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The Hilbert–Schmidt theorem formulation of the R-matrix theory

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Abstract. Using the Hilbert–Schmidt theorem, we reformulate the non-relativistic R-matrix theory in terms of a uniformly and absolutely convergent expansion. Term-by-term differentiation is possible with this expansion in the neighbourhood of the surface. Methods for improving the convergence are discussed when the R-function series is truncated for practical applications.

1. Introduction

Since 1937, boundary condition methods (BCM) have played an important role for many quantum mechanical problems [1–43]. In the BCM formulation, configuration space is divided into two parts: internal and external regions. In the external region, the interaction is usually known and in many cases the effective two-body equation is exactly solvable. A boundary condition matrix is defined in terms of the independent external wavefunctions and their derivates at a boundary. From this information (boundary condition matrix) and the known solution in the external region, the S-matrix and the cross section can be calculated. There are two boundary condition matrices: R-matrix and P-matrix. The R-matrix is the inverse of the logarithmic derivative of the external channel wavefunction at the surface. A detailed account of the R-matrix theory of nuclear reactions is given in [5]. The P-matrix is the logarithmic derivation matrix. The P-matrix formulation of nuclear reactions has not been used extensively except for the nucleon–nucleon scattering problem [5–10]. We note that in some papers this matrix is called the B-matrix or Y-matrix.

The R-matrix theory is extensively employed for describing energy dependence of the cross section for various binary nuclear processes including both elementary and composite nuclear particles [5, 13–19] and is often used to extrapolate experimental data for the cross section which are dominated by the contributions from a few resonance or bound states.

In atomic physics, the exchange interaction, which is the most difficult part of the problem to calculate accurately, is only in the internal region, and interactions in the external region reduce to long-range local potentials [20]. The R-matrix code is a very powerful computation code [21, 22] for calculating electron–atom collisions and photoabsorption processes. For example, the inner-shell photoionization cross sections calculated by the R-matrix code [23, 24] are in excellent agreement with the recent experimental measurements [44].

The R-matrix method for studying low-energy electron–molecule collisions was developed in [25–27]. It has been used to describe elastic scattering, electronic excitation, vibrational excitation [29] and dissociative attachment [31]. For an extensive review of

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physical applications of the BCM in atomic physics see [40]; for a more mathematical treatment see [41].

The R-matrix method is based upon expanding the total wavefunction Ψ for any energy in the internal region in terms of the complete set of eigenfunctions X_λ,

$$\Psi = \sum_\lambda A_\lambda X_\lambda \tag{1}$$

where X_λ are defined by the equation

$$HX_\lambda = E_\lambda X_\lambda \tag{2}$$

and satisfy certain R-matrix boundary conditions on the surface [5]. It is known that there is a formal problem with the wavefunction expansion used in the conventional approach for the R-matrix theory. Either the expansion given by equation (1) is not uniformly convergent in the neighbourhood of the surface, or term-by-term differentiation of the expansion is not admissible [5, 20]. To avoid these difficulties variational formalisms [32–38] were proposed with basis functions which do not satisfy the R-matrix boundary conditions.

The non-relativistic R-matrix theory is rigorous and therefore, there remains, from the formal point of view, a problem of how to formulate the R-matrix method in terms of a uniformly and absolutely convergent expansion.

In this paper we present solutions of this formal problem and discuss various approximations of the R-function. In section 2, we describe in some detail the conventional formulation of R-function in terms of the expansion given by equations (1) and (2). In section 3, we reformulate the R-matrix theory based on the Hilbert–Schmidt theorem to obtain the R-function in terms of a series which is uniformly and absolutely convergent. In section 4, we discuss methods of improving the convergence of the R-function series when it is truncated for practical applications. In section 5 we present an illustrative numerical example (low-energy n–^{12}C interaction) supporting our theoretical results. A summary and conclusions are given in section 6.

2. R-function

In order to describe the formal procedure employed in the R-matrix theory, we consider the simplest case of potential scattering for spinless particles with only the elastic scattering channel being open.

The radial wavefunction $u_\ell(r)$ in the interior region $0 \leqslant r \leqslant a$ satisfies the Schrödinger equation

$$-\frac{\mathrm{d}^2 u_\ell}{\mathrm{d}r^2} + \left(\frac{2\mu V(r)}{\hbar^2} + \frac{\ell(\ell+1)}{r^2}\right) u_\ell(r) = k^2 u_\ell(r) \tag{3}$$

where μ is the reduced mass, $V(r)$ is the interaction potential in the internal region $0 \leqslant r \leqslant a$, and $k^2 = 2\mu E/\hbar^2$.

In the conventional theory [5, 20, 39], $u_\ell(r)$ in the internal region ($0 \leqslant r \leqslant a$) is expanded in terms of complete set of states $u_\lambda^\ell(r)$ given within the region $0 \leqslant r \leqslant a$. These states are the solutions of the equation

$$-\frac{\mathrm{d}^2 u_\lambda^\ell}{\mathrm{d}r^2} + \left(\frac{2\mu V(r)}{\hbar^2} + \frac{\ell(\ell+1)}{r^2}\right) u_\lambda^\ell(r) = k_\lambda^2 u_\lambda^\ell(r) \tag{4}$$

satisfying the R-matrix boundary conditions

$$u_\lambda^\ell(0) = 0$$
$$\frac{a}{u_\lambda^\ell(a)}\left(\frac{\mathrm{d}u_\lambda^\ell}{\mathrm{d}r}\right)_{r=a} = B \tag{5}$$

and the orthonormality conditions

$$\int_o^a u_\lambda^\ell(r)u_{\lambda'}^\ell(r)\,\mathrm{d}r = \delta_{\lambda\lambda'}. \tag{6}$$

In the region $0 \leqslant r \leqslant a$, $u_\ell(r)$ may be expanded in terms of the eigenfunctions $u_\lambda^\ell(r)$

$$u_\ell(r) = \sum_{\lambda=1}^{\infty} c_\lambda^\ell u_\lambda^\ell(r) \qquad (0 \leqslant r \leqslant a) \tag{7}$$

where

$$c_\lambda^\ell = \int_o^a \mathrm{d}r\, u_\ell(r)u_\lambda^\ell(r). \tag{8}$$

As we show below, either: (i) expansion (7) does not converge uniformly, or (ii) term-by-term differentiation is not admissible [5, 20], or both (i) and (ii) may be applicable. From Green's theorem [5, 20] and the boundary conditions (5), we find

$$c_\lambda^\ell = \frac{1}{a}\frac{u_\lambda^\ell(a)}{k_\lambda^2 - k^2}\left[a\frac{\mathrm{d}u_\ell}{\mathrm{d}r} - Bu_\ell\right]_{r=a}. \tag{9}$$

Substitution of equation (7) into equation (6) gives

$$\tilde{u}_l(r, k^2) = u_\ell(r)\left[a\frac{\mathrm{d}u_\ell}{\mathrm{d}r} - Bu_\ell\right]_{r=a}^{-1} = \frac{1}{a}\sum_{\lambda=1}^{\infty}\frac{u_\lambda^\ell(r)u_\lambda^\ell(a)}{k_\lambda^2 - k^2}. \tag{10}$$

If we now define

$$R^{(B)} = \frac{1}{a}\sum_{\lambda=1}^{\infty}\frac{(u_\lambda^\ell(a))^2}{k_\lambda^2 - k^2} \tag{11}$$

and assume that

$$\lim_{r\to a^-}\left[\sum_{\lambda=1}^{\infty}\frac{u_\lambda^\ell(r)u_\lambda^\ell(a)}{k_\lambda^2 - k^2}\right] = \sum_{\lambda=1}^{\infty}\frac{(u_\lambda^\ell(a))^2}{k_\lambda^2 - k^2} \tag{12}$$

we find that $R^{(B)}$ relates the amplitude of u_ℓ to its derivative at the boundary by the relation

$$R^{(B)} = u_\ell(a)\left[a\frac{\mathrm{d}u_\ell}{\mathrm{d}r} - Bu_\ell\right]_{r=a}^{-1}. \tag{13}$$

Once $R^{(B)}$ has been calculated, the K-matrix and cross section can be easily determined.

From the fact that

$$G_\ell(r, r') = -\sum_{\lambda=1}^{\infty}\frac{u_\lambda^\ell(r)u_\lambda^\ell(r')}{k_\lambda^2 - k^2} \tag{14a}$$

and

$$G_\ell(r, r') = \begin{cases} u_\ell(r)Y_\ell(r') & r \leqslant r' \\ u_\ell(r')Y_\ell(r) & r' \leqslant r \end{cases} \tag{14b}$$

with

$$Y_\ell(r) = \frac{y_\ell(a) B u_\ell(r)}{\left[a\frac{\mathrm{d}u_\ell}{\mathrm{d}r} - Bu_\ell\right]_{r=a}} + y_\ell(r) \tag{15}$$

where $y_\ell(r)$ is the irregular solution of equation (3) with boundary conditions $(\frac{\mathrm{d}y_\ell}{\mathrm{d}r})_{r=a} = 0$, and $u'_\ell y_\ell - y'_\ell u_\ell = 1$, it can be seen that equations (7) and (10) can be obtained from the spectral decomposition, equation (14*a*), of Green's function $G_\ell(r, r')$. This bilinear series, equation (14*a*), converges in $L_2(0 < r < a)$.

We note that the completeness of the states u_λ^ℓ does not guarantee validity of equation (12). To demonstrate this statement, let us first consider a special case of boundary conditions $B = \infty$, or

$$u_\lambda^\ell(0) = u_\lambda^\ell(a) = 0. \tag{16}$$

Using equation (5), equation (9) can be written as

$$c_\lambda^\ell = \left[\frac{u_\lambda^\ell(a)}{k_\lambda^2 - k^2}\,\frac{\mathrm{d}u_l(r)}{\mathrm{d}r} + \frac{u_l(a)}{k^2 - k_\lambda^2}\,\frac{\mathrm{d}u_l^\lambda(r)}{\mathrm{d}r}\right]_{r=a}. \tag{17a}$$

For the $u_\lambda^\ell(a) = 0$ case, equation (17*a*) is

$$c_\lambda^\ell = \frac{u_\ell(a)}{k^2 - k_\lambda^2}\left(\frac{\mathrm{d}u_\lambda^\ell}{\mathrm{d}r}\right)_{r=a} \tag{17b}$$

and substitution of equation (17) into equation (7) gives

$$\frac{u_\ell(r)}{u_\ell(a)} = \sum_{\lambda=1}^{\infty} \frac{u_\lambda^\ell(r)}{k^2 - k_\lambda^2}\left(\frac{\mathrm{d}u_\lambda^\ell}{\mathrm{d}r}\right)_{r=a}. \tag{18}$$

If one tries to obtain this value of $\lim_{r\to a}\frac{u_\ell(r)}{u_\ell(a)} = 1$ from the right-hand side of equation (18) taking the limit term by term, one obtains a null result, because of equation (16).

In the case of the boundary conditions (5) we can obtain from equation (10), that

$$\eta(r) = \frac{1}{a}\left(a\frac{\mathrm{d}}{\mathrm{d}r} - B\right)\sum_{\lambda=1}^{\infty}\frac{u_\lambda^\ell(r)u_\lambda^\ell(a)}{k_\lambda^2 - k^2} \tag{19}$$

where

$$\eta(r) = \left[a\frac{\mathrm{d}u_\ell(r)}{\mathrm{d}r} - Bu_\ell(r)\right] \Big/ \left[a\frac{\mathrm{d}u_\ell}{\mathrm{d}r} - Bu_\ell\right]_{r=a}. \tag{20}$$

Once again we obtain a null result for $\eta(a) = 1$ by differentiating term by term and taking the limit term by term of the sum in equation (19) and using equation (5). The explanation for these paradoxes is that either (i) the expansion (7) or (ii) its derivative series, obtained by differentiating the individual terms of the expansion (7), is not uniformly convergent in the neighbourhood of the surface. Or they may be due to both (i) and (ii). This difficulty associated with expansion (7) has been known for many years [5, 20]. We note that the possibility of the interchange of the operations $\lim_{r\to a^-}$ and $\sum_\lambda$ in equation (12) has been studied [42].

3. The Hilbert–Schmidt theorem formulation of the R-matrix theory

Let us rewrite equation (3) in an integral form

$$u_\ell(r) = \phi_\ell(r) + (k^2 - \kappa^2)\int_0^a K_\ell(r, r')u_\ell(r')\,\mathrm{d}r' \tag{21}$$

with

$$K_\ell(r, r') = -\begin{cases} \tilde{X}_\ell(r)\tilde{Y}_\ell(r') & r \leqslant r' \\ \tilde{Y}_\ell(r)\tilde{X}_\ell(r') & r' \leqslant r \end{cases} \tag{22}$$

where $\tilde{X}_\ell(r)$ and $\tilde{Y}_\ell(r)$ are regular and irregular solutions, respectively, of the following equation

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2} + \left[\frac{2\mu V(r)}{\hbar^2} + \frac{\ell(\ell+1)}{r^2}\right]\psi = \kappa^2\psi \tag{23}$$

and satisfy the following conditions

$$\begin{aligned} &\tilde{X}_\ell(0) = 0 \\ &\frac{a}{\tilde{Y}_\ell(a)}\left(\frac{\mathrm{d}\tilde{Y}_\ell}{\mathrm{d}r}\right)_{r=a} = B \end{aligned} \tag{24}$$

and

$$\frac{\mathrm{d}\tilde{Y}_\ell(r)}{\mathrm{d}r}\tilde{X}_\ell(r) - \frac{\mathrm{d}\tilde{X}_\ell(r)}{\mathrm{d}r}\tilde{Y}_\ell(r) = -1.$$

B is the same as one the introduced in equation (5). κ^2 is an energy independent constant satisfying a condition

$$\kappa^2 \neq k_\lambda^2 \qquad (\lambda = 1, 2, \ldots) \tag{25}$$

and $\phi_\ell(r)$ is related to $\tilde{X}_\ell(r)$ by

$$\phi_\ell(r) = \alpha\tilde{X}_\ell(r) \tag{26a}$$

where α is an energy-dependent constant given by

$$\alpha = \left[a\frac{\mathrm{d}u_\ell}{\mathrm{d}r} - Bu_\ell(r)\right]_{r=a} \Bigg/ \left[a\frac{\mathrm{d}\tilde{X}_\ell(r)}{\mathrm{d}r} - B\tilde{X}_\ell(r)\right]_{r=a}. \tag{26b}$$

The integral equation (21), which is not the Lippmann–Schwinger-type equation, was first introduced in [11] for the $\kappa^2 = 0, B = \infty$ case. Equation (21) has a unique solution, since

$$\int_0^a \int_0^a K_\ell^2(r, r')\,\mathrm{d}r\,\mathrm{d}r' < \infty$$

i.e. $K_\ell(r, r')$ is completely continuous and self-adjoint kernel [45]. Let $\gamma_\lambda(\lambda = 1, 2, \ldots)$ be eigenvalues of the Hermitian continuous kernel $K_\ell(r, r')$

$$u_\lambda^\ell(r) = \gamma_\lambda \int_0^a K_\ell(r, r')u_\lambda^\ell(r')\,\mathrm{d}r' \tag{27a}$$

with

$$\gamma_\lambda = k_\lambda^2 - \kappa^2. \tag{27b}$$

As it is well known, the eigenvalues γ_λ are real, and the functions $u_\ell(r)$ and $u_\lambda^\ell(r)$ are continuous. Due to the Hilbert–Schmidt theorem [45], the following expansion

$$\int_0^a K_\ell(r,r')u_\ell(r')\,\mathrm{d}r' = \sum_{\lambda=1}^{\infty} \tilde{c}_\lambda^\ell u_\lambda^\ell(r) \tag{28}$$

converges uniformly and absolutely over $0 \leqslant r \leqslant a$, and, if $k^2 \neq k_\lambda^2$, the unique solution $u_\ell(r)$ of the integral equation (21) appears in the following form of a series which is uniformly and absolutely convergent over $0 \leqslant r \leqslant a$ (by Schmidt's formula):

$$u_\ell(r)\left[a\frac{\mathrm{d}u_\ell}{\mathrm{d}r} - Bu_\ell\right]_{r=a}^{-1} = \frac{\tilde{X}_\ell(r)}{\left[a\frac{\mathrm{d}\tilde{X}_\ell(r)}{\mathrm{d}r} - B\tilde{X}_\ell(r)\right]_{r=a}} + \frac{k^2-\kappa^2}{a}\sum_{\lambda=1}^{\infty}\frac{u_\lambda^\ell(r)u_\lambda^\ell(a)}{(k_\lambda^2-\kappa^2)(k_\lambda^2-k^2)}. \tag{29}$$

If we now define

$$R^{(B)}(k^2) = R^{(B)}(\kappa^2) + \frac{(k^2-\kappa^2)}{a}\sum_{\lambda=1}^{\infty}\frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2-\kappa^2)(k_\lambda^2-k^2)} \tag{30}$$

where

$$R^{(B)}(\kappa^2) = \frac{\tilde{X}_\ell(a)}{\left[a\frac{\mathrm{d}\tilde{X}_\ell(r)}{\mathrm{d}r} - B\tilde{X}_\ell(r)\right]_{r=a}} \tag{31}$$

we find that $R^{(B)}(k^2)$ relates the amplitudes u_ℓ to its derivative on the boundary by the relation (13). Because the series (29) converges uniformly and absolutely, the following equation

$$\lim_{r\to a^-}\left[\sum_{\lambda=1}^{\infty}\frac{u_\lambda^\ell(r)u_\lambda^\ell(a)}{(k_\lambda^2-k^2)(k_\lambda^2-k^2)}\right] = \sum_{\lambda=1}^{\infty}\frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2-k^2)(k_\lambda^2-k^2)} \tag{32}$$

is valid [46], and hence the expansion (29) is free of difficulties encountered in the expansions given by equations (7) and (10). Series (29) can be also obtained from the standard Wigner's expansion (9) by separating the energy independent term $\tilde{u}_l(r,\kappa^2)$ in $\tilde{u}_l(r,k^2)$, equation (10), with κ^2 satisfying condition (25). Our derivation has shown that the dispersion expansion (30) converges absolutely, and exhibits the general energy dependence of the R-function. The expansion given by equation (29) is a main result of this paper. The proof of the absolute convergence of the series (30) in case $\kappa^2 = 0$ was given by Schiffer and Bargmann. Their proof is reproduced in [47].

4. Improving the convergence

In general, the R-function has an infinite number of pole terms. According to Courant's minimax considerations, if $V(r)$ is bounded, no k_λ^2 differs from the corresponding value of k_λ^2, $(k_\lambda^{(0)})^2$, for noninteracting case ($V(r) = 0$) by more than the bound [5]. Consequently, the general term of the series (11) for fixed k^2 behaves as $1/\lambda^2$ since $(k_\lambda^{(0)})^2 \propto \lambda^2$, while the general term of the series (30) behaves as $1/\lambda^4$ as $\lambda \to \infty$. For the case of the dispersion formula (11), truncation of the R-function by a finite number (N) of terms gives

$$R_N^{(B)} = \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2-k^2)}. \tag{33}$$

While for the case of the dispersion formula (30), we have

$$R_N^{(B)}(k^2) = R_0^{(N)} + \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2 - k^2)} \tag{34}$$

where

$$R_0^{(N)} = R^{(B)}(\kappa^2) - \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2 - \kappa^2)}. \tag{35}$$

The general method of improving the convergence is to separate and sum the slowly converging parts of the series [48]. An alternative approach leading to a smooothly convergent R-matrix was proposed in [43]. It is obvious that there are many possibilities to obtain a rapid convergence. For example, the expansion (30) can be represented in the form

$$\begin{aligned} R^{(B)}(k^2) = {} & R^{(B)}(\kappa^2) + \frac{k^2-\kappa^2}{(k_0^2-\kappa^2)}(R^{(B)}(k_0^2) - R^{(B)}(\kappa^2)) \\ & + \frac{(k^2-\kappa^2)(k^2-k_0^2)}{a}\sum_{\lambda=1}^{\infty}\frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2-\kappa^2)(k_\lambda^2-k^2)(k_\lambda^2-k_0^2)} \end{aligned} \tag{36}$$

where k_0^2 is an energy-independent constant ($k_0^2 \neq \kappa^2, k_0^2 \neq k_\lambda^2, \lambda = 1, 2, \ldots$). Expansion (36) converges much faster than (30) (the general term behaves as $1/\lambda^6$), and truncation of equation (36) by a finite number of terms gives

$$R_N^{(B)}(k^2) = \overset{\approx}{R}{}_0^{(N)} + k^2 R_1^{(N)} + \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(u_\ell^\lambda(a))^2}{k_\lambda^2 - k^2} \tag{37}$$

where

$$\overset{\approx}{R}{}_0^{(N)} = R^{(B)}(\kappa^2) - \frac{\kappa^2}{k_0^2-\kappa^2}(R^{(B)}(k_0^2) - R^{(B)}(\kappa^2)) + \frac{\kappa^2 - k_0^2 - k_\lambda^2}{a}\sum_{\lambda=1}^{N}\frac{(u_\ell^\lambda(a))^2}{(k_\lambda^2-\kappa^2)(k_\lambda^2-k_0^2)} \tag{38}$$

and

$$R_1^{(N)} = \frac{1}{k_0^2-\kappa^2}(R^{(B)}(k_0^2) - R^{(B)}(\kappa^2)) - \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(u_\ell^\lambda(a))^2}{(k_\lambda^2-\kappa^2)(k_\lambda^2-k_0^2)}. \tag{39}$$

However, for the case of equation (37), we have introduced an additional parameter $R_1^{(N)}$, and we do not expect a weak dependence of equation (37) on this.

To obtain a faster convergence, we introduce a trial potential $\tilde{V}(r)$ and remove the corresponding R-function $\tilde{R}^{(B)}(k^2)$ obtained with $\tilde{V}(r)$:

$$\tilde{R}^{(B)}(k^2) = \tilde{R}^{(B)}(\kappa^2) + \frac{k^2-\kappa^2}{a}\sum_{\lambda=1}^{\infty}\frac{(\tilde{u}_\lambda^\ell(a))^2}{(\tilde{k}_\lambda^2-\kappa^2)(\tilde{k}_\lambda^2-k^2)}. \tag{40}$$

For the case of the dispersion formula (11), this method has been used in many papers [13, 17, 20]. For the case of equation (30), we have

$$\begin{aligned} R^{(B)}(k^2) = {} & R^{(B)}(\kappa^2) + \tilde{R}^{(B)}(k^2) - \tilde{R}^{(B)}(\kappa^2) \\ & + \frac{k^2-\kappa^2}{a}\sum_{\lambda=1}^{\infty}\left(\frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2-\kappa^2)(k_\lambda^2-k^2)} - \frac{(\tilde{u}_\lambda^\ell(a))^2}{(\tilde{k}_\lambda^2-\kappa^2)(\tilde{k}_\lambda^2-k^2)}\right). \end{aligned} \tag{41}$$

It can be shown (see the appendix) that the general term of equation (41) behaves as $1/\lambda^6$ for any bound $\tilde{V}(r)$, and hence we expect a weak $\tilde{V}(r)$ dependence for the following approximation

$$R_N^{(B)}(k^2) = R_0^{(N)} + g_N(k^2) + \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(u_\lambda^\ell(a))^2}{k_\lambda^2 - k^2} \tag{42}$$

where

$$g_N(k^2) = \tilde{R}^{(B)}(k^2) - \tilde{R}_0^{(N)} - \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(\tilde{u}_\lambda^\ell(a))^2}{\tilde{k}_\lambda^2 - k^2} \tag{43}$$

$$\tilde{R}_0^{(N)} = \tilde{R}^{(B)}(\kappa^2) - \frac{1}{a}\sum_{\lambda=1}^{N}\frac{(\tilde{u}_\lambda^\ell(a))^2}{\tilde{k}_\lambda^2 - \kappa^2} \tag{44}$$

and $\tilde{u}_\lambda^\ell(r)$ are solutions of equation (4) with the trial potential $\tilde{V}(r)$. Note that the case of $\tilde{V}(r) = 0$ was considered in [11, 49]. For practical calculations of the R-matrix with the approximation (42) for an incident nucleon, it is possible to use a simple squared-well potential

$$\tilde{V}(r) = -\tilde{V}_0\theta(a - r) \tag{45}$$

where $\tilde{V}_0 = \frac{\hbar^2 K_0^2}{2\mu}$. The wavenumber K_0 is independent of the mass number A and is approximately the same for all nuclei ($K_0 \approx 1$ fm) [50].

5. Numerical test of the convergence

As an illustration of our method, we consider the case of a square-well potential for low-energy n–^{12}C interactions,

$$V(r) = -V_0\theta(a - r) \tag{46}$$

for which the R-function and its parameters are determined in explicit form [5]. We restrict our discussion to the S-wave interaction ($\ell = 0$). The low-energy parameters (the scattering length A, the effective radius r_0, and the binding energy ϵ of $\ell = 0, s = \frac{1}{2}$ state of ^{13}C) in the case of potential given by equation (1) are determined from the R-function $R(E)$ by the following formulae

$$A = a(1 - R(0)) \tag{47}$$

$$r_0 = 2a(1 - a/A + a^2/(3A^2) - \hbar^2 R'(0)/(2\mu A^2)) \tag{48}$$

$$1 + \chi_\epsilon a R(\epsilon) = 0 \tag{49}$$

where μ is the reduced mass,

$$R(0) = \tan(\chi a)/\chi a \qquad R(\epsilon) = \tan(\chi_\epsilon a)/(\chi_\epsilon a) \tag{50}$$

$$R'(0) = \frac{1}{2V_0}\left[\frac{1}{\cos^2(\chi a)} - R(0)\right] \tag{51}$$

and

$$\chi = \sqrt{2\mu V_0/\hbar^2} \qquad \chi_\epsilon = \sqrt{2\mu(V_0 + \epsilon)/\hbar^2}. \tag{52}$$

The parameters V_0 and a are taken as

$$V_0 = 34.997 \text{ MeV} \qquad a = 4.071 \text{ fm}. \tag{53}$$

These parameters correspond to the following values of the scattering length A, the effective radius r_0 and the binding energy ϵ of the $\ell = 0, s = \frac{1}{2}$ state of ^{13}C:

$$A = 6.140 \text{ fm} \qquad r_0 = 3.377 \text{ fm} \qquad \epsilon = -1.860 \text{ MeV} \tag{54}$$

which are in good agreement with low-energy parameters obtained in [51]

$$A = 6.140 \text{ fm} \qquad r_0 = 3.367 \text{ fm} \qquad \epsilon = -1.860 \text{ MeV}. \tag{55}$$

It is also necessary to mention the good agreement of the calculated values of the elastic cross section with experimental values [52] up to energies of the order of 2 MeV in the laboratory system.

We note that [51] uses a model with

$$V_0 = 41.3 \text{ MeV} \qquad a = 3.72 \text{ fm} \tag{56}$$

which corresponds to

$$A = 5.862 \text{ fm} \qquad r_0 = 3.128 \text{ fm} \qquad \epsilon = 1.880 \text{ MeV} \tag{57}$$

and leads to a low-energy cross section, which is about 8% smaller than experimental values.

For the potential (46) we have investigated the convergence of the two-particle low-energy parameters (A and r_0) to their exact values as a function of the number of pole terms in the expansion for the R-function using three different R-function expansions: (a) without background terms, dispersion formula (33), (b) with a constant background term, dispersion formula (34) and (c) with removal of the R-function generated from the trial potential $\tilde{V}(r) = 0$ (corresponding to the case of free motion) dispersion formula (42). Approximations (a) and (b) are the conventional methods used previously, while the proposed method with approximation (c) is new to the best of our knowledge.

In the calculation we used the following value of the boundary condition parameter B (equation (5))

$$B = -\sqrt{\frac{2\mu|\epsilon|}{\hbar^2}}a. \tag{58}$$

With approximations (a)–(c) for the R-function, we have calculated the scattering length A and the effective radius r_0. Our numerical calculations show that approximation (b) yields a much faster convergence than that with approximation (a). We note that parametrization with a constant background term (approximation (b)) was used for fitting of the $^{12}\text{C} + n$ scattering and reaction cross section in [53].

We also find that the removal of a term corresponding to the free motion in the R-function substantially improves the convergences (approximation (c)). Here the inclusion of only one pole term in the expansion yields the exact reproduction of the effective radius (relative error is about 0.01%), whereas 25 and 10 terms are required to obtain the effective radius within accuracies of $\sim$0.3% for approximations (a) and (b), respectively. It is important to note that this removal procedure does not introduce any additional parameters in comparison with approximation (b).

6. Summary and conclusions

Using the Hilbert–Schmidt theorem and the integral equation, equation (21), we have reformulated the R-function theory in terms of the expansion given by equation (29) which is uniformly and absolutely convergent for all values of $0 \leqslant r \leqslant a$. This expansion, equation (29), can be differentiated term by term in the neighbourhood of the surface. Our reformulation solves the existing formal problem of how to formulate the R-matrix theory

without the use of expansions which are not uniformly convergent. A possible method for improving the convergence of the R-function series is given when the series is truncated for practical applications.

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Appendix

In this appendix, we show that the general term of equation (41) behaves as $1/\lambda^6$. We rewrite equation (4) in a form of the Volterra integral equation

$$u_\lambda^\ell(r) = \phi_{0\lambda}^\ell(r) + \int_0^r \tilde{K}(r,r')u_\lambda^\ell(r')\,\mathrm{d}r' \tag{A1}$$

where

$$\tilde{K}(r,r') = [\chi_{0\lambda}^\ell(r)\phi_{0\lambda}^\ell(r') - \phi_{0\lambda}^\ell(r)\chi_{0\lambda}^\ell(r')]\omega(r') \tag{A2}$$

with

$$\omega(r) = \frac{2\mu}{\hbar^2}V(r) - [k_\lambda^2 - (k_\lambda^{(0)})^2].$$

$\phi_{0\lambda}^\ell$ in equation (A1) is a regular solution of the Schrödinger equation for the noninteracting case

$$-\frac{\mathrm{d}^2\phi_{0\lambda}^\ell}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2}\phi_{0\lambda}^\ell(r) = (k_\lambda^{(0)})^2\phi_{0\lambda}^\ell(r) \tag{A3}$$

satisfying the R-matrix boundary conditions (5) and the orthonormality conditions (6). $\chi_{0\lambda}^\ell$ in equation (A2) is the irregular solution of equation (A3)

$$\chi_{0\lambda}^\ell(r) = \phi_{0\lambda}^\ell(r)\int_0^r [\phi_{0\lambda}^\ell(x)]^{-2}\mathrm{d}x$$

and k_λ^2 is defined from the condition

$$\int_0^a \chi_{0\lambda}^\ell(r)\omega(r)u_\lambda^\ell(r)\,\mathrm{d}r = 0. \tag{A4}$$

For any bound and continuous $V(r)$, $\tilde{K}(r,r')$ is also continuous and bound, and hence the Neumann series (iteration series)

$$u_\lambda^\ell(r) = \sum_{p=0}^{\infty}(\tilde{K}^p\phi_{0\lambda}^\ell)(r) \tag{A5}$$

converges uniformly and absolutely over $0 \leqslant r \leqslant a$ [39], where $\tilde{K}^p$ is a product of the operators $\tilde{K}$ and the function $\tilde{K}(r,r')$ is the kernel of the linear integral operator $\tilde{K}$.

From equation (A5), we can obtain

$$\lim_{\lambda\to\infty} u_\lambda^\ell(a) = \phi_{0\lambda}^\ell(a) + \mathrm{O}\left(\frac{1}{\lambda^2}\right) \tag{A6}$$

and hence the general term of equation (41) behaves as $1/\lambda^6$ for any bound and continuous $V(r)$ and $\tilde{V}(r)$.

We note an important fact that we do not need 'smallness' of $V(r)$ for the convergence of the Neumann series, equation (A5), in contrast to the conventional perturbation expansion.

References

[1] Kapur P L and Peierls R 1938 *Proc. R. Soc.* A **166** 277
[2] Wigner E P 1946 *Phys. Rev.* **70** 15 606
[3] Wigner E P and Eisenbud L 1947 *Phys. Rev.* **72** 29
[4] Breit G and Bouricius W G 1949 *Phys. Rev.* **75** 1029
[5] Lane A M and Thomas R G 1958 *Rev. Mod. Phys.* **30** 257
[6] Bloch C 1957 *Nucl. Phys.* **4** 503
[7] Feshbach H and Lomon E L 1956 *Phys. Rev.* **102** 891
Feshbach H and Lomon E L 1964 *Ann. Phys., NY* **29** 19
[8] Kim Y E and Tubis A 1970 *Phys. Rev.* C **1** 414
Kim Y E and Tubis A 1970 *Phys. Rev.* C **2** 2118
Kim Y E and Tubis A 1973 *Phys. Rev. Lett.* **31** 952
[9] Efimov V N and Schulz H 1976 *Sov. J. Part. Nucl.* **7** 349
[10] Jaffe R L and Low F E 1979 *Phys. Rev.* D **19** 2105
[11] Abdurakhmanov A, Zubarev A L, Latipov A Sh and Nasyrov M 1987 *Sov. J. Nucl. Phys.* **46** 217
[12] Babenko V A, Petrov N M and Sitenko A G 1991 *Can. J. Phys.* **70** 252
[13] Buttle P J A 1967 *Phys. Rev.* **160** 719
[14] Barker F C, Hay H J and Treacy P B 1968 *Aust. J. Phys.* **21** 239
[15] Barker F C 1972 *Aust. J. Phys* **25** 341
Barker F C 1995 *Nucl. Phys.* A **588** 693
[16] Barker F C and Kajino T 1991 *Aust. J. Phys.* **44** 369
[17] Koonin S E, Tombrello T A and Fox G 1974 *Nucl. Phys.* A **220** 221
[18] Knox H D, Resler D A and Lane R O 1987 *Nucl. Phys.* A **466** 245
[19] Hale G M, Brown R E and Jarmie N 1987 *Phys. Rev. Lett.* **59** 763
[20] Burke P G and Robb W D 1975 *Adv. At. Mol. Phys.* **11** 143
[21] Berrington K A, Burke P G, Le Dourneu M, Robb W D, Taylor K T and Lan Vo Ky 1978 *Comput. Phys. Commun.* **14** 346
[22] Berrington K A, Burke P G, Butler K, Seaton M J, Storey P Y, Taylor K T and Yan Yu 1987 *J. Phys. B: At. Mol. Phys.* **20** 6379
[23] Lisini A, Burke P G and Hibbert A 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 3767
[24] Lan Vo Ky, Saraph H E, Eissner W, Liu Z W and Kelly H P 1992 *Phys. Rev.* A **46** 3945
[25] Schneider B 1975 *Chem. Phys. Lett.* **31** 237
[26] Schneider B 1975 *Phys. Rev.* A **11** 1957
[27] Burke P G, Mackey I and Shimamura I 1977 *J. Phys. B: At. Mol. Phys.* **10** 2497
[28] Schneider B I, LeDourneuf M and Burke P G 1979 *J. Phys. B: At. Mol. Phys.* **12** L365
[29] Schneider B I, LeDourneuf M and Vo Ky Lan 1979 *Phys. Rev. Lett.* **43** 1926
[30] Schneider B I 1983 *Electron–Atom and Electron–Molecule Collisions* ed J Hinze (New York: Plenum) p 121
[31] Burke P G and Noble C J 1986 *Comment. At. Mol. Phys.* **18** 181
[32] Lane A M and Robson D 1968 *Phys. Rev.* **178** 1715
[33] Oberoi R S and Nesbet R K 1973 *Phys. Rev.* A **8** 215
[34] Oberoi R S and Nesbet R K 1974 *Phys. Rev.* A **9** 2804
[35] Schlessinger L and Payne G L 1974 *Phys. Rev.* A **10** 1559
[36] Fano U and Lee C M 1973 *Phys. Rev. Lett.* **31** 1573
[37] Lee C M 1974 *Phys. Rev.* A **10** 584
[38] Nesbet R K 1980 *Variational Method in Electron–Atom Scattering Theory* (New York: Plenum)
[39] Sitenko A G 1990 *Theory of Nuclear Reactions* (Singapore: World Scientific)
[40] Aymar M, Greene C and Luc-Koenig E 1996 *Rev. Mod. Phys.* **68** 1015
[41] Szmytkowski R 1997 *J. Phys. A: Math. Gen.* **30** 4413
[42] Szmytkowski R and Hinze 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 761
Szmytkowski R and Hinze 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 3800 (erratum)
[43] Szmytkowski R 1998 *Phys. Lett.* A **23** 319
[44] Kiernan L M, Lee M K, Sonntag B F, Zimmerman P, Costello J T, Kennedy E T, Gray A and Lan Vo Ky 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** L181
[45] Vladimirov V S 1971 *Equation of Mathematical Physics* (New York: Dekker)
Kolmogorov A N and Fomin S V 1961 *Elements of the Theory of Functions and Functional Analysis* (New York: Graylock)
[46] Knopp K 1947 *Theory and Application of Infinite Series* (New York: Hefner)

[47] Wigner E 1951 *Ann. Math.* **53** 36
[48] Kantorovich L V and Krylov V I 1958 *Approximate Methods of Higher Analysis* (New York: Interscience)
[49] Babenko V A and Petrov N M 1987 *Sov. J. Nucl. Phys.* **45** 1004
[50] Blatt J M and Weisskopf V F 1963 *Theoretical Nuclear Physics* (New York: Wiley)
[51] Lane R O, Koshel R D and Monahan J E 1969 *Phys. Rev.* **188** 1618
[52] Fu C Y and Perey F G 1978 *At. Data Nucl. Data Tables* **22** 249
[53] Knox H D and Lane R O 1982 *Nucl. Phys.* A **378** 503