G_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') = G_0^{(\pm)}(E, \boldsymbol{r}', \boldsymbol{r}), \tag{6.68}$$

following directly from Eq. (6.5), from Eq. (6.25) one easily deduces that in the case considered here it holds

$$\Psi^{(\pm)*}(E, \boldsymbol{n}_0, \boldsymbol{r}) = \Psi^{(\mp)}(E, -\boldsymbol{n}_0, \boldsymbol{r}). \tag{6.69}$$

Similarly, application of (6.31), (6.62), (6.63), and (6.68) to Eq. (6.30) yields

$$G^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') = G^{(\pm)}(E, \boldsymbol{r}', \boldsymbol{r}). \tag{6.70}$$

Combining Eq. (6.70) with the asymptotic relations (6.34) and (6.35) is another way of obtaining Eq. (6.69).

7. Application to Dirac particles

7.1. Eigenchannel bispinor wave functions and eigenchannel bispinor harmonics

For a free Dirac particle in three spatial dimensions the matrix Green functions

$$\mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') \equiv \langle \boldsymbol{r} | \hat{G}_0^{(\pm)}(E) | \boldsymbol{r}' \rangle \tag{7.1}$$

are these 4×4 matrix solutions to the inhomogeneous Dirac equation ($|E| > mc^2$, $\boldsymbol{r}'$ fixed)

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + mc^2\beta - E\mathscr{I}]\mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') = \delta^3(\boldsymbol{r} - \boldsymbol{r}')\mathscr{I} \tag{7.2}$$

which asymptotically obey the following counterparts of the Sommerfeld conditions (6.3):

$$r\left[\boldsymbol{n} \cdot \boldsymbol{\alpha}_+ \mp \frac{c\hbar k}{E + mc^2}\beta_+\right]\mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') \overset{r\to\infty}{\longrightarrow} 0 \tag{7.3}$$

or *equivalently*

$$r\left[\boldsymbol{n} \cdot \boldsymbol{\alpha}_- \mp \frac{c\hbar k}{E - mc^2}\beta_-\right]\mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') \overset{r\to\infty}{\longrightarrow} 0. \tag{7.4}$$

In Eq. (7.2) $\boldsymbol{\alpha}$ and β are the standard 4×4 Dirac matrices, $\mathscr{I}$ is the 4×4 unit matrix, the 4×4 matrices $\boldsymbol{\alpha}_\pm$ and $\beta_\pm$ appearing in Eqs. (7.3) and (7.4) are defined as

$$\beta_\pm = \frac{1}{2}(\mathscr{I} \pm \beta), \qquad \boldsymbol{\alpha}_\pm = \beta_\pm \boldsymbol{\alpha}, \tag{7.5}$$

while the Dirac wave number is

$$k = \mathrm{sgn}(E)\frac{\sqrt{E^2 - (mc^2)^2}}{c\hbar}. \tag{7.6}$$

Explicitly one has

$$\mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') = \frac{-\mathrm{i}c\hbar\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + mc^2\beta + E\mathscr{I}}{4\pi c^2\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r} - \boldsymbol{r}'|}. \tag{7.7}$$

The functions (7.7) may be represented as

$$\mathscr{G}_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') = \mathscr{G}_0^{(0)}(E,\boldsymbol{r},\boldsymbol{r}') \pm \mathrm{i}\mathscr{D}_0(E,\boldsymbol{r},\boldsymbol{r}') \tag{7.8}$$

with

$$\mathscr{G}_0^{(0)}(E,\boldsymbol{r},\boldsymbol{r}') \equiv \langle\boldsymbol{r}|\hat{G}_0^{(0)}(E)|\boldsymbol{r}'\rangle = \frac{-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta + E\mathscr{I}}{4\pi c^2\hbar^2}\,\frac{\cos(k|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|} \tag{7.9}$$

and

$$\mathscr{D}_0(E,\boldsymbol{r},\boldsymbol{r}') \equiv \langle\boldsymbol{r}|\hat{D}_0(E)|\boldsymbol{r}'\rangle = \frac{-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta + E\mathscr{I}}{4\pi c^2\hbar^2}\,\frac{\sin(k|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{7.10}$$

For a given Hermitian short range potential operator $\hat{V}$, the eigenchannel bispinor wave functions

$$X_\gamma(E,\boldsymbol{r}) \equiv \langle\boldsymbol{r}|X_\gamma(E)\rangle \tag{7.11}$$

are solutions to the integral eigenproblem

$$X_\gamma(E,\boldsymbol{r}) = -\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\left[\mathscr{G}_0^{(0)}(E,\boldsymbol{r},\boldsymbol{r}') + \cot\delta_\gamma(E)\mathscr{D}_0(E,\boldsymbol{r},\boldsymbol{r}')\right]\hat{V}X_\gamma(E,\boldsymbol{r}') \tag{7.12}$$

with $-\cot\delta_\gamma(E)$ being the eigenvalue. In virtue of Eqs. (7.7)–(7.10), Eq. (7.12) may be equivalently rewritten as

$$X_\gamma(E,\boldsymbol{r}) = \frac{1}{2\mathrm{i}\sin\delta_\gamma(E)} \times \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\left[\mathrm{e}^{-\mathrm{i}\delta_\gamma(E)}\mathscr{G}_0^{(-)}(E,\boldsymbol{r},\boldsymbol{r}') - \mathrm{e}^{\mathrm{i}\delta_\gamma(E)}\mathscr{G}_0^{(+)}(E,\boldsymbol{r},\boldsymbol{r}')\right] \times \hat{V}X_\gamma(E,\boldsymbol{r}') \tag{7.13}$$

or

$$X_\gamma(E,\boldsymbol{r}) = -\frac{1}{\sin\delta_\gamma(E)}\,\frac{-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta + E\mathscr{I}}{4\pi c^2\hbar^2} \times \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\,\frac{\sin[k|\boldsymbol{r}-\boldsymbol{r}'| + \delta_\gamma(E)]}{|\boldsymbol{r}-\boldsymbol{r}'|}\hat{V}X_\gamma(E,\boldsymbol{r}'). \tag{7.14}$$

It follows from Eqs. (7.13) and (7.2) that the eigenchannel wave functions obey the Dirac equation

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta + \hat{V} - E\mathscr{I}]X_\gamma(E,\boldsymbol{r}) = 0. \tag{7.15}$$

Hereafter, we shall be assuming that the eigenchannel wave functions have been orthonormalized in the sense

$$\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\,X_\gamma^\dagger(E,\boldsymbol{r})\hat{V}\mathscr{D}_0(E,\boldsymbol{r},\boldsymbol{r}')\hat{V}X_{\gamma'}(E,\boldsymbol{r}') = \delta_{\gamma\gamma'} \tag{7.16}$$

(cf. Eq. (3.10)), where the dagger denotes the matrix Hermitian conjugation. Then Eq. (7.12) yields

$$\cot\delta_\gamma(E) = -\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\,X_\gamma^\dagger(E,\boldsymbol{r})\hat{V}X_\gamma(E,\boldsymbol{r}) - \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\,X_\gamma^\dagger(E,\boldsymbol{r})\hat{V}\mathscr{G}_0^{(0)}(E,\boldsymbol{r},\boldsymbol{r}')\hat{V}X_\gamma(E,\boldsymbol{r}'). \tag{7.17}$$

To investigate behaviors of the eigenchannel wave functions for $r \to \infty$, one needs the asymptotic representations of the Green functions (7.7). The representations

$$\mathscr{G}_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \stackrel{r\to\infty}{\longrightarrow} \frac{E}{2\pi c^2\hbar^2}\mathscr{P}(E,\pm\boldsymbol{n})\mathrm{e}^{\mp\mathrm{i}k\boldsymbol{n}\cdot\boldsymbol{r}'}\frac{\mathrm{e}^{\pm\mathrm{i}kr}}{r}, \tag{7.18}$$

where

$$\mathscr{P}(E,\boldsymbol{n}) = \frac{c\hbar k\boldsymbol{n}\cdot\boldsymbol{\alpha} + mc^2\beta + E\mathscr{I}}{2E}, \tag{7.19}$$

following directly from Eq. (7.7), must be transformed before they become convenient for our purposes. To this end, we introduce two bispinors

$$\mathcal{U}_i(E,\boldsymbol{n}) = (1+\varepsilon^2)^{-1/2}\begin{pmatrix} u_i \\ \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}u_i \end{pmatrix} \qquad (i=1,2), \tag{7.20}$$

where $\boldsymbol{n} = \boldsymbol{r}/r$,

$$\varepsilon = \sqrt{\frac{E-mc^2}{E+mc^2}}, \tag{7.21}$$

while the two-component $\boldsymbol{n}$-independent spinors $\{u_i\}$ obey

$$u_i^\dagger u_{i'} = \delta_{ii'} \qquad (i,i'=1,2), \tag{7.22}$$

$$\sum_{i=1}^{2} u_i u_i^\dagger = I, \tag{7.23}$$

where I is the 2×2 unit matrix. It is easy to verify that the bispinors (7.20) are solutions to the homogeneous algebraic system

$$[c\hbar k\boldsymbol{n}\cdot\boldsymbol{\alpha} + mc^2\beta - E\mathscr{I}]\mathcal{U}_i(E,\boldsymbol{n}) = 0 \tag{7.24}$$

and possess the properties

$$\mathcal{U}_i^\dagger(E,\boldsymbol{n})\mathcal{U}_{i'}(E,\boldsymbol{n}) = \delta_{ii'} \qquad (i,i'=1,2), \tag{7.25}$$

$$\sum_{i=1}^{2}\mathcal{U}_i(E,\boldsymbol{n})\mathcal{U}_i^\dagger(E,\boldsymbol{n}) = \mathscr{P}(E,\boldsymbol{n}). \tag{7.26}$$

The property (7.26) allows us to rewrite Eq. (7.18) in the sought convenient form

$$\mathscr{G}_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \stackrel{r\to\infty}{\longrightarrow} \frac{E}{2\pi c^2\hbar^2}\sum_{i=1}^{2}\mathcal{U}_i(E,\pm\boldsymbol{n})\Phi_i^\dagger(E,\pm\boldsymbol{n},\boldsymbol{r}')\frac{\mathrm{e}^{\pm\mathrm{i}kr}}{r}, \tag{7.27}$$

with

$$\Phi_i(E,\boldsymbol{n},\boldsymbol{r}') = \mathcal{U}_i(E,\boldsymbol{n})\mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot\boldsymbol{r}'}. \tag{7.28}$$

Then, with the aid of Eq. (7.27), from Eq. (7.13) we deduce that for $r\to\infty$ it holds

$$X_\gamma(E,\boldsymbol{r}) \stackrel{r\to\infty}{\longrightarrow} \mathrm{sgn}(E)\sqrt{\frac{E}{2c^2\hbar^2k}}\frac{1}{\mathrm{i}\sin\delta_\gamma(E)}\left[\frac{\mathrm{e}^{-\mathrm{i}kr-\mathrm{i}\delta_\gamma(E)}}{r}\mathcal{Y}_\gamma(E,-\boldsymbol{n}) - \frac{\mathrm{e}^{\mathrm{i}kr+\mathrm{i}\delta_\gamma(E)}}{r}\mathcal{Y}_\gamma(E,\boldsymbol{n})\right] \tag{7.29}$$

with the eigenchannel *bispinor* harmonics defined as

$$\mathcal{Y}_{\gamma}(E,\boldsymbol{n}) = \sqrt{\frac{Ek}{8\pi^2c^2\hbar^2}}\sum_{i=1}^{2}\mathcal{U}_i(E,\boldsymbol{n})\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\,\Phi_i^{\dagger}(E,\boldsymbol{n},\boldsymbol{r}')\hat{V}X_{\gamma}(E,\boldsymbol{r}'). \tag{7.30}$$

For the sake of later applications, we observe here that the bispinor harmonics (7.30) have the structure

$$\mathcal{Y}_{\gamma}(E,\boldsymbol{n}) = (1+\varepsilon^2)^{-1/2}\begin{pmatrix}\Upsilon_{\gamma}(E,\boldsymbol{n})\\ \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}\Upsilon_{\gamma}(E,\boldsymbol{n})\end{pmatrix}, \tag{7.31}$$

where the eigenchannel *spinor* harmonics $\Upsilon_{\gamma}(E,\boldsymbol{n})$ are

$$\Upsilon_{\gamma}(E,\boldsymbol{n}) = \sqrt{\frac{Ek}{8\pi^2c^2\hbar^2}}\sum_{i=1}^{2}u_i\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}'\,\Phi_i^{\dagger}(E,\boldsymbol{n},\boldsymbol{r}')\hat{V}X_{\gamma}(E,\boldsymbol{r}'). \tag{7.32}$$

In Appendix C.2 we prove the orthonormality relation

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}\,\mathcal{Y}_{\gamma}^{\dagger}(E,\boldsymbol{n})\mathcal{Y}_{\gamma'}(E,\boldsymbol{n}) = \delta_{\gamma\gamma'}, \tag{7.33}$$

which, in virtue of Eq. (7.31), is equivalent to the relation

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}\,\Upsilon_{\gamma}^{\dagger}(E,\boldsymbol{n})\Upsilon_{\gamma'}(E,\boldsymbol{n}) = \delta_{\gamma\gamma'}. \tag{7.34}$$

7.2. Eigenchannel expansions of bispinor wave functions and matrix Green functions

Consider the wave functions

$$\Psi^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n}_0,\boldsymbol{r}) \equiv \langle\boldsymbol{r}|\Psi^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n}_0)\rangle \tag{7.35}$$

defined as these solutions to the Dirac equation

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta + \hat{V} - E\mathcal{I}]\Psi^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n}_0,\boldsymbol{r}) = 0 \tag{7.36}$$

for which asymptotically it holds

$$\Psi^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n}_0,\boldsymbol{r}) \overset{r\to\infty}{\to} \lim_{r\to\infty}\Phi(E,\boldsymbol{v}_0,\boldsymbol{n}_0,\boldsymbol{r}) + \mathcal{A}^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)\frac{\mathrm{e}^{\pm\mathrm{i}kr}}{r}. \tag{7.37}$$

In Eq. (7.37)

$$\Phi(E,\boldsymbol{v}_0,\boldsymbol{n}_0,\boldsymbol{r}) \equiv \langle\boldsymbol{r}|\Phi(E,\boldsymbol{v}_0,\boldsymbol{n}_0)\rangle = \mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}_0)\mathrm{e}^{\mathrm{i}k\boldsymbol{n}_0\cdot\boldsymbol{r}} \tag{7.38}$$

is a monochromatic Dirac plane wave, while $\mathcal{A}^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)$ are bispinor far-field amplitudes. The bispinor plane-wave amplitude appearing in Eq. (7.38) is of the form

$$\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}_0) = (1+\varepsilon^2)^{-1/2}\begin{pmatrix}u(\boldsymbol{v}_0)\\ \varepsilon\boldsymbol{n}_0\cdot\boldsymbol{\sigma}u(\boldsymbol{v}_0)\end{pmatrix}, \tag{7.39}$$

where $\boldsymbol{\sigma}$ is the vector composed of the Pauli matrices, while the two-component spinor $u(\boldsymbol{v}_0)$, describing particle's spin pointing in the direction $\boldsymbol{v}_0$, is normalized according to

$$u^{\dagger}(\boldsymbol{v}_0)u(\boldsymbol{v}_0) = 1 \tag{7.40}$$

and obeys

$$\boldsymbol{v}_0 \cdot \boldsymbol{\sigma} u(\boldsymbol{v}_0) = u(\boldsymbol{v}_0). \tag{7.41}$$

Alternatively, the functions (7.35) are defined as solutions to the Lippmann–Schwinger equation

$$\Psi^{(\pm)}(E, \boldsymbol{v}_0, \boldsymbol{n}_0, \boldsymbol{r}) = \Phi(E, \boldsymbol{v}_0, \boldsymbol{n}_0, \boldsymbol{r}) - \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, \mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}')\hat{V}\Psi^{(\pm)}(E, \boldsymbol{v}_0, \boldsymbol{n}_0, \boldsymbol{r}'). \tag{7.42}$$

It follows from Eqs. (7.42), (2.25), (7.11), (7.30), and (4.10) that the eigenchannel representations of the functions (7.35) are

$$\begin{aligned}\Psi^{(\pm)}(E, \boldsymbol{v}_0, \boldsymbol{n}_0, \boldsymbol{r}) = \Phi(E, \boldsymbol{v}_0, \boldsymbol{n}_0, \boldsymbol{r}) &+ \sqrt{\frac{8\pi^2 c^2 \hbar^2}{Ek}} \sum_{\gamma} \mathrm{e}^{\pm \mathrm{i}\delta_{\gamma}(E)} \\ &\times \sin\delta_{\gamma}(E) \mathcal{Y}_{\gamma}^{\dagger}(E, \boldsymbol{n}_0)\mathcal{U}(E, \boldsymbol{v}_0, \boldsymbol{n}_0) \\ &\times \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'\, \mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}')\hat{V}X_{\gamma}(E, \boldsymbol{r}').\end{aligned} \tag{7.43}$$

It is also of interest to find eigenchannel representations of the Green functions

$$\mathscr{G}^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') \equiv \langle \boldsymbol{r}|\hat{G}^{(\pm)}(E)|\boldsymbol{r}'\rangle, \tag{7.44}$$

defined as these solutions to the Dirac equation ($\boldsymbol{r}'$ fixed)

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta + \hat{V} - E\mathscr{I}]\mathscr{G}^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') = \delta^3(\boldsymbol{r} - \boldsymbol{r}')\mathscr{I} \tag{7.45}$$

for which

$$r\left[\boldsymbol{n}\cdot\boldsymbol{\alpha}_{+} \mp \frac{c\hbar k}{E + mc^2}\beta_{+}\right]\mathscr{G}^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') \stackrel{r\to\infty}{\longrightarrow} 0 \tag{7.46}$$

or equivalently

$$r\left[\boldsymbol{n}\cdot\boldsymbol{\alpha}_{-} \mp \frac{c\hbar k}{E - mc^2}\beta_{-}\right]\mathscr{G}^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') \stackrel{r\to\infty}{\longrightarrow} 0 \tag{7.47}$$

(cf. Eqs. (7.2)–(7.4)). Alternatively, $\mathscr{G}^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}')$ may be defined as solutions to

$$\mathscr{G}^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') = \mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}') - \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}''\, \mathscr{G}_0^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}'')\hat{V}\mathscr{G}^{(\pm)}(E, \boldsymbol{r}'', \boldsymbol{r}). \tag{7.48}$$

In view of Eqs. (7.48), (2.34), (7.44), (7.11), and (4.11), the sought eigenchannel representations of $\mathscr{G}^{(\pm)}(E, \boldsymbol{r}, \boldsymbol{r}')$ are

$$\begin{aligned}\mathscr{G}^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') = \mathscr{G}_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') &+ \sum_{\gamma} \mathrm{e}^{\pm \mathrm{i}\delta_{\gamma}(E)} \sin\delta_{\gamma}(E) \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}''\, \mathscr{G}_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}'')\hat{V}X_{\gamma}(E,\boldsymbol{r}'') \\ &\times \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'''\, X_{\gamma}^{\dagger}(E,\boldsymbol{r}''')\hat{V}\mathscr{G}_0^{(\pm)}(E,\boldsymbol{r}''',\boldsymbol{r}').\end{aligned} \tag{7.49}$$

From Eq. (7.49) and from the relations

$$\mathscr{G}_0^{(\pm)\dagger}(E,\boldsymbol{r},\boldsymbol{r}') = \mathscr{G}_0^{(\mp)}(E,\boldsymbol{r}',\boldsymbol{r}) \tag{7.50}$$

easily deducible from Eq. (7.7), one finds that $\mathscr{G}^{(\pm)\dagger}(E,\boldsymbol{r},\boldsymbol{r}')$ obey the analogous relations:

$$\mathscr{G}^{(\pm)\dagger}(E,\boldsymbol{r},\boldsymbol{r}') = \mathscr{G}^{(\mp)}(E,\boldsymbol{r}',\boldsymbol{r}). \tag{7.51}$$

Moreover, shifting in Eq. (7.49) either the source ($\boldsymbol{r}'$) or the observation ($\boldsymbol{r}$) point to the infinity and making use of Eqs. (7.27) and (7.30) yields

$$\mathscr{G}^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \overset{r\to\infty}{\longrightarrow} \frac{E}{2\pi c^2\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}kr}}{r}\sum_{i=1}^{2}\mathcal{U}_i(E,\pm\boldsymbol{n})\Psi_i^{(\mp)\dagger}(E,\pm\boldsymbol{n},\boldsymbol{r}') \tag{7.52}$$

and

$$\mathscr{G}^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}') \overset{r'\to\infty}{\longrightarrow} \frac{E}{2\pi c^2\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}kr'}}{r'}\sum_{i=1}^{2}\Psi_i^{(\pm)}(E,\pm\boldsymbol{n}',\boldsymbol{r})\mathcal{U}_i^{\dagger}(E,\mp\boldsymbol{n}'), \tag{7.53}$$

with the functions $\Psi_i^{(\pm)}(E,\boldsymbol{n}',\boldsymbol{r})$ defined as

$$\Psi_i^{(\pm)}(E,\boldsymbol{n}',\boldsymbol{r}) = \Phi_i(E,\boldsymbol{n}',\boldsymbol{r}) + \sqrt{\frac{8\pi^2c^2\hbar^2}{Ek}}\sum_{\gamma}\mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma^{\dagger}(E,\boldsymbol{n}')\mathcal{U}_i(E,\boldsymbol{n}')$$
$$\times\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}''\,\mathscr{G}_0^{(\pm)}(E,\boldsymbol{r},\boldsymbol{r}'')\hat{V}X_\gamma(E,\boldsymbol{r}'') \tag{7.54}$$

(cf. the definition (7.43)).

7.3. Far-field amplitudes

If the limiting passage $r\to\infty$ is made in Eq. (7.43) and the result is transformed with the aid of Eqs. (7.27) and (7.30), comparison with Eq. (7.37) shows that the far-field amplitudes $\mathcal{A}^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)$ may be expressed as

$$\mathcal{A}^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0) = \mathscr{A}^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}_0) \tag{7.55}$$

with

$$\mathscr{A}^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0) = \frac{4\pi}{k}\sum_{\gamma}\mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma(E,\pm\boldsymbol{n})\mathcal{Y}_\gamma^{\dagger}(E,\boldsymbol{n}_0). \tag{7.56}$$

From the definition (7.56), in the way completely analogous to that adopted in Section 6.3, one may infer the following properties of the matrix amplitudes $\mathscr{A}^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)$:

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}_0\,\mathscr{A}^{(\pm)}(E,\pm\boldsymbol{n},\boldsymbol{n}_0)\mathcal{Y}_\gamma(E,\boldsymbol{n}_0) = \frac{4\pi}{k}\mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)\mathcal{Y}_\gamma(E,\boldsymbol{n}), \tag{7.57}$$

$$\mathscr{A}^{(\pm)\dagger}(E,\boldsymbol{n},\boldsymbol{n}_0)=\mathscr{A}^{(\mp)}(E,\mp\boldsymbol{n}_0,\pm\boldsymbol{n}), \tag{7.58}$$

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}'\,\mathscr{A}^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}')\mathscr{A}^{(\pm)\dagger}(E,\boldsymbol{n}_0,\boldsymbol{n}') = \pm\frac{2\pi}{\mathrm{i}k}\left[\mathscr{A}^{(\pm)}(E,\boldsymbol{n},\pm\boldsymbol{n}_0)-\mathscr{A}^{(\pm)\dagger}(E,\boldsymbol{n}_0,\pm\boldsymbol{n})\right], \tag{7.59}$$

$$\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}'\,\mathscr{A}^{(\pm)\dagger}(E,\boldsymbol{n}',\boldsymbol{n})\mathscr{A}^{(\pm)}(E,\boldsymbol{n}',\boldsymbol{n}_0) = \pm\frac{2\pi}{\mathrm{i}k}\left[\mathscr{A}^{(\pm)}(E,\pm\boldsymbol{n},\boldsymbol{n}_0)-\mathscr{A}^{(\pm)\dagger}(E,\pm\boldsymbol{n}_0,\boldsymbol{n})\right]. \tag{7.60}$$

Moreover, from Eqs. (7.56) and (7.31) it follows that $\mathscr{A}^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)$ may be written in the form

$$\mathscr{A}^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)=(1+\varepsilon^2)^{-1}\begin{pmatrix} A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0) & \varepsilon A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)\boldsymbol{n}_0\cdot\boldsymbol{\sigma} \\ \pm\varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0) & \pm\varepsilon^2\boldsymbol{n}\cdot\boldsymbol{\sigma}A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)\boldsymbol{n}_0\cdot\boldsymbol{\sigma}\end{pmatrix}, \tag{7.61}$$

where $A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)$ are the 2×2 matrix amplitudes defined through the expansion

$$A^{(\pm)}(E,\boldsymbol{n},\boldsymbol{n}_0)=\frac{4\pi}{k}\sum_{\gamma}\mathrm{e}^{\pm\mathrm{i}\delta_\gamma(E)}\sin\delta_\gamma(E)\Upsilon_\gamma(E,\pm\boldsymbol{n})\Upsilon_\gamma^\dagger(E,\boldsymbol{n}_0). \tag{7.62}$$

Concluding, we observe that the counterpart of the nonrelativistic formula (6.43) is

$$\mathcal{A}^{(\pm)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)=-\frac{E}{2\pi c^2\hbar^2}\sum_{i=1}^{2}\mathcal{U}_i(E,\pm\boldsymbol{n})\langle\Phi_i(E,\pm\boldsymbol{n})|\hat{T}^{(\pm)}(E)|\Phi(E,\boldsymbol{v}_0,\boldsymbol{n}_0)\rangle. \tag{7.63}$$

7.4. 2 × 2 scattering kernel

Let $\Psi(E,\boldsymbol{r})$ be an arbitrary regular solution to the Dirac equation

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+mc^2\beta+\hat{V}-E\mathscr{I}]\Psi(E,\boldsymbol{r})=0. \tag{7.64}$$

Asymptotically, $\Psi(E,\boldsymbol{r})$ is of the form

$$\Psi(E,\boldsymbol{r})\overset{r\to\infty}{\longrightarrow}\mathcal{F}_-(E,\boldsymbol{n})\frac{\mathrm{e}^{-\mathrm{i}kr}}{r}-\mathcal{F}_+(E,\boldsymbol{n})\frac{\mathrm{e}^{\mathrm{i}kr}}{r}, \tag{7.65}$$

where $\mathcal{F}_\pm(E,\boldsymbol{n})$ are angle-dependent bispinor amplitudes.

In the complete analogy with the nonrelativistic case (cf. Section 6.4), one might look for a 4×4 scattering kernel $\mathscr{S}(E,\boldsymbol{n},\boldsymbol{n}')$ such that

$$\mathcal{F}_+(E,\boldsymbol{n})=\oint_{4\pi}\mathrm{d}^2\boldsymbol{n}'\,\mathscr{S}(E,\boldsymbol{n},-\boldsymbol{n}')\mathcal{F}_-(E,\boldsymbol{n}'). \tag{7.66}$$

It may be shown, however, that because $\mathcal{F}_{\pm}(E,\boldsymbol{n})$ are of the forms

$$\mathcal{F}_{\pm}(E,\boldsymbol{n}) = \begin{pmatrix} F_{\pm}(E,\boldsymbol{n}) \\ \pm\varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}F_{\pm}(E,\boldsymbol{n}) \end{pmatrix}, \tag{7.67}$$

where $F_{\pm}(E,\boldsymbol{n})$ are spinor amplitudes, Eq. (7.66) does not define $\mathscr{S}(E,\boldsymbol{n},\boldsymbol{n}')$ uniquely. Therefore, rather than working with $\mathscr{S}(E,\boldsymbol{n},\boldsymbol{n}')$, one introduces a 2×2 scattering kernel $S(E,\boldsymbol{n},\boldsymbol{n}')$ such that

$$F_{+}(E,\boldsymbol{n}) = \oint_{4\pi} \mathrm{d}^2\boldsymbol{n}'\, S(E,\boldsymbol{n},-\boldsymbol{n}')F_{-}(E,\boldsymbol{n}'). \tag{7.68}$$

To determine $S(E,\boldsymbol{n},\boldsymbol{n}')$, we choose

$$\Psi(E,\boldsymbol{r}) = \Psi^{(+)}(E,\boldsymbol{v}_0,\boldsymbol{n}',\boldsymbol{r}) \tag{7.69}$$

and employ Eq. (7.37) together with the asymptotic formula

$$\Phi(E,\boldsymbol{v}_0,\boldsymbol{n}',\boldsymbol{r}) \overset{r\to\infty}{\to} \frac{2\pi\mathrm{i}}{k}\delta^2(\boldsymbol{n}+\boldsymbol{n}')\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}')\frac{\mathrm{e}^{-\mathrm{i}kr}}{r} - \frac{2\pi\mathrm{i}}{k}\delta^2(\boldsymbol{n}-\boldsymbol{n}')\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}')\frac{\mathrm{e}^{\mathrm{i}kr}}{r} \tag{7.70}$$

and Eq. (7.55). This gives

$$\Psi^{(+)}(E,\boldsymbol{v}_0,\boldsymbol{n}',\boldsymbol{r}) \overset{r\to\infty}{\to} \frac{2\pi\mathrm{i}}{k}\delta^2(\boldsymbol{n}+\boldsymbol{n}')\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}')\frac{\mathrm{e}^{-\mathrm{i}kr}}{r} - \frac{2\pi\mathrm{i}}{k}\left[\delta^2(\boldsymbol{n}-\boldsymbol{n}')\mathscr{I} + \frac{\mathrm{i}k}{2\pi}\mathscr{A}^{(+)}(E,\boldsymbol{n},\boldsymbol{n}')\right]\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}')\frac{\mathrm{e}^{\mathrm{i}kr}}{r}. \tag{7.71}$$

Hence, after invoking Eqs. (7.39) and (7.61), one finds that in this particular case

$$F_{-}(E,\boldsymbol{n}) = \frac{2\pi\mathrm{i}}{k}(1+\varepsilon^2)^{-1/2}\delta^2(\boldsymbol{n}+\boldsymbol{n}')u(\boldsymbol{v}_0), \tag{7.72}$$

$$F_{+}(E,\boldsymbol{n}) = \frac{2\pi\mathrm{i}}{k}(1+\varepsilon^2)^{-1/2}\left[\delta^2(\boldsymbol{n}-\boldsymbol{n}')I + \frac{\mathrm{i}k}{2\pi}A^{(+)}(E,\boldsymbol{n},\boldsymbol{n}')\right]u(\boldsymbol{v}_0), \tag{7.73}$$

and substitution of Eqs. (7.72) and (7.73) into the definition (7.68) leads to

$$S(E,\boldsymbol{n},\boldsymbol{n}')u(\boldsymbol{v}_0) = \left[\delta^2(\boldsymbol{n}-\boldsymbol{n}')I + \frac{\mathrm{i}k}{2\pi}A^{(+)}(E,\boldsymbol{n},\boldsymbol{n}')\right]u(\boldsymbol{v}_0). \tag{7.74}$$

Since the initial spin orientation $\boldsymbol{v}_0$ may be arbitrary, from Eq. (7.74) we infer that

$$S(E,\boldsymbol{n},\boldsymbol{n}') = \delta^2(\boldsymbol{n}-\boldsymbol{n}')I + \frac{\mathrm{i}k}{2\pi}A^{(+)}(E,\boldsymbol{n},\boldsymbol{n}'), \tag{7.75}$$

and further, after applying the expansion (7.62),

$$S(E,\boldsymbol{n},\boldsymbol{n}') = \delta^2(\boldsymbol{n}-\boldsymbol{n}')I + \sum_{\gamma}\left[\mathrm{e}^{2\mathrm{i}\delta_\gamma(E)} - 1\right]\Upsilon_\gamma(E,\boldsymbol{n})\Upsilon_\gamma^\dagger(E,\boldsymbol{n}'). \tag{7.76}$$

Exploiting the representation (7.76) and the orthonormality relation (7.34), one easily deduces the following properties of the Dirac 2×2 scattering kernel:

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}'\, S(E,\boldsymbol{n},\boldsymbol{n}')\Upsilon_\gamma(E,\boldsymbol{n}') = \mathrm{e}^{2\mathrm{i}\delta_\gamma(E)}\Upsilon_\gamma(E,\boldsymbol{n}), \tag{7.77}$$

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}'\, S(E,\boldsymbol{n},\boldsymbol{n}')S^\dagger(E,\boldsymbol{n}_0,\boldsymbol{n}') = \delta^2(\boldsymbol{n}-\boldsymbol{n}_0)I, \tag{7.78}$$

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}'\, S^\dagger(E,\boldsymbol{n}',\boldsymbol{n})S(E,\boldsymbol{n}',\boldsymbol{n}_0) = \delta^2(\boldsymbol{n}-\boldsymbol{n}_0)I, \tag{7.79}$$

analogous to the properties (6.52)–(6.54) of the Schrödinger scattering kernel. Moreover, if the potential $\hat{V}$ is such that the eigenchannel spinor harmonics obey (cf., however, the remark preceding Eq. (6.65))

$$\sum_\gamma \Upsilon_\gamma(E,\boldsymbol{n})\Upsilon_\gamma^\dagger(E,\boldsymbol{n}') = \delta^2(\boldsymbol{n}-\boldsymbol{n}')I, \tag{7.80}$$

Eq. (7.76) simplifies to

$$S(E,\boldsymbol{n},\boldsymbol{n}') = \sum_\gamma \mathrm{e}^{2\mathrm{i}\delta_\gamma(E)}\Upsilon_\gamma(E,\boldsymbol{n})\Upsilon_\gamma^\dagger(E,\boldsymbol{n}'). \tag{7.81}$$

7.5. Scattering cross-sections

Similarly to the nonrelativistic case, knowledge of the asymptotics of the wave function $\Psi^{(+)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)$ enables one to obtain the differential cross-section:

$$\frac{\mathrm{d}^2Q(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)}{\mathrm{d}^2\boldsymbol{n}} = \frac{\mathcal{A}^{(+)\dagger}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)\boldsymbol{n}\cdot\boldsymbol{\alpha}\mathcal{A}^{(+)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)}{\mathcal{U}^\dagger(E,\boldsymbol{v}_0,\boldsymbol{n}_0)\boldsymbol{n}_0\cdot\boldsymbol{\alpha}\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}_0)}. \tag{7.82}$$

Since

$$\mathcal{U}^\dagger(E,\boldsymbol{v}_0,\boldsymbol{n}_0)\boldsymbol{n}_0\cdot\boldsymbol{\alpha}\mathcal{U}(E,\boldsymbol{v}_0,\boldsymbol{n}_0) = \frac{c\hbar k}{E} \tag{7.83}$$

and

$$\mathcal{A}^{(+)\dagger}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)\boldsymbol{n}\cdot\boldsymbol{\alpha}\mathcal{A}^{(+)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0) = \frac{c\hbar k}{E}\mathcal{A}^{(+)\dagger}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)\mathcal{A}^{(+)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0), \tag{7.84}$$

Eq. (7.82) may be simplified to

$$\frac{\mathrm{d}^2Q(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)}{\mathrm{d}^2\boldsymbol{n}} = \mathcal{A}^{(+)\dagger}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)\mathcal{A}^{(+)}(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0) \tag{7.85}$$

and further, after applying Eqs. (7.55), (7.20), and (7.61), to

$$\frac{\mathrm{d}^2Q(E,\boldsymbol{v}_0,\boldsymbol{n},\boldsymbol{n}_0)}{\mathrm{d}^2\boldsymbol{n}} = u^\dagger(\boldsymbol{v}_0)A^{(+)\dagger}(E,\boldsymbol{n},\boldsymbol{n}_0)A^{(+)}(E,\boldsymbol{n},\boldsymbol{n}_0)u(\boldsymbol{v}_0). \tag{7.86}$$

The total cross-section, for the given direction of incidence $\boldsymbol{n}_0$ and the given initial spin orientation $\boldsymbol{v}_0$ is

$$Q(E, \boldsymbol{v}_0, \boldsymbol{n}_0) = \oint_{4\pi} \mathrm{d}^2\boldsymbol{n} \, \frac{\mathrm{d}^2 Q(E, \boldsymbol{v}_0, \boldsymbol{n}, \boldsymbol{n}_0)}{\mathrm{d}^2\boldsymbol{n}}, \tag{7.87}$$

which, after combining with Eq. (7.62) and the orthogonality relation (7.54), becomes

$$Q(E, \boldsymbol{v}_0, \boldsymbol{n}_0) = \frac{16\pi^2}{k^2} \sum_{\gamma} \sin^2 \delta_\gamma(E) |u^\dagger(\boldsymbol{v}_0) \Upsilon_\gamma(E, \boldsymbol{n}_0)|^2. \tag{7.88}$$

Since

$$u(\boldsymbol{v}_0) u^\dagger(\boldsymbol{v}_0) = \frac{1}{2}[I + \boldsymbol{\sigma} \cdot \boldsymbol{v}_0], \tag{7.89}$$

the equivalent form of Eq. (7.88) is

$$Q(E, \boldsymbol{v}_0, \boldsymbol{n}_0) = \frac{8\pi^2}{k^2} \sum_{\gamma} \sin^2 \delta_\gamma(E) \Upsilon_\gamma^\dagger(E, \boldsymbol{n}_0)[I + \boldsymbol{\sigma} \cdot \boldsymbol{v}_0] \Upsilon_\gamma(E, \boldsymbol{n}_0). \tag{7.90}$$

From Eq. (7.90) one finds that the total cross-section averaged over all initial spin orientations,

$$Q(E, \boldsymbol{n}_0) = \frac{1}{4\pi} \oint_{4\pi} \mathrm{d}^2\boldsymbol{v}_0 \, Q(E, \boldsymbol{v}_0, \boldsymbol{n}_0), \tag{7.91}$$

is

$$Q(E, \boldsymbol{n}_0) = \frac{8\pi^2}{k^2} \sum_{\gamma} \sin^2 \delta_\gamma(E) \Upsilon_\gamma^\dagger(E, \boldsymbol{n}_0) \Upsilon_\gamma(E, \boldsymbol{n}_0). \tag{7.92}$$

From this, after employing the orthonormality relation (7.34), the total cross-section averaged over initial spin orientations and directions of incidence,

$$Q(E) = \frac{1}{4\pi} \oint_{4\pi} \mathrm{d}^2\boldsymbol{n}_0 \, Q(E, \boldsymbol{n}_0), \tag{7.93}$$

is found to be

$$Q(E) = \frac{2\pi}{k^2} \sum_{\gamma} \sin^2 \delta_\gamma(E). \tag{7.94}$$

8. Conclusions

Augusiak [57] has applied the approach presented in this work to scattering of Schrödinger and Dirac particles from a class of separable potentials. His results will be published elsewhere.

There are at least four directions in which the formalism proposed in the present work may be extended. First, it would be desirable to generalize it so that it becomes also applicable to scattering from long range potentials, in particular from potentials with Coulomb tails. Although in principle such a generalization does not seem difficult, being formally realized by including a long range component of the potential into the Hamiltonian $\hat{H}_0$, in practice some subtleties appear which require a more thorough study. Second, the formalism might be extended to scattering from non-Hermitian potentials. Third, it would be interesting to study consequences on the formalism resulting from admitting complex energies. Finally, the approach presented in this work deserves generalization to reactive scattering. We work on these subjects and any significant progress will be reported in future publications.

Acknowledgments

Discussions with Mr. R. Augusiak are acknowledged. I am grateful to Professor R. J. Garbacz for sending me a copy of his thesis [39] and reprints of relevant publications. This work was supported by the Polish State Committee for Scientific Research and by the Gdańsk University of Technology.

Appendix A. Dependencies of $\lambda_\gamma(E)$ and $\delta_\gamma(E)$ on the potential strength

In this appendix we shall investigate the dependence of eigenvalues of the eigenchannel spectral problem (3.1) on the strength of the potential $\hat{V}$.

The following substitutions:

$$\hat{V} \to \mu \hat{V} \qquad (\mu \in \mathbb{R} \setminus \{0\}), \tag{A.1}$$

$$|X_\gamma(E)\rangle \to |X_\gamma(E,\mu)\rangle, \tag{A.2}$$

$$\lambda_\gamma(E) \to \lambda_\gamma(E,\mu), \tag{A.3}$$

transform Eqs. (3.1), (3.10), and (3.11) into

$$\left[\mu^{-1}\hat{I} + \hat{G}_0^{(0)}(E)\hat{V}\right]|X_\gamma(E,\mu)\rangle = \lambda_\gamma(E,\mu)\hat{D}_0(E)\hat{V}|X_\gamma(E,\mu)\rangle, \tag{A.4}$$

$$\mu^2\langle X_\gamma(E,\mu)|\hat{V}\hat{D}_0(E)\hat{V}|X_\gamma(E,\mu)\rangle = 1, \tag{A.5}$$

and

$$\lambda_\gamma(E,\mu) = \langle X_\gamma(E,\mu)|\mu\hat{V} + \mu^2\hat{V}\hat{G}_0^{(0)}(E)\hat{V}|X_\gamma(E,\mu)\rangle, \tag{A.6}$$

respectively. Differentiating Eq. (A.6) with respect to the potential strength μ, after making use of Eq. (A.4), yields

$$\frac{\partial \lambda_\gamma(E,\mu)}{\partial \mu} = -\langle X_\gamma(E,\mu)|\hat{V}|X_\gamma(E,\mu)\rangle + \frac{\partial}{\partial \mu}\left[\mu^2\langle X_\gamma(E,\mu)|\hat{V}\hat{D}_0(E)\hat{V}|X_\gamma(E,\mu)\rangle\right], \tag{A.7}$$

which, in virtue of Eq. (A.5), simplifies to

$$\frac{\partial \lambda_\gamma(E,\mu)}{\partial \mu} = -\langle X_\gamma(E,\mu)|\hat{V}|X_\gamma(E,\mu)\rangle. \tag{A.8}$$

Since

$$\lambda_\gamma(E,\mu) = -\cot\delta_\gamma(E,\mu), \tag{A.9}$$

Eq. (A.8) implies

$$\frac{\partial\delta_\gamma(E,\mu)}{\partial\mu} = -\sin^2\delta_\gamma(E,\mu)\langle X_\gamma(E,\mu)|\hat{V}|X_\gamma(E,\mu)\rangle. \tag{A.10}$$

From Eqs. (A.8) and (A.10) one infers that if the potential $\hat{V}$ is definite then the eigenvalues $\{\lambda_\gamma(E,\mu)\}$ and the eigenphases $\{\delta_\gamma(E,\mu)\}$ are monotonic functions of the potential strength μ; in particular:

$$\hat{V} \text{ positive definite } \Rightarrow \frac{\partial\lambda_\gamma(E,\mu)}{\partial\mu} < 0, \quad \frac{\partial\delta_\gamma(E,\mu)}{\partial\mu} \leqslant 0, \tag{A.11}$$

$$\hat{V} \text{ negative definite } \Rightarrow \frac{\partial\lambda_\gamma(E,\mu)}{\partial\mu} > 0, \quad \frac{\partial\delta_\gamma(E,\mu)}{\partial\mu} \geqslant 0. \tag{A.12}$$

Appendix B. Construction of the functional (5.3)

We begin with rewriting the spectral problem (3.1) as

$$[\hat{I} + \hat{G}_0^{(0)}(E)\hat{V} - \lambda(E)\hat{D}_0(E)\hat{V}]|X(E)\rangle = 0 \tag{B.1}$$

(for brevity, throughout this appendix indices labeling eigensolutions will be omitted). Following the prescription of Gerjuoy et al. [55], considering Eq. (B.1) as a constraint, we shall seek the functional $\mathscr{F}_1$ in the form

$$\mathscr{F}_1[\overline{\lambda}, |\overline{X}\rangle, \langle\overline{\Theta}|] = \overline{\lambda} + \langle\overline{\Theta}|\hat{I} + \hat{G}_0^{(0)}(E)\hat{V} - \overline{\lambda}\hat{D}_0(E)\hat{V}|\overline{X}\rangle. \tag{B.2}$$

Here $\overline{\lambda}$ and $|\overline{X}\rangle$ are some estimates of $\lambda(E)$ and $|X(E)\rangle$, respectively, while $\langle\overline{\Theta}|$ is a Lagrange bra which at this stage is arbitrary. It is evident that if eigensolutions to Eq. (B.1) are substituted into the functional (B.2), for arbitrary $\langle\overline{\Theta}|$ we have

$$\mathscr{F}_1[\lambda(E), |X(E)\rangle, \langle\overline{\Theta}|] = \lambda(E). \tag{B.3}$$

Consider now the first variation of the functional (B.2) due to unconstrained variations in its arguments around $\lambda(E)$, $|X(E)\rangle$, and some $\langle\Theta|$ (which is at our disposal), respectively. The variation is

$$\begin{aligned} &\delta\mathscr{F}_1[\lambda(E), |X(E)\rangle, \langle\Theta|] \\ &\quad = \delta\lambda + \langle\delta\Theta|\hat{I} + \hat{G}_0^{(0)}(E)\hat{V} - \lambda(E)\hat{D}_0(E)\hat{V}|X(E)\rangle - \delta\lambda\langle\Theta|\hat{D}_0(E)\hat{V}|X(E)\rangle \\ &\qquad + \langle\Theta|\hat{I} + \hat{G}_0^{(0)}(E)\hat{V} - \lambda(E)\hat{D}_0(E)\hat{V}|\delta X\rangle \end{aligned} \tag{B.4}$$

and, because of Eq. (B.1), may be simplified to

$$\begin{aligned} \delta\mathscr{F}_1[\lambda(E), |X(E)\rangle, \langle\Theta|] &= \delta\lambda[1 - \langle\Theta|\hat{D}_0(E)\hat{V}|X(E)\rangle] \\ &\quad + \langle\Theta|\hat{I} + \hat{G}_0^{(0)}(E)\hat{V} - \lambda(E)\hat{D}_0(E)\hat{V}|\delta X\rangle. \end{aligned} \tag{B.5}$$

At this moment we demand that $\langle\Theta|$ is such that

$$\delta\mathscr{F}_1[\lambda(E), |X(E)\rangle, \langle\Theta|] = 0. \tag{B.6}$$

In view of arbitrariness of the variations $\delta\lambda$ and $|\delta X\rangle$, this yields

$$1 - \langle\Theta|\hat{D}_0(E)\hat{V}|X(E)\rangle = 0 \tag{B.7}$$

and

$$\langle\Theta|[\hat{I} + \hat{G}_0^{(0)}(E)\hat{V} - \lambda(E)\hat{D}_0(E)\hat{V}] = 0. \tag{B.8}$$

Since $\lambda(E)$ is real and $\hat{V}$ is Hermitian, the Hermitian adjoint to Eq. (B.8) is

$$[\hat{I} + \hat{V}\hat{G}_0^{(0)}(E) - \lambda(E)\hat{V}\hat{D}_0(E)]|\Theta\rangle = 0. \tag{B.9}$$

Comparison of Eqs. (B.1) and (B.3) shows that $|\Theta\rangle$ may be chosen as

$$|\Theta\rangle = \eta\hat{V}|X(E)\rangle, \tag{B.10}$$

where η is some numerical constant. Hence, we deduce that

$$\langle\Theta| = \eta^*\langle X(E)|\hat{V} \tag{B.11}$$

and substitution of Eq. (B.11) into Eq. (B.7) yields

$$\eta = \eta^* = \frac{1}{\langle X(E)|\hat{V}\hat{D}_0(E)\hat{V}|X(E)\rangle}. \tag{B.12}$$

Consequently, we infer that

$$\langle\Theta| = \frac{1}{\langle X(E)|\hat{V}\hat{D}_0(E)\hat{V}|X(E)\rangle}\langle X(E)|\hat{V}. \tag{B.13}$$

Guided by Eq. (B.13), in the functional (B.2) we choose

$$\langle\overline{\Theta}| = \frac{1}{\langle\overline{X}|\hat{V}\hat{D}_0(E)\hat{V}|\overline{X}\rangle}\langle\overline{X}|\hat{V}, \tag{B.14}$$

which results in

$$\mathscr{F}_1\left[|\overline{X}\rangle, \langle\overline{X}|\right] = \frac{\langle\overline{X}|\hat{V} + \hat{V}\hat{G}_0^{(0)}(E)\hat{V}|\overline{X}\rangle}{\langle\overline{X}|\hat{V}\hat{D}_0(E)\hat{V}|\overline{X}\rangle}. \tag{B.15}$$

Appendix C. Orthonormality of eigenchannel harmonics

C.1. Schrödinger eigenchannel harmonics

Consider the scalar product of two Schrödinger eigenchannel harmonics over the unit sphere:

$$I_{\gamma\gamma'}(E) = \oint_{4\pi} d^2\boldsymbol{n}\, Y_\gamma^*(E, \boldsymbol{n})Y_{\gamma'}(E, \boldsymbol{n}). \tag{C.1}$$

On making use of the definitions (6.19) and (6.17), we rewrite this integral as

$$I_{\gamma\gamma'}(E) = \frac{mk}{8\pi^2\hbar^2} \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}' \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'' X_\gamma^*(E,\boldsymbol{r}')\hat{V}\left(\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot(\boldsymbol{r}'-\boldsymbol{r}'')} \right) \hat{V} X_{\gamma'}(E,\boldsymbol{r}''). \tag{C.2}$$

Elementary integration yields

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot(\boldsymbol{r}'-\boldsymbol{r}'')} = 4\pi \frac{\sin(k|\boldsymbol{r}'-\boldsymbol{r}''|)}{k|\boldsymbol{r}'-\boldsymbol{r}''|}, \tag{C.3}$$

which, after making use of Eq. (6.8), becomes

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot(\boldsymbol{r}'-\boldsymbol{r}'')} = \frac{8\pi^2\hbar^2}{mk} D_0(E,\boldsymbol{r}',\boldsymbol{r}''). \tag{C.4}$$

Consequently, we have

$$I_{\gamma\gamma'}(E) = \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}' \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'' X_\gamma^*(E,\boldsymbol{r}')\hat{V} D_0(E,\boldsymbol{r}',\boldsymbol{r}'')\hat{V} X_{\gamma'}(E,\boldsymbol{r}''), \tag{C.5}$$

which, in virtue of Eq. (6.14), gives

$$I_{\gamma\gamma'}(E) = \delta_{\gamma\gamma'}. \tag{C.6}$$

C.2. Dirac eigenchannel bispinor harmonics

Application of Eqs. (7.30) and (7.26) transforms the integral

$$I_{\gamma\gamma'}(E) = \oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathcal{Y}_\gamma^\dagger(E,\boldsymbol{n})\mathcal{Y}_{\gamma'}(E,\boldsymbol{n}) \tag{C.7}$$

into

$$I_{\gamma\gamma'}(E) = \frac{Ek}{8\pi^2c^2\hbar^2} \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}' \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'' X_\gamma^\dagger(E,\boldsymbol{r}')\hat{V}\left(\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathscr{P}(E,\boldsymbol{n})\mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot(\boldsymbol{r}'-\boldsymbol{r}'')} \right) \hat{V} X_{\gamma'}(E,\boldsymbol{r}''). \tag{C.8}$$

In virtue of Eq. (7.19) one has

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathscr{P}(E,\boldsymbol{n})\mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot(\boldsymbol{r}'-\boldsymbol{r}'')} = \frac{-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}' + mc^2\beta + E\mathscr{I}}{2E} \oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot(\boldsymbol{r}'-\boldsymbol{r}'')}, \tag{C.9}$$

which, after employing Eqs. (C.3) and (7.10), may be converted into

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \mathscr{P}(E,\boldsymbol{n})\mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot(\boldsymbol{r}'-\boldsymbol{r}'')} = \frac{8\pi^2c^2\hbar^2}{Ek} \mathscr{D}_0(E,\boldsymbol{r}',\boldsymbol{r}''). \tag{C.10}$$

Equations (C.8) and (C.10) imply that

$$I_{\gamma\gamma'}(E) = \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}' \int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}'' X_\gamma^\dagger(E,\boldsymbol{r}')\hat{V} \mathscr{D}_0(E,\boldsymbol{r}',\boldsymbol{r}'')\hat{V} X_{\gamma'}(E,\boldsymbol{r}'') \tag{C.11}$$

and combining this result with Eq. (7.16) leads to

$$I_{\gamma\gamma'}(E) = \delta_{\gamma\gamma'}. \tag{C.12}$$

References

[1] H. Faxén, J. Holtsmark, Z. Phys. 45 (1927) 307.
[2] J. Holtsmark, Z. Phys. 55 (1929) 437.
[3] H.Ch. Stier, Z. Phys. 76 (1932) 439.
[4] J.B. Fisk, Phys. Rev. 49 (1936) 167.
[5] D.I. Abramov, I.V. Komarov, Teor. Mat. Fiz. 22 (1975) 253.
[6] I.V. Komarov, L.I. Ponomarev, S.Yu. Slavianov, Spheroidal and Coulomb Spheroidal Wave Functions, Nauka, Moscow, 1976, Sec. III.3 (in Russian).
[7] T. Levitina, E.J. Brändas, Int. J. Quantum Chem. Quantum Chem. Symp. 30 (1996) 5.
[8] T. Levitina, E.J. Brändas, Int. J. Quantum Chem. 65 (1997) 601.
[9] T. Levitina, E.J. Brändas, Comput. Phys. Commun. 126 (2000) 107.
[10] T.V. Levitina, E.J. Brändas, Comput. Chem. 25 (2001) 55.
[11] B.A. Lippmann, J. Schwinger, Phys. Rev. 79 (1950) 469.
[12] J.M. Blatt, L.C. Biedenharn, Rev. Mod. Phys. 24 (1952) 258.
[13] L.C. Biedenharn, H.B. Willard, Proc. Phys. Soc. 72 (1958) 874.
[14] H.B. Willard, L.C. Biedenharn, P. Huber, E. Baumgartner, in: J.B. Marion, J.L. Fowler (Eds.), Fast Neutron Physics. Part II: Experiments and Theory, Interscience, New York, 1963, p. 1217.
[15] R.G. Newton, Scattering Theory of Waves and Particles, second ed., Springer, New York, 1982, Sections 10.3.3, 15.1.3, and 15.2.3.
[16] R.G. Newton, Phys. Rev. Lett. 62 (1989) 1811; erratum: 63 (1989) 103.
[17] R.G. Newton, Ann. Phys. (N.Y.) 194 (1989) 173.
[18] R.G. Newton, in: R. Pike, P. Sabatier (Eds.), Scattering. Scattering and Inverse Scattering in Pure and Applied Science, Academic, San Diego, 2002, Chapter 2.1.2, Section 9.
[19] M. Danos, W. Greiner, Phys. Rev. 146 (1966) 708.
[20] C. Mahaux, H.A. Weidenmüller, Phys. Rev. 170 (1968) 847.
[21] C. Toepffer, W. Greiner, Ann. Phys. (N.Y.) 47 (1968) 285.
[22] H.G. Wahsweiler, W. Greiner, M. Danos, Phys. Rev. 170 (1968) 893.
[23] P.P. Delsanto, M.F. Roetter, H.G. Wahsweiler, Z. Phys. 222 (1969) 67.
[24] W. Greiner, in: M. Jean (Ed.), Cargèse Lectures in Physics, Gordon and Breach, London, vol. 3, 1969, p. 535.
[25] C. Toepffer, W. Greiner, Phys. Rev. 186 (1969) 1044.
[26] C. Mahaux, H.A. Weidenmüller, Shell-model Approach to Nuclear Reactions, North-Holland, Amsterdam, 1969, Sections 8.14 and 8.15.
[27] B. Greiner, Z. Naturforsch. A 25 (1970) 170.
[28] R.F. Barrett, L.C. Biedenharn, M. Danos, P.P. Delsanto, W. Greiner, H.G. Wahsweiler, Rev. Mod. Phys. 45 (1973) 44.
[29] U. Fano, Phys. Rev. A 2 (1970) 353.
[30] K.T. Lu, Phys. Rev. A 4 (1971) 579.
[31] C.M. Lee, Phys. Rev. A 10 (1974) 584.
[32] C.M. Lee, Phys. Rev. A 11 (1975) 1692.
[33] U. Fano, J. Opt. Soc. Am. 65 (1975) 979.
[34] C.M. Lee, W.R. Johnson, Phys. Rev. A 22 (1980) 979.
[35] C.W. Clark, K.T. Taylor, J. Phys. B 15 (1982) L213.
[36] C.H. Greene, Ch. Jungen, Adv. At. Mol. Phys. 21 (1985) 51.
[37] C.-W. Lee, Phys. Rev. A 58 (1998) 4581.
[38] R.J. Garbacz, Proc. IEEE 53 (1965) 856.
[39] R.J. Garbacz, Ph. D. Thesis, Ohio State University, 1968.
[40] R.F. Harrington, J.R. Mautz, IEEE Trans. Antennas Propagat. 19 (1971) 622.
[41] R.F. Harrington, J.R. Mautz, IEEE Trans. Antennas Propagat. 20 (1972) 194.
[42] R.F. Harrington, in: R. Mittra (Ed.), Numerical and Asymptotic Techniques in Electromagnetics, Springer, Berlin, 1975, p. 51.

[43] N.N. Voitovich, B.Z. Katsenelenbaum, E.N. Korshunova, A.N. Sivov, Radiotekh. Elektron. 20 (1975) 1129.
[44] N.N. Voitovich, B.Z. Katsenelenbaum, A.N. Sivov, Usp. Fiz. Nauk 118 (1976) 709, Sec. 3.e.
[45] N.N. Voitovich, B.Z. Katsenelenbaum, A.N. Sivov, Generalized Method of Eigenoscillations in Diffraction Theory, Nauka, Moscow, 1977, Sections II.13, III.17.5, IV.20, IV.27, and IV.28 (in Russian).
[46] M.S. Agranovich, Spectral Properties of Diffraction Problems (Appendix to Ref. [45]), Sec. 39 (in Russian).
[47] M.S. Agranovich, B.Z. Katsenelenbaum, A.N. Sivov, N.N. Voitovich, Generalized Method of Eigenoscillations in Diffraction Theory, Wiley-VCH, Berlin, 1999, Sections 2.5, 3.4, 4.2, 4.9, 4.10, and 5.10.
[48] Yu.N. Demkov, V.S. Rudakov, Zh. Eksp. Teor. Fiz. 59 (1970) 2035.
[49] Yu.N. Demkov, V.N. Ostrovskii, Zero-radius Potentials Method in Atomic Physics, Izdatelstvo Leningradskogo Universiteta, Leningrad, 1975, Chapter 4 (in Russian).
[50] W. John, P. Ziesche, Phys. Stat. Sol. B 47 (1971) K83.
[51] W. John, P. Ziesche, Phys. Stat. Sol. B 47 (1971) 555.
[52] W. John, Phys. Stat. Sol. B 49 (1972) K57.
[53] W. John, G. Lehmann, P. Ziesche, Phys. Stat. Sol. B 53 (1972) 287.
[54] P. Ziesche, J. Phys. C 7 (1974) 1085.
[55] R. Szmytkowski, Phys. Lett. A 319 (2003) 233.
[56] E. Gerjuoy, A.R.P. Rau, L. Spruch, Rev. Mod. Phys. 55 (1983) 725.
[57] R. Augusiak, M.Sc. Thesis, Gdańsk University of Technology, 2003.