Non-relativistic quantum scattering from non-local separable potentials: the eigenchannel approach

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Abstract

A recently formulated version of the eigenchannel method [R. Szmytkowski, Ann. Phys. (N.Y.) 311, 503 (2004)] is applied to quantum scattering of Schrödinger particles from non-local separable potentials. Eigenchannel vectors and negative cotangents of eigenphase-shifts are introduced as eigensolutions to some weighted matrix spectral problem, without a necessity of prior construction and diagonalization of the scattering matrix. Explicit expressions for the scattering amplitude, the total cross section in terms of the eigenchannel vectors and the eigenphase-shifts are derived. An illustrative example is provided.

1 Introduction

Recently, Szmytkowski [1] (see also [2]), inspired by works of Garbacz [3] and Harrington and Mautz [4] has presented a general formulation of the eigenchannel method for quantum scattering from Hermitian short-range potentials. This formulation, exploiting the formalism of integral equations, is alternative to that proposed in 1960’s by Danos and Greiner [5], who based on wave equations written in differential forms.

While various theoretical aspects of the new approach to the eigenchannel method have been considered in detail in Ref. [1], no explicit illustrative applications of the formalism have been provided therein. It is the purpose of the present paper to fill in this gap by applying the formalism to non-relativistic scattering from non-local separable potentials.

Separable potentials have proved to be useful in many branches of physics such as atomic [6], molecular [7] and solid state [8] physics. Still, the most extensive use of the separable potentials seems to be made in nuclear physics for describing nucleon-nucleon interactions [9]. The utility of separable potentials stems from two facts. Firstly, the Lippman-Schwinger [10] equation with a separable potential may be solved by employing algebraic methods. Secondly, methods are known which allow one to construct separable approximations to arbitrary local potentials [11]. Here, the crucial role plays the method proposed by Ernst, Shakin and Thaler [12] (see also [13]).

The arrangement of the paper is as follows. Section 2 contains some basic notions of quantum theory of potential scattering. In Section 3 we focus on scattering from separable potentials. In Section 4 we define **eigenchannel vectors** as eigenvectors of some weighted spectral problem and investigate some of their properties. We introduce

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also eigenphaseshifts using eigenvalues of the same spectral problem. Then, we derive formulas for a scattering amplitude in terms of eigenchannel vectors and calculate a total cross section and an averaged total cross section. Finally, in Section 5 we consider an illustrative example. The paper ends with two appendices.

2 Non-relativistic quantum scattering from non-local potentials

Consider a Schrödinger particle described by the monochromatic plane wave

\[ \phi_i(r) \equiv \langle r | k_i \rangle = e^{i k_i \cdot r} \]  

(2.1)

with \( \hbar k_i \) denoting its initial momentum, scattered elastically, i.e. \( |k_i| = |k_f| = k \) (\( \hbar k_f \) is a momentum of the scattered particle) by a non-local Hermitian potential with a kernel \( V(r, r') \).

It was shown by Lippmann and Schwinger [10] that such processes can be described by the following integral equation:

\[ \psi(r) = \phi_i(r) - \int_{\mathbb{R}^3} d^3r' \int_{\mathbb{R}^3} d^3r'' G(E, r, r') V(r', r'') \psi(r''), \]  

(2.2)

where \( G(E, r, r') \) is the well-known free-particle outgoing Green function and is of the form

\[ G(E, r, r') = \frac{m}{2\pi \hbar^2} \frac{e^{ik|r-r'|}}{|r-r'|}. \]  

(2.3)

As usual, during considerations concerning scattering processes we tend to find asymptotical behavior of the wave function \( \psi(r) \). To aim this we firstly need to find asymptotical form of Green function (2.3) for \( r \to \infty \). After straightforward movements we have:

\[ G(E, r, r') \overset{r \to \infty}{\longrightarrow} \frac{m}{2\pi \hbar^2} \frac{e^{ikr}}{r} e^{-ik_f \cdot r'}, \quad k_f = k \frac{r}{r}. \]  

(2.4)

and therefore

\[ \psi(r) \overset{r \to \infty}{\longrightarrow} e^{ik_i \cdot r} + A(k_f \leftarrow k_i) \frac{e^{ikr}}{r}. \]  

(2.5)

The quantity \( A(k_f \leftarrow k_i) \) appearing above is called scattering amplitude and is of the form

\[ A(k_f \leftarrow k_i) = -\frac{m}{2\pi \hbar^2} \int_{\mathbb{R}^3} d^3r' \int_{\mathbb{R}^3} d^3r'' e^{-ik_f \cdot r'} V(r', r'') \psi(r''). \]  

(2.6)

In terms of the scattering amplitude the differential cross section for scattering from the direction \( k_i \) into the direction \( k_f \) is

\[ \frac{d\sigma}{d\Omega_f}(k_f \leftarrow k_i) = |A(k_f \leftarrow k_i)|^2. \]  

(2.7)

Moreover, one defines the total cross section in the following way

\[ \sigma(k_i) = \int_{4\pi} d^2\hat{k}_f |A(k_f \leftarrow k_i)|^2. \]  

(2.8)

Then averaging the total cross section by all directions of incidence \( k_i \), one gets the so-called averaged total cross section:

\[ \sigma_t(E) = \frac{1}{4\pi} \int_{4\pi} d^2\hat{k}_i \int_{4\pi} d^2\hat{k}_f |A(k_f \leftarrow k_i)|^2. \]  

(2.9)
3 The special class of non-local separable potentials

In this section we focus on the special class of Hermitian separable potentials given by the following kernel:

\[ V(r, r') = \sum_\mu \omega_\mu v_\mu(r)v_\mu^*(r') \quad (\forall \mu : \omega_\mu \in \mathbb{R} \setminus \{0\}), \tag{3.1} \]

where \( \mu \) may, in general, denote an arbitrary finite set of countable indices \( \mu_i \), i.e., \( \mu = \{\mu_1, \ldots, \mu_k\} \) and asterisk stands for the complex conjugation.

Application of Eq. (3.1) to Eq. (2.2) leads us to the Lippmann–Schwinger equation for the separable potentials:

\[ \psi(r) = \phi_i(r) - \sum_\mu \omega_\mu \int_{\mathbb{R}^3} d^3 r' G(E, r, r')v_\mu(r') \int_{\mathbb{R}^3} d^3 r'' v_\mu^*(r'')\psi(r''). \tag{3.2} \]

Similarly, substitution of Eq. (3.1) to Eq. (2.6) gives us the scattering amplitude of the form

\[ A(k_f \leftarrow k_i) = -\frac{m}{2\pi\hbar^2} \sum_\mu \omega_\mu \int_{\mathbb{R}^3} d^3 r' e^{-ik_f r'} v_\mu(r') \int_{\mathbb{R}^3} d^3 r'' v_\mu^*(r'')\psi(r''). \tag{3.3} \]

For the sake of convenience, henceforth we shall use the Dirac notation. Then, the above formula reads

\[ A(k_f \leftarrow k_i) = -\frac{m}{2\pi\hbar^2} \sum_\mu \langle k_f | v_\mu \rangle \omega_\mu \langle v_\mu | \psi \rangle. \tag{3.4} \]

The fact that \( \mu \) is an element of an arbitrary countable set, implies that we can put all scalar products \( \langle v_\mu | \psi \rangle \) into a sequence. Therefore, for further simplicity we can employ the following notations:

\[ \langle \nu | \varphi \rangle = \begin{pmatrix} \langle v_1 | \varphi \rangle \\ \langle v_2 | \varphi \rangle \\ \vdots \end{pmatrix}, \quad \langle \varphi | \nu \rangle = \langle \nu | \varphi \rangle^* = (\langle \varphi | v_1 \rangle \langle \varphi | v_2 \rangle \ldots ) \tag{3.5} \]

and

\[ \Omega = \text{diag}[\omega_1, \omega_2, \ldots], \tag{3.6} \]

where the dagger denotes the matrix Hermitian conjugation. Note that from Eqs. (3.1) and (3.6) it is evident that the matrix \( \Omega \) is invertible. We keep this fact for purposes of further considerations. In the light of Eqs. (3.5) and (3.6) we may rewrite the scattering amplitude (3.4) in the following form:

\[ A(k_f \leftarrow k_i) = -\frac{m}{2\pi\hbar^2} \langle k_f | \nu \rangle \Omega \langle \nu | \psi \rangle. \tag{3.7} \]

In the last step we need to calculate the scalar product \( \langle \nu | \psi \rangle \). To this end, we transform Lippmann–Schwinger equation for the separable potentials (3.2) to a set of linear algebraic equations. Hence, after some elementary movements, we have

\[ \sum_\mu [\delta_{\nu\mu} + G_{\nu\mu}\omega_\mu] \langle v_\mu | \psi \rangle = \langle v_\nu | k_i \rangle, \tag{3.8} \]

where

\[ G_{\nu\mu} = \int_{\mathbb{R}^3} d^3 r \int_{\mathbb{R}^3} d^3 r' v_\mu^*(r)G(E, r, r')v_\mu(r'). \tag{3.9} \]
Finally, application of Eqs. (3.8) and (3.9) to Eq. (3.7) yields
\[
(1 + G \Omega) \langle v | \psi \rangle = \langle v | k_i \rangle \quad \Rightarrow \quad \langle v | \psi \rangle = (1 + G \Omega)^{-1} \langle v | k_i \rangle, \tag{3.10}
\]
where I stands for the identity matrix and G denotes a matrix with the elements $G_{\nu \mu}$. Substitution of Eq. (3.10) to Eq. (3.7) gives the expression for the scattering amplitude
\[
A(k_f \leftarrow k_i) = -\frac{m}{2\pi \hbar^2} \langle k_f | v \rangle \Omega (1 + G \Omega)^{-1} \langle v | k_i \rangle. \tag{3.11}
\]
Since $(MN)^{-1} = N^{-1}M^{-1}$ for all invertible matrices $M$ and $N$, we can conclude that
\[
A(k_f \leftarrow k_i) = -\frac{m}{2\pi \hbar^2} \langle k_f | v \rangle (\Omega^{-1} + G)^{-1} \langle v | k_i \rangle. \tag{3.12}
\]

4 The eigenchannel method

Here, we turn to the formulation of the eigenchannel method proposed by Szymtowski [1]. This author has shown that the eigenchannels provide a powerful mathematical tool to the quantum theory of scattering. Moreover, in this approach we do not need to construct the scattering matrix to obtain the formula for an averaged total cross section.

In the first step we rewrite the matrix $\Omega^{-1} + G$ as a sum of its Hermitian and non–Hermitian parts. Hence, we have
\[
\Omega^{-1} + G = A + iB, \tag{4.1}
\]
where the matrices $A$ and $B$ are defined by the relations:
\[
A = \frac{1}{2} [\Omega^{-1} + G + (\Omega^{-1} + G)^\dagger] = \Omega^{-1} + \frac{1}{2} (G + G^\dagger) \tag{4.2}
\]
and
\[
B = \frac{1}{2i} [\Omega^{-1} + G - (\Omega^{-1} + G)^\dagger] = \frac{1}{2i} (G - G^\dagger), \tag{4.3}
\]
respectively. From the definitions (4.2) and (4.3) it is evident that both matrices $A$ and $B$ are Hermitian, i.e., $A = A^\dagger$ and $B = B^\dagger$. Moreover, straightforward calculations with the aid of Eqs. (4.2) and (4.3) allow us to express their elements as
\[
[A]_{\nu \mu} = \frac{1}{\omega_{\nu}} \delta_{\nu \mu} + \frac{m}{2\pi \hbar^2} \int_{\mathbb{R}^3} d^3 r \int_{\mathbb{R}^3} d^3 r' v_{\nu}^*(r) \frac{\cos(k |r - r'|)}{|r - r'|} v_{\mu}(r'), \tag{4.4}
\]
\[
[B]_{\nu \mu} = \frac{m}{2\pi \hbar^2} \int_{\mathbb{R}^3} d^3 r \int_{\mathbb{R}^3} d^3 r' v_{\nu}^*(r) \frac{\sin(k |r - r'|)}{|r - r'|} v_{\mu}(r'). \tag{4.5}
\]
Following [1] let us consider the following weighted spectral problem
\[
AX_{\gamma}(E) = \lambda_{\gamma}(E)BX_{\gamma}(E), \tag{4.6}
\]
where $X_{\gamma}(E)$ and $\lambda_{\gamma}(E)$ are, respectively, its eigenvectors and eigenvalues. Throughout the rest of the present paper, the eigenvectors $X_{\gamma}(E)$ will be called eigenchannel vectors. They constitute a representation of eigenchannels, defined in [1] as state vectors, in subspace spanned by the potential functions $v_{\mu}(r)$. In fact, the knowledge of eigenvectors $X_{\gamma}(E)$ allows us, by some elementary steps, to construct the eigenchannels.

By virtue of the fact that both $A$ and $B$ are Hermitian with the aid of positive semidefiniteness of the matrix $B$ (for a proof, cf. Appendix A), we infer that $\lambda_{\gamma}(E) =$
\( \lambda_\gamma(E) \) for all \( \gamma \). Moreover, it is easy to show that eigenvectors \( X_\gamma(E) \) satisfy the weighted orthogonality relation

\[
X_{\gamma'}^\dagger(E) B X_\gamma(E) = 0 \quad (\gamma' \neq \gamma).
\]

Hence, it is natural to assume the following normalization:

\[
X_{\gamma'}^\dagger(E) B X_\gamma(E) = \delta_{\gamma'\gamma},
\]

or, using the matrices \( A \) and \( \Omega^{-1} + G \):

\[
X_{\gamma'}^\dagger(E) A X_\gamma(E) = \lambda_\gamma(E) \delta_{\gamma'\gamma}, \quad X_{\gamma'}^\dagger(E) (\Omega^{-1} + G) X_\gamma(E) = [i + \lambda_\gamma(E)] \delta_{\gamma'\gamma}.
\]

Since the eigenvectors \( X_\gamma(E) \) are solutions of the Hermitian eigenproblem, they should obey the following closure relations:

\[
\sum_\gamma X_\gamma(E) X_\gamma^\dagger(E) B = 1, \quad \sum_\gamma \lambda_{\gamma}^{-1} X_\gamma(E) X_\gamma^\dagger(E) A = 1
\]

and

\[
\sum_\gamma \frac{1}{i + \lambda_\gamma(E)} X_\gamma(E) X_\gamma^\dagger(E) (\Omega^{-1} + G) = 1.
\]

Henceforth, we shall be assuming that the potential \( \text{(4.11)} \) is such that the above relations are satisfied. Therefore, it is possible to express the matrix \( (\Omega^{-1} + G)^{-1} \) in terms of the eigenchannel vectors \( X_\gamma(E) \). Indeed, using Eq. \( (4.11) \) we have

\[
(\Omega^{-1} + G)^{-1} = \sum_\gamma \frac{1}{i + \lambda_\gamma(E)} X_\gamma(E) X_\gamma^\dagger(E).
\]

Application of Eq. \( (4.12) \) to Eq. \( (3.12) \) yields

\[
A(k_f \leftarrow k_i) = -\frac{m}{2\pi \hbar^2} \sum_\gamma \frac{1}{i + \lambda_\gamma(E)} \langle k_f | \psi \rangle X_\gamma(E) X_\gamma^\dagger(E) \langle \psi | k_i \rangle
\]

or equivalently

\[
A(k_f \leftarrow k_i) = -\frac{m}{2\pi \hbar^2} \sum_\gamma \frac{1}{i + \lambda_\gamma(E)} \sum_\mu \langle k_f | \psi_\mu \rangle X_\gamma \mu(E) \sum_\nu X_\gamma^\mu(E) \langle \psi_\nu | k_i \rangle.
\]

Because of the very symmetrical form of the scattering amplitude, it is useful to define the following functions:

\[
\mathcal{Y}_\gamma(k) = \sqrt{\frac{mk}{8\pi^2 \hbar^2}} \sum_\mu \langle k | \psi_\mu \rangle X_\gamma \mu(E) = \sqrt{\frac{mk}{8\pi^2 \hbar^2}} \langle k | \psi \rangle X_\gamma(E),
\]

hereafter termed eigenchannel harmonics. It follows from their definition that they are orthonormal on the unit sphere (cf. Appendix B), i.e.,

\[
\int_{4\pi} d^2 k \, \mathcal{Y}_\gamma^\ast (k) \mathcal{Y}_\gamma(k) = \delta_{\gamma'\gamma}.
\]

After substitution of Eq. \( (4.13) \) to Eq. \( (4.14) \), one finds

\[
A(k_f \leftarrow k_i) = -\frac{4\pi}{k} \sum_\gamma \frac{1}{i + \lambda_\gamma(E)} \mathcal{Y}_\gamma(k_f) \mathcal{Y}_\gamma^\ast (k_i).
\]
Further, it is convenient to express the eigenvalues \( \lambda_\gamma(E) \) in terms of so-called eigenphaseshifts \( \delta_\gamma(E) \) by the relation

\[
\lambda_\gamma(E) = -\cot \delta_\gamma(E),
\]

which after application to the scattering amplitude (4.17) gives

\[
A(k_f \leftarrow k_i) = \frac{4\pi}{k} \sum_\gamma e^{i\delta_\gamma(E)} \sin \delta_\gamma(E) Y_\gamma^*(k_f) Y_\gamma(k_i). \tag{4.19}
\]

As already mentioned the above result was obtained without prior construction of the scattering matrix. It is also necessary to emphasize that the method used gives formula for the scattering amplitude which has a similar form to that obtained for potentials with spherical symmetry \( V(r) \) \[16\]. For such potentials the functions \( Y_\gamma(k) \) reduce to the spherical harmonics \( Y_{lm}(\hat{k}) \). Subsequently, combining relation (4.19) with (2.8) we have

\[
\sigma(k_i) = \frac{16\pi^2}{k^2} \sum_\gamma \sin^2 \delta_\gamma(E) Y_\gamma^*(k_i) Y_\gamma(k_i). \tag{4.20}
\]

Finally, after substitution of Eq. (4.19) to Eq. (2.9) one obtains

\[
\sigma_t(E) = \frac{4\pi}{k^2} \sum_\gamma \sin^2 \delta_\gamma(E). \tag{4.21}
\]

Thus, we have arrived at the well-known formula for the averaged total cross section.

5 Example

To illustrate the method, let us consider scattering from a pair of identical spheres, of radii \( R \). The symmetry of this target allows us to locate the origin of a coordinate system in the midpoint of the interval joining the centers of spheres. Thus, we may choose the spheres to be centered at points \( r = \pm \rho \). However, due to the assumption of non-locality we may simulate this collision process by potential

\[
V(r, r') = \omega \left[ v_+(r)v_+^*(r') + v_-(r)v_-^*(r') \right] \tag{5.1}
\]

with

\[
v_\pm(r) = \frac{1}{\sqrt{4\pi}} \frac{\delta(|r \pm \rho| - R)}{R^2}. \tag{5.2}
\]

It should be noticed that potential defined by the Eqs. (5.1) and (5.2) is the special case of that proposed recently by de Prunelé \[13\] (see also \[8\]). As one can notice, for further simplicity the strengths of both spheres were taken to be equal and have value \( \omega \). Therefore, the matrix \( \Omega \) defined by Eq. (3.6) may be rewritten as

\[
\Omega = \begin{pmatrix} \omega & 0 \\ 0 & \omega \end{pmatrix} = \omega I_2, \tag{5.3}
\]

where \( I_2 \) is the \( 2 \times 2 \) identity matrix. Moreover, straightforward integrations in Eq. (3.9) with the aid of the expansion

\[
e^{ik|r-r'|}/|r-r'| = 4\pi k \sum_{l=0}^{\infty} \sum_{m=-l}^{l} h_{l}^{(+)}(kr_>)j_l(kr_<)Y_{lm}(r)Y_{lm}^*(r')
\]

\[
(r_> = \max\{r, r'\}, r_< = \min\{r, r'\}). \tag{5.4}
\]
where its eigenvalues \( \lambda \) the scattering amplitude is of the form

\[
G = \eta j_0(kR) \begin{pmatrix}
    h_0^+(kR) & j_0(kR)h_0^+(2kR) \\
    j_0(kR)h_0^+(2kR) & h_0^+(kR)
\end{pmatrix},
\]

(5.5)

where \( \eta = 2m/\hbar^2 \), \( j_i(z) \) stand for spherical Bessel functions and \( h_0^{(+)}(z) \) stand for Hankel functions of the first kind. Then, utilizing Eqs. (4.10) and (5.13) one finds

\[
A = \begin{pmatrix}
    \omega^{-1} - \eta j_0(kR)y_0(kR) & -\eta j_0(kR)y_0(2kR) \\
    -\eta j_0(kR)y_0(2kR) & \omega^{-1} - \eta j_0(kR)y_0(kR)
\end{pmatrix}
\]

(5.6)

and

\[
B = \eta j_0^2(kR) \begin{pmatrix}
    1 & j_0(2kR) \\
    j_0(2kR) & 1
\end{pmatrix}
\]

(5.7)

with \( y_l(z) \) denoting spherical Neumann functions. Note that, in general

\[
j_0(z) = \frac{\sin z}{z}, \quad y_0(z) = -\frac{\cos z}{z}, \quad h_0^{(+)}(z) = -\frac{e^{iz}}{z}.
\]

(5.8)

As one can see the eigenvalue problem (4.6) reduces to

\[
AX_{\pm}(E) = \lambda_{\pm}BX_{\pm}(E),
\]

(5.9)

where its eigenvalues \( \lambda_{\pm}(E) \) are

\[
\lambda_{\pm}(E) = \frac{\omega^{-1} - \eta j_0(kR)[y_0(kR) \pm j_0(kR)y_0(2kR)]}{\eta j_0^2(kR)[1 \pm j_0(2kR)]}
\]

(5.10)

and respective eigenvectors

\[
X_{\pm}(E) = \left\{2\eta j_0^2(kR)[1 \pm j_0(2kR)]\right\}^{-1/2} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}.
\]

(5.11)

Since for arbitrary \( k \):

\[
\langle v|k \rangle = \begin{pmatrix}
    \langle v_+|k \rangle \\
    \langle v_-|k \rangle
\end{pmatrix} = \sqrt{4\pi} j_0(kR) \begin{pmatrix} e^{-ik\cdot e} \\ e^{ik\cdot e} \end{pmatrix}
\]

(5.12)

and by virtue of Eqs. (5.15) and (5.11) the eigenchannel harmonics may be expressed as

\[
\mathcal{Y}_{\pm}(k) = \frac{1}{2\sqrt{2\pi}} [1 \pm j_0(2kR)]^{-1/2}(e^{-ik\cdot e} \pm e^{ik\cdot e}).
\]

(5.13)

and therefore, after substitution of Eqs. (5.10) and (5.13) to Eq. (5.14) we infer that the scattering amplitude is of the form

\[
A(k_f \leftarrow k_i) = -2\eta j_0^2(kR) \left[ \frac{\cos(k_f \cdot \cdot e)\cos(k_i \cdot \cdot e)}{\omega^{-1} + \eta j_0(kR)[h_0^+(kR) + j_0(kR)h_0^+(2kR)]} \\
+ \frac{\sin(k_f \cdot \cdot e)\sin(k_i \cdot \cdot e)}{\omega^{-1} + \eta j_0(kR)[h_0^+(kR) - j_0(kR)h_0^+(2kR)]} \right].
\]

(5.14)

After application of the above to Eq. (2.3) and integration over all directions of scattering \( k_f \) we infer

\[
\sigma(k_i) = 8\eta^2 j_0^4(kR) \times \left[ \frac{[1 + j_0(2kR)]\cos^2(k_i \cdot e)}{[\omega^{-1} - \eta j_0(kR)[y_0(kR) + j_0(kR)y_0(2kR)]] + \eta^2 k^2 j_0^4(kR)[1 + j_0(2kR)]^2} \\
+ \frac{[1 - j_0(2kR)]\sin^2(k_i \cdot e)}{[\omega^{-1} - \eta j_0(kR)[y_0(kR) - j_0(kR)y_0(2kR)]] + \eta^2 k^2 j_0^4(kR)[1 - j_0(2kR)]^2} \right].
\]

(5.15)
Then averaging Eq. (5.10) over all directions of incidence \( k \), and using the fact that
\[
\int_{4\pi} d^2 k_i \cos^2(k_i \cdot \varrho) = 2\pi[1 + j_0(2k\varrho)]
\]
(5.16)
and
\[
\int_{4\pi} d^2 k_i \sin^2(k_i \cdot \varrho) = 2\pi[1 - j_0(2k\varrho)],
\]
(5.17)
we obtain the averaged total cross section
\[
\sigma_t(E) = 4\pi\eta^2 j_0^2(kR)
\]
\text{[B.1]}
\[
\times \left[ \frac{[1 + j_0(2k\varrho)]^2}{\{\omega^{-1} - \eta k j_0(kR)\alpha_0(kR) + j_0(kR)\alpha_0(2k\varrho)\}^2 + \eta^2 k^2 j_0^2(kR)[1 + j_0(2k\varrho)]^2}
\right. \\
+ \left. \frac{[1 - j_0(2k\varrho)]^2}{\{\omega^{-1} - \eta k j_0(kR)\alpha_0(kR) - j_0(kR)\alpha_0(2k\varrho)\}^2 + \eta^2 k^2 j_0^2(kR)[1 - j_0(2k\varrho)]^2} \right].
\]
(5.18)

Note that the results (5.17) and (5.18) may be equivalently obtained after application of Eqs. (5.10) and (5.13), respectively, to Eqs. (4.20) and (4.21).

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A  Positive semidefiniteness of the matrix \( B \)

The proof is due to R. Szmytkowski [17]. Below we show that the matrix \( B \) given by Eq. (4.3) is such that, the inequality
\[
X^\dagger(\mathbf{E})B X(\mathbf{E}) \geq 0
\]
(A.1)
is satisfied. Since
\[
\int_{4\pi} d^2 \mathbf{k} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} = 4\pi \frac{\sin \mathbf{k}|\mathbf{r}-\mathbf{r}'|}{|\mathbf{r}-\mathbf{r}'|}
\]
(A.2)
we may rewrite Eq. (4.3) in the form
\[
[B]_{\nu\mu} = \frac{m k}{8\pi^2 \hbar^2} \int_{4\pi} d^2 \mathbf{k} \int_{\mathbb{R}^3} d^3 \mathbf{r} \nu^\dagger(\mathbf{r}) \mathbf{e}^{i\mathbf{k}\mathbf{r}} \int_{\mathbb{R}^3} d^3 \mathbf{r}' \nu(\mathbf{r}') e^{-i\mathbf{k}\mathbf{r}'},
\]
(A.3)
which after application to Eq. (A.1) yields
\[
X^\dagger(\mathbf{E})B X(\mathbf{E}) = \frac{m k}{8\pi^2 \hbar^2} \int_{4\pi} d^2 \mathbf{k} \left| \sum_{\nu} X^\dagger_{\gamma\nu}(\mathbf{E}) \int_{\mathbb{R}^3} d^3 \mathbf{r} \nu^\dagger(\mathbf{r}) \mathbf{e}^{i\mathbf{k}\mathbf{r}} \int_{\mathbb{R}^3} d^3 \mathbf{r}' \nu(\mathbf{r}') e^{-i\mathbf{k}\mathbf{r}'} \right|^2 \geq 0.
\]
(A.4)

Obviously, the above statement finishes the proof.

B  Proof of orthonormality relation (4.16)

Substituting Eq. (4.15) to Eq. (4.16) and reorganizing terms one finds
\[
\int_{4\pi} d^2 \mathbf{k} \, \nu^\dagger_{\gamma\nu}(\mathbf{k}) \nu_{\gamma}(\mathbf{k}) = \frac{m k}{8\pi^2 \hbar^2} \\
\times \sum_{\nu'\mu} X^\dagger_{\nu'\nu}(\mathbf{E}) \int_{\mathbb{R}^3} d^3 \mathbf{r} \nu^\dagger(\mathbf{r}) \int_{\mathbb{R}^3} d^3 \mathbf{r}' \nu(\mathbf{r}') \int_{4\pi} d^2 \mathbf{k} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}') X_{\gamma\mu}(\mathbf{E})}.
\]
(B.1)
In virtue of Eq. (A.2), Eq. (B.1) may be rewritten in the form

$$\oint_{4\pi} d^2 \hat{k} \gamma'_\gamma(k) \gamma_\gamma(k) = \frac{m}{2\pi \hbar^2} \times \sum_{\nu\mu} X_{\gamma'\nu}(E) \left[ \int_{\mathbb{R}^3} d^3 r \int_{\mathbb{R}^3} d^3 r' \psi^*_\nu(r) \frac{\sin|k| r - r'|}{|r - r'|} \psi_\mu(r') \right] X_{\gamma\mu}(E).$$

(B.2)

As one can notice with the aid of Eq. (4.5), the expression in square brackets is proportional to an element of the matrix $B$. Hence, we arrive at

$$\oint_{4\pi} d^2 \hat{k} \gamma'_\gamma(k) \gamma_\gamma(k) = X_{\gamma'\gamma}^\dagger(E)BX_{\gamma\gamma}(E),$$

(B.3)

which after comparison with Eq. (4.8) completes the proof.

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