The Hilbert-Schmidt Theorem Formulation of the R-Matrix Theory

Yeong E. Kim and Alexander L. Zubarev
Department of Physics, Purdue University
West Lafayette, IN 47907

Abstract

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

I. Introduction

Since 1947, boundary condition methods (BCM) have played an important role for many quantum mechanical problems [1-37]. 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 wave functions and their derivatives 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, which is the inverse of the logarithmic derivative of the external channel wave function at the surface, was first introduced by Wigner and Eisenbud in 1947 [1]. A detailed account of the R-matrix theory of nuclear reactions is given in [3]. The P-matrix is the inverse of the R-matrix. The P-matrix formulation of nuclear reactions has not been used extensively except for the nucleon-nucleon scattering problem [5-10].

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 [3, 11-17] 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 [18]. The R-matrix code is a very powerful computation code [19, 20] for calculating electron-atom collisions and photoabsorption processes. For example, the inner-shell photoionization cross-sections calculated by the R-matrix code [21, 22] are in excellent agreement with the recent experimental measurements [38].

The R-matrix method for studying low-energy electron-molecule collisions was developed in [23-25]. It has been used to describe elastic scattering, electronic excitation, vibrational excitation [27] and dissociative attachment [29].

The R-matrix method is based upon expanding the total wave function \( \Psi \) for any energy in the internal region in terms of the complete set of eigenfunction \( X_\lambda \) of that region,

\[
\Psi = \sum_\lambda A_\lambda X_\lambda, \tag{1}
\]

where \( X_\lambda \) are defined by the equation

\[
HX_\lambda = E_\lambda X_\lambda, \tag{2}
\]

and satisfy certain R-matrix boundary conditions on the surface [3]. It is known that there is a formal problem with the wave function expansion used in the conventional approach for the R-matrix theory. Either the expansion given by Eq. (1) is not uniformly convergent in the neighborhood of the surface, or term-by-term differentiation of the expansion is not admissible [3,18]. To avoid these difficulties variational formalisms [30-36] were proposed with basis functions which do not satisfy the R-matrix boundary conditions.

The 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 II, we describe in some detail the conventional formulation of R-function in terms of the expansion given by Eq. (1) and (2). In Section III, 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 IV, we discuss methods of improving the convergence of the R-function series when it is truncated for practical applications. A summary and conclusions are given in Section V.

II. 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 wave function \( u_\ell(r) \) in the interior region \( 0 \leq r \leq a \) satisfies the Schrödinger equation

\[
-\frac{d^2 u_\ell}{dr^2} + \left( \frac{2\mu V(r)}{\hbar^2} + \frac{\ell(\ell + 1)}{r^2} \right) u_\ell(r) = k^2 u_\ell(r),
\]

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

In the conventional theory [3, 18, 37], \( u_\ell(r) \) in the internal region \( 0 \leq r \leq a \) is expanded in terms of complete set of states \( u_\ell^\lambda(r) \) given within the region \( 0 \leq r \leq a \). These states are the solutions of the equation

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

satisfying the R-matrix boundary conditions

\[
u_\lambda^\ell(0) = 0, \quad \frac{a}{u_\lambda^\ell(a)} \frac{du_\ell^\lambda}{dr}(r=a) = B, \tag{5}\]

and the orthonormality conditions

\[
\int_0^a u_\lambda^\ell(r)u_\lambda^\ell(r)dr = \delta_{\lambda\lambda'} \tag{6}\]

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

\[
u_\ell(r) = \sum_{\lambda=1}^{\infty} c_\lambda^\ell u_\lambda^\ell(r), \quad (0 \leq r \leq a), \tag{7}\]
where

\[ c_\lambda^\ell = \int_0^a dr u_\ell(r) u_\lambda^\ell(r). \]  

(8)

As we show below, either (i) the expansion (7) does not converge uniformly, or (ii) term-by-term differentiation is not admissible [3, 18], or both (i) and (ii) may be applicable. From Green’s theorem [3, 18] and the boundary conditions (5), we find

\[ c_\lambda^\ell = \frac{1}{a} \left[ \frac{u_\lambda^\ell(a)}{k_\lambda^2 - k^2} \right] - Bu_\ell \big|_{r=a}. \]  

(9)

Substitution of Eq. (7) into Eq. (6) gives

\[ u_\ell(r) \left[ \frac{du_\ell}{dr} - Bu_\ell \right]^{-1} = \frac{1}{a} \sum_{\lambda=1}^\infty \frac{u_\lambda^\ell(r) u_\lambda^\ell(a)}{k_\lambda^2 - k^2}. \]  

(10)

If we now define

\[ R^{(B)} = \frac{1}{a} \sum_{\lambda=1}^\infty \frac{(u_\lambda^\ell(a))^2}{k_\lambda^2 - k^2}, \]  

(11)

and assume that

\[ \left[ \sum_{\lambda=1}^\infty \frac{u_\lambda^\ell(r) u_\lambda^\ell(a)}{k_\lambda^2 - k^2} \right]_{r=a} = \sum_{\lambda=1}^\infty \frac{(u_\lambda^\ell(a))^2}{k_\lambda^2 - k^2}, \]  

(12)

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

\[ R^{(B)} = u_\ell(a) \left[ \frac{du_\ell}{dr} - Bu_\ell \right]^{-1}. \]  

(13)

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

From the fact that

\[ G_\ell(r, r') = -\sum_{\lambda=1}^\infty \frac{u_\lambda^\ell(r) u_\lambda^\ell(r')}{k_\lambda^2 - k^2} \]  

(14a)

and

\[ G_\ell(r, r') = \begin{cases} u_\ell(r) Y_\ell(r'), & r \leq r', \\ u_\ell(r') Y_\ell(r), & r' \leq r, \end{cases} \]  

(14b)
with

\[ Y_\ell(r) = \frac{y_\ell(a)Bu_\ell(r)}{[a\frac{du_\ell}{dr} - Bu_\ell]_{r=a}} + y_\ell(r), \tag{15} \]

where \(y_\ell(r)\) is the irregular solution of Eq. (3) with boundary conditions \((\frac{du}{dr})_{r=a} = 0\), and \(u'_\ell y_\ell - y'_\ell u_\ell = 1\), it can be seen that Eqs. (7) and (10) can be obtained from the spectral decomposition, Eq. (14a), of Green’s function \(G_\ell(r, r')\). This bilinear series, Eq. (14a), converges in \(L^2(0 < r < a)\).

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

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

In this case, we can find from Eq. (9) that

\[ c_\lambda^\ell = \frac{u_\lambda^\ell(a)}{k^2 - k_\lambda^2} \left( \frac{du_\lambda^\ell}{dr} \right)_{r=a}, \tag{17} \]

and substitution of Eq. (17) into Eq. (7) gives

\[ \frac{u_\ell(r)}{u_\ell(a)} = \sum_{\lambda=1}^{\infty} \frac{u_\lambda^\ell(r)}{k^2 - k_\lambda^2} \left( \frac{du_\lambda^\ell}{dr} \right)_{r=a}. \tag{18} \]

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

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

\[ \eta(r) = \frac{1}{a} (a \frac{d}{dr} - B) \sum_{\lambda=1}^{\infty} \frac{u_\lambda^\ell(r) u_\lambda^\ell(a)}{k^2_{\lambda} - k^2}, \tag{19} \]

where

\[ \eta(r) = [a\frac{du_\ell}{dr} - Bu_\ell(r)]/[a\frac{du_\ell}{dr} - Bu_\ell]_{r=a}. \tag{20} \]

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 Eq. (19) and using Eq. (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 neighborhood of the surface. Or they may be due to both (i) and (ii). This difficulty associated with the expansion (7) has been known for many years [3,18].

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

Let us rewrite Eq. (3) in an integral form

\[ u_\ell(r) = \phi_\ell(r) + (k^2 - \kappa^2) \int_0^a K_\ell(r, r') u_\ell(r') dr', \]  

(21)

with

\[ K_\ell(r, r') = \begin{cases} \tilde{X}_\ell(r)\tilde{Y}_\ell(r'), & r \leq r', \\
\tilde{Y}_\ell(r)\tilde{X}_\ell(r'), & r' \leq r, \end{cases} \]  

(22)

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

\[ -\frac{d^2\psi}{dr^2} + \frac{2\mu V(r)}{\hbar^2} + \frac{\ell(\ell + 1)}{r^2} \psi = \kappa^2 \psi, \]  

(23)

and satisfy the following conditions

\[ \tilde{X}_\ell(0) = 0, \]

(24)

\[ \frac{a}{\tilde{Y}_\ell(a)} \left( \frac{d\tilde{Y}_\ell}{dr} \right)_{r=a} = B, \]

and

\[ \frac{d\tilde{Y}_\ell(r)}{dr} \tilde{X}_\ell(r) - \frac{d\tilde{X}_\ell(r)}{dr} \tilde{Y}_\ell(r) = -1. \]

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

\[ \kappa^2 \neq k_\lambda^2 \quad (\lambda = 1, 2, \ldots), \]  

(25)

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

\[ \phi_\ell(r) = \alpha \tilde{X}_\ell(r), \]  

(26a)
where $\alpha$ is an energy dependent constant given by

$$\alpha = [(a \frac{du_\ell}{dr} - Bu_\ell(r)]_{r=a}/[a \frac{d\tilde{X}_\ell(r)}{dr} - B\tilde{X}_\ell(r)]_{r=a}. \quad (26b)$$

The integral equation (21), which is not the Lippmann-Schwinger type equation, was first introduced in [9] for the $\kappa^2 = 0, B = \infty$ case. Eq. (21) has a unique solution, since

$$\int_0^a \int_0^a K_\ell^2(r, r') dr dr' < \infty,$$

i.e. $K_\ell(r, r')$ is completely continuous and self-adjoint kernel [39]. Let $\gamma_\lambda(\lambda = 1, 2, \ldots)$ be eigenvalues of the Hermitian continuous kernel $K_\ell(r, r')$

$$u_\lambda^\ell(r) = \gamma_\lambda \int_0^a K_\ell(r, r') u_\lambda^\ell(r') dr', \quad (27a)$$

with

$$\gamma_\lambda = k_\lambda^2 - \kappa^2. \quad (27b)$$

As it is well known, the eigenvalues $\gamma_\lambda$ are real, and the functions $u_\ell(r)$ and $u_\lambda^\ell(r)$ are continuous. Due to the Hilbert-Schmidt theorem [39], the following expansion

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

converges uniformly and absolutely over $0 \leq r \leq a$, 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 $0 \leq r \leq a$ (by Schmidt’s formula):

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

If we now define

$$R^{(B)}(k^2) = R^{(B)}(\kappa^2) + \frac{(k^2 - \kappa^2)}{a} \sum_{\lambda=1}^\infty \frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2 - \kappa^2)(k_\lambda^2 - k^2)}, \quad (30)$$
where
\[ R^{(B)}(\kappa^2) = \frac{\tilde{X}_\ell(a)}{[a\frac{d\tilde{X}_\ell(r)}{dr} - B\tilde{X}_\ell(r)]_{r=a}} \]  
we find that \( R^{(B)}(\kappa^2) \) relates the amplitudes \( u_\ell \) to its derivative on the boundary by the relation (13). Because the series (29) converges uniformly and absolutely, the following equation
\[ \sum_{\lambda=1}^{\infty} \frac{u^{\ell}_\lambda(r)u^{\ell}_\lambda(a)}{(k^2_\lambda - \kappa^2)(k^2_\lambda - k^2)} \bigg|_{r=a} = \sum_{\lambda=1}^{\infty} \frac{(u^{\ell}_\lambda(a))^2}{(k^2_\lambda - \kappa^2)(k^2_\lambda - k^2)} \]  
is valid [40], and hence the expansion (29) is free of difficulties encountered in the expansions given by Eqs. (7) and (10). Series (30) can be also obtained from the dispersion formula (11) by separating the energy independent term \( R^{(B)}(\kappa^2) \) in the R-function, Eq. (11), with \( \kappa^2 \) 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 Eq. (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 M. Schiffer and V. Bargmann. Their proof is reproduced in [41].

IV. 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 \( k^2_\lambda \) differs from the corresponding value of \( k^2_\lambda, (k^{(0)}_\lambda)^2 \), for noninteracting case \( (V(r) = 0) \) by more than the bound [3]. Consequently, the general term of the series (11) for fixed \( k^2 \) behaves as \( 1/\lambda^2 \) since \( (k^{(0)}_\lambda)^2 \propto \lambda^2 \), 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
\[ R^{(B)}_N = \frac{1}{a} \sum_{\lambda=1}^{N} \frac{(u^{\ell}_\lambda(a))^2}{(k^2_\lambda - k^2)} \]  
While for the case of the dispersion formula (30), we have
\[ R^{(B)}_N(k^2) = R^{(N)}_0 + \frac{1}{a} \sum_{\lambda=1}^{N} \frac{(u^{\ell}_\lambda(a))^2}{(k^2_\lambda - k^2)} \]  
where
\[ R^{(N)}_0 = R^{(B)}(\kappa^2) - \frac{1}{a} \sum_{\lambda=1}^{N} \frac{(u^{\ell}_\lambda(a))^2}{(k^2_\lambda - \kappa^2)} \]
The general method of improving the convergence is to separate and sum the slowly converging parts of the series [42]. It is obvious that there are many possibilities to obtain a rapid convergence. For example, the expansion (30) can be represented in the form

\[
R^{(B)}(k^2) = R^{(B)}(\kappa^2) + \frac{k^2 - \kappa^2}{(k_0^2 - \kappa^2)} (R^{(B)}(k_0^2) - R^{(B)}(\kappa^2)) + \frac{(k^2 - \kappa^2)(k^2 - k_0^2)}{a} \sum_{\lambda=1}^{\infty} \frac{(u^\lambda_{\ell}(a))^2}{(k_\lambda^2 - \kappa^2)(k_\lambda^2 - k_0^2)}.
\]

(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) (general term behaves as \(1/\lambda^6\)), and truncation of Eq. (36) by a finite number of terms gives

\[
R_{N}^{(B)}(k^2) \approx R_0 + k^2 R_{1}^{(N)} + \frac{1}{a} \sum_{\lambda=1}^{N} \frac{(u^\lambda_{\ell}(a))^2}{k_\lambda^2 - k^2}.
\]

(37)

where

\[
R_{0}^{(N)} = R^{(B)}(\kappa^2) - \frac{\kappa^2}{k_0^2 - \kappa^2} (R^{(B)}(k_0^2) - R^{(B)}(\kappa^2)) + \frac{k^2 - k_0^2 - k_\lambda^2}{a} \sum_{\lambda=1}^{N} \frac{(u^\lambda_{\ell}(a))^2}{(k_\lambda^2 - \kappa^2)(k_\lambda^2 - k_0^2)}.
\]

(38)

and

\[
R_{1}^{(N)} = \frac{1}{k_0^2 - \kappa^2} (R^{(B)}(k_0^2) - R^{(B)}(\kappa^2)) - \frac{1}{a} \sum_{\lambda=1}^{N} \frac{(u^\lambda_{\ell}(a))^2}{(k_\lambda^2 - \kappa^2)(k_\lambda^2 - k_0^2)}.
\]

(39)

However, for the case of Eq. (37), we have introduced an additional parameter \(R_{1}^{(N)}\), and we do not expect a weak dependence of Eq. (37) on this parameter \(R_{1}^{(N)}\).

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 \(\tilde{V}(r)\):

\[
\tilde{R}^{(B)}(k^2) = \tilde{R}^{(B)}(\kappa^2) + \frac{k^2 - \kappa^2}{a} \sum_{\lambda=1}^{\infty} \frac{(\tilde{u}^\lambda_{\ell}(a))^2}{(k_\lambda^2 - \kappa^2)(k_\lambda^2 - k_0^2)}.
\]

(40)
For the case of the dispersion formula (11), this method has been used in many papers [11, 15, 18]. For the case of Eq. (30), we have

\[ R(B) = R(B)(k^2) + \tilde{R}(B)(k^2) - \tilde{R}(B)(\kappa^2) \]

\[ + \frac{k^2 - \kappa^2}{a} \sum_{\lambda=1}^{\infty} \frac{(u_\lambda^\ell(a))^2}{(k_\lambda^2 - \kappa^2)(k_\lambda^2 - k^2)} - \frac{(\tilde{u}_\lambda^\ell(a))^2}{(\kappa_\lambda^2 - \kappa^2)(\kappa_\lambda^2 - k^2)} \].

(41)

It can be shown (see Appendix) that the general term of Eq. (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

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

(42)

where

\[ g_N(k^2) = \tilde{R}(B)(k^2) - \tilde{R}_0^{(N)} - \frac{1}{a} \sum_{\lambda=1}^{N} \frac{(\tilde{u}_\lambda^\ell(a))^2}{k_\lambda^2 - k^2}, \]

(43)

\[ \tilde{R}_0^{(N)} = \tilde{R}(B)(\kappa^2) - \frac{1}{a} \sum_{\lambda=1}^{N} \frac{(\tilde{u}_\lambda^\ell(a))^2}{k_\lambda^2 - \kappa^2}, \]

(44)

and \( \tilde{u}_\lambda^\ell(r) \) are solutions of Eq. (4) with the trial potential \( \tilde{V}(r) \). Note that the case of \( \tilde{V}(r) = 0 \) was considered in [9, 43]. 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

\[ \tilde{V}(r) = -V_0 \theta(a - r), \]

(45)

where \( V_0 = \frac{K_0^2 k_0^2}{2\mu} \). The wave number \( K_0 \) is independent of the mass number \( A \) and is approximately the same for all nuclei \( (K_0 \approx 1 fm) \) [44].

V. Summary and Conclusions

Using the Hilbert-Schmidt theorem and the integral equation, Eq. (21), we have reformulated the R-function theory in terms of the expansion given by Eq. (29) which is uniformly and absolutely convergent for all values of \( 0 \leq r \leq a \). This expansion, Eq. (29), can be differentiated term by term in the neighborhood 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.

Acknowledgments

One of the authors (A.L.Z.) acknowledges Drs. L.A.P. Balazs, M.S. Goldshtein and S. Khlebnikov for helpful discussions.
Appendix

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

$$u_\lambda^\ell(r) = \phi_0^\ell(r) + \int_0^r \tilde{K}(r, r')u_\lambda^\ell(r')dr',$$

(A.1)

where

$$\tilde{K}(r, r') = [\chi_0^\ell(r)\phi_0^\ell(r') - \phi_0^\ell(r)\chi_0^\ell(r')]\omega(r'),$$

(A.2)

with

$$\omega(r) = \frac{2\mu}{\hbar^2}V(r) - [k_\lambda^2 - (k_0^{(0)})^2].$$

(A.3)

$\phi_0^\ell$ in Eq. (A.1) is a regular solution of the Schrödinger equation for noninteracting case

$$-\frac{d^2\phi_0^\ell}{dr^2} + \frac{\ell(\ell + 1)}{r^2}\phi_0^\ell(r) = (k_\lambda^{(0)})^2\phi_0^\ell(r),$$

(A.4)

satisfying the R-matrix boundary conditions (5) and the orthonormality conditions (6). $\chi_0^\ell$ in Eq. (A.2) is the irregular solution of Eq. (A.3)

$$\chi_0^\ell(r) = \phi_0^\ell(r)\int_0^r [\phi_0^\ell(x)]^{-2}dx,$$

and $k_\lambda^2$ is defined from the condition

$$\int_0^a \chi_0^\ell(r)\omega(r)u_\lambda^\ell(r)dr = 0.$$

(A.4)

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

$$u_\lambda^\ell(r) = \sum_{p=0}^\infty (\tilde{K}^p\phi_0^\ell)(r)$$

(A.5)

converges uniformly and absolutely over $0 \leq r \leq a$ [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 Eq. (A.5), we can obtain

$$\lim_{\lambda \to \infty} u^\ell_\lambda(a) = \phi^\ell_{0\lambda}(a) + O\left(\frac{1}{\lambda^2}\right), \quad (A.6)$$

and hence the general term of Eq. (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, Eq. (A.5), in contrast to the conventional perturbation expansion.
References

1. E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947).
2. G. Breit and W. G. Bouricius, Phys. Rev. 75, 1029 (1949).
3. A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30, 257 (1958).
4. C. Bloch, Nucl. Phys. 4, 503 (1957).
5. H. Feshbach and E. L. Lomon, Phys. Rev. 102, 891 (1956); Ann. Phys. (N.Y.) 29, 19 (1964).
6. Y. E. Kim and A. Tubis, Phys. Rev. C1, 414 (1970); Phys. Rev. C2, 2118 (1970); Phys. Rev. Lett. 31, 952 (1973).
7. V. N. Efimov and H. Schulz, Sov. J. Part. Nucl. 7, 349 (1976).
8. R. L. Jaffe and F. E. Low, Phys. Rev. D19, 2105 (1979).
9. A. Abdurakhmanov, A. L. Zubarev, A. Sh. Latipov, and M. Nasyrov, Sov. J. Nucl. Phys. 46, 217 (1987).
10. V. A. Babenko, N. M. Petrov and A. G. Sitenko, Can. J. Phys. 70, 252 (1991).
11. P.J.A. Buttle, Phys. Rev. 160, 719 (1967).
12. F. C. Barker, H. J. Hay and P. B. Treacy, Aust. J. Phys. 21, 239 (1968).
13. F. C. Barker, Aust. J. Phys 25, 341 (1972); Nucl. Phys. A588, 693 (1995).
14. F. C. Barker and T. Kajino, Aust. J. Phys. 44, 369 (1991).
15. S. E. Koonin, T. A. Tombrello, and G. Fox, Nucl. Phys. A220, 221 (1974).
16. H. D. Knox, D. A. Resler and R. O. Lane, Nucl. Phys. A466, 245 (1987).
17. G. M. Hale, R. E. Brown, and N. Jarmie, Phys. Rev. Lett. 59, 763 (1987).
18. P. G. Burke and W. D. Robb, Adv. in Atomic and Molecular Phys. 11, 143 (1975).

19. K. A. Berrington, P. G. Burke, M. LeDournef, W. D. Robb, K. T. Taylor, and Lan Vo Ky, Comput. Phys. Commun. 14, 346 (1978).

20. K. A. Berrington, P. G. Burke, K. Butler, M. J. Seaton, P. Y. Storey, K. T. Taylor, and Yan Yu, J. Phys. B20, 6379 (1987).

21. A. Lisini, P. G. Burke, and A. Hilbert, J. Phys. B23, 3767 (1990).

22. Lan Vo Ky, N. E. Saraph, W. Eissner, Z. W. Liu, and H. P. Kelly, Phys. Rev. A46, 3945 (1992).

23. B. Schneider, Chem. Phys. Lett. 31, 237 (1975).

24. B. Schneider, Phys. Rev. A11, 1957 (1975).

25. P. G. Burke, I. Mackey, and I. Shimamura, J. Phys. B10, 2497 (1977).

26. B. I. Schneider, M. LeDourneuf, and P. G. Burke, J. Phys. B12, L365 (1979).

27. B. I. Schneider, M. LeDourneuf, and Vo Ky Lan, Phys. Rev. Lett. 43, 1926 (1979).

28. B. I. Schneider, Electron-Atom and Electron-Molecule Collisions, Ed. by J. Hinze (Plenum Publishing Corporation, 1983), p. 121.

29. P. G. Burke and C. J. Noble, Comments At. Mol. Phys. 18, 181 (1986).

30. A. M. Lane and D. Robson, Phys. Rev. 178, 1715 (1968).

31. R. S. Oberoi and R. K. Nesbet, Phys. Rev. A8, 2115 (1973).

32. R. S. Oberoi and R. K. Nesbet, Phys. Rev. A9, 2804 (1974).

33. L. Schlessinger and G. L. Payne, Phys. Rev. A10, 1559 (1974).

34. U. Fano and C. M. Lee, Phys. Rev. Lett. 31, 1573 (1973).

35. C. M. Lee, Phys. Rev. A10, 584 (1974).

36. R. K. Nesbet, Variational Method in Electron-Atom Scattering Theory (Plenum Press, New York, 1980).
37. A. G. Sitenko, *Theory of Nuclear Reactions* (World Scientific, Singapore, 1990).

38. L. M. Kiernan, M. K. Lee. B. F. Sonntag, P. Zimmerman, J. T. Costello, E. T. Kennedy, A. Gray, and Lan Vo Ky, J. Phys. B29, L21 (1996).

39. V. S. Vladimirov, *Equation of Mathematical Physics* (Marcel Dekker, Inc., New York, 1971); A.N. Kolmogorov and S.V. Fomin, *Elements of the Theory of Functions and Functional Analysis* (Graylock Press, Albany, N.Y., 1961).

40. K. Knopp, *Theory and Application of Infinite Series* (Hefner Publishing Company, New York 1947).

41. E. Wigner, Ann. Math. 53, 36 (1951).

42. L.V. Kantorovich and V.I. Krylov, *Approximate Methods of Higher Analysis* (Interscience Publisher, Inc., N.Y., 1958).

43. V.A. Babenko and N. M. Petrov, Sov. J. Nucl. Phys. 45, 1004 (1987).

44. J. M. Blatt and V.F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, N.Y., 1963).