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Regularization in the J-matrix method of scattering revisited

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Abstract

We present an alternative, but equivalent, approach to the regularization of the reference problem in the J-matrix method of scattering. After identifying the regular solution of the reference wave equation with the "sine-like" solution in the J-matrix approach we proceed by *direct integration* to find the expansion coefficients in an L^2 basis set that ensures a tridiagonal representation of the reference Hamiltonian. A differential equation in the energy is then deduced for these coefficients. The second independent solution of this equation, called the "cosine-like" solution, is derived by requiring it to pertain to the L^2 space. These requirements lead to solutions that are exactly identical to those obtained in the classical J-matrix approach. We find the present approach to be more direct and transparent than the classical *differential approach* of the J-matrix method.

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1. Introduction

The J-matrix is an algebraic method of quantum scattering with substantial success in atomic and nuclear physics [1]. Its structure in function space is endowed with formal and computational analogy to the R-matrix method in configuration space [2]. The method yields scattering information over a continuous range of energy for a model potential obtained by truncating the given scattering potential in a finite subset of an L^2 basis set, $\{\phi_n\}_{n=0}^{\infty}$. In other words, it is assumed that the scattering potential is short-range and is well represented by its matrix elements in the N-dimensional subspace spanned by $\{\phi_n\}_{n=0}^{N-1}$. The method was extended to multi-channel [3] as well as relativistic scattering [4]. For a large class of problems that model realistic physical systems, the Hamiltonian could be written as the sum of two components: $H = H_\infty + V$ where H_∞ is the free Hamiltonian. The potential can be written as $V = V_0 + \tilde{V}$ where $\tilde{V}$ is the short range part of the scattering potential while V_0 is the part of the potential that, when added to H_∞, gives the "reference Hamiltonian" $H_0 = H_\infty + V_0$ which, most importantly, admits an analytic solution. The exact analytical solvability of the reference wave equation is the main criterion behind the selective choice of the part of the potential, V_0, which could be included in H_0. The basis $\{\phi_n\}_{n=0}^{\infty}$ is chosen such that it gives a tridiagonal matrix representation of the reference wave operator $J = H_0 - E$. The analytic part of the J-matrix approach is, thus, limited to finding the asymptotic solutions of the reference H_0-problem defined by $H_0|\chi\rangle = E|\chi\rangle$. The solution to this problem is of fundamental importance since it will be the carrier of scattering information generated by the scattering potential $\tilde{V}$ and transmitted asymptotically by this solution.

Typically, the realization of H_0 in configuration space is given by a second order differential operator. Therefore, the reference H_0-problem has two independent solutions. Both behave asymptotically as free particles. That is, they have sinusoidal behavior as sine-like and cosine-like solutions. However, one of these two solutions is singular (irregular); typically, around the origin of configuration space. The regularization of the singular

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solution is of prime importance in the J-matrix approach, which deals only with square integrable function space. These two independent solutions are essential in scattering calculations where they are augmented by the contribution of the scattering potential $\tilde{V}$ to give the phase shift [5]. The regular solution of the reference problem, $\chi_{\sin}$, could be written as a linear combination of the basis elements $\chi_{\sin}(\vec{r},E)=\sum_n s_n(E)\phi_n(\vec{r})$. The expansion coefficients $\{s_n\}_{n=0}^{\infty}$ are written in terms of orthogonal polynomials that satisfy a three term recursion relation resulting from the matrix representation of the reference wave equation $\sum_{m=n,n\pm1} J_{nm}s_m=0$. Subsequently, we show that these sine-like expansion coefficients satisfy a second order linear differential equation in the energy. Hence, we look for another independent set of solutions to this equation; called $\{c_n(E)\}_{n=0}^{\infty}$. However, we find out that these expansion coefficients satisfy the same three-term recursion relation except for the initial relation ($n=0$). That is, $\sum_m J_{nm}c_m=\gamma\delta_{n0}$, where γ is a real energy dependent regularization constant. Therefore, the corresponding wavefunction, $\chi_{\cos}(\vec{r},E)=\sum_n c_n(E)\phi_n(\vec{r})$, satisfies a regularized non-homogeneous reference wave equation that reads

$$(H_0-E)|\chi_{\cos}\rangle=\gamma(E)|\tilde{\phi}_0\rangle, \tag{1.1}$$

where $\tilde{\phi}_0$ is an element of the set $\{\tilde{\phi}_n\}_{n=0}^{\infty}$ which is orthogonal to $\{\phi_n\}_{n=0}^{\infty}$ (i.e., $\langle\phi_n|\tilde{\phi}_m\rangle=\langle\tilde{\phi}_n|\phi_m\rangle=\delta_{nm}$) and $\lim_{r\to\infty}\tilde{\phi}_0(r)=0$.

In Section 2, we consider the three-dimensional problem with spherical symmetry where the reference Hamiltonian is the partial ℓ-wave free Hamiltonian. We take advantage of a recently obtained integral formula [6] to calculate the sine-like expansion coefficients $\{s_n(E)\}_{n=0}^{\infty}$. This is a direct integration approach, which differs from the differential approach of the original J-matrix method. We then obtain a second order differential equation in the energy satisfied by $s_n(E)$. The second independent solution of this equation is identified with the expansion coefficients $\{c_n\}_{n=0}^{\infty}$ of the "regularized" cosine-like wavefunction. We show that this wavefunction satisfies the regularized reference wave equation (1.1) and has the correct asymptotic behavior. Finally, in Section 3, we summarize our findings and discuss the results.

2. Solution to the reference problem

The time-independent radial Schrödinger equation for a scalar particle in the field of a central potential $V(r)$ reads as follows

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{2r^2}+V(r)-E\right]\psi_\ell(r,E)=0, \tag{2.1}$$

where ℓ is the angular momentum quantum number and we have used the atomic units $\hbar=m=1$. Now, we assume that the range of the potential is finite and thus take the reference Hamiltonian H_0 to be the free kinetic energy operator, $H_0=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{2r}$. Therefore, the wave equation that defines the reference problem is

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{2r^2}-E\right]\chi^\ell(r,E)=J\chi^\ell(r,E)=0, \tag{2.2}$$

where J defines the J-matrix operator (H_0-E). The two independent scattering solutions (for $E>0$) of this equation which are also energy eigenfunctions of H_0, could be found in most standard textbooks on quantum mechanics [7]. They are written in terms of the spherical Bessel and Neumann functions as follows:

$$\chi^\ell_{\text{reg}}(r,E)=\frac{2}{\sqrt{\pi}}(kr)j_\ell(kr), \tag{2.3a}$$

$$\chi^\ell_{\text{irr}}(r,E)=\frac{2}{\sqrt{\pi}}(kr)n_\ell(kr), \tag{2.3b}$$

where $k=\sqrt{2E}$. The regular solution is energy-normalized, $\langle\chi^\ell_{\text{reg}}|\chi'^\ell_{\text{reg}}\rangle=\delta(k-k')$, whereas the irregular solution is not square integrable (with respect to the integration measure, dr). Near the origin they behave as $\chi^\ell_{\text{reg}}\to r^{\ell+1}$ and $\chi^\ell_{\text{irr}}\to r^{-\ell}$. On the other hand, asymptotically ($r\to\infty$) they are sinusoidal: $\chi^\ell_{\text{reg}}\to\frac{2}{\sqrt{\pi}}\sin(kr-\pi\ell/2)$ and $\chi^\ell_{\text{irr}}\to-\frac{2}{\sqrt{\pi}}\cos(kr-\pi\ell/2)$. Now, we look for a complete L^2 basis functions, $\{\phi_n\}_{n=0}^{\infty}$, that could also support an infinite tridiagonal matrix representation for the reference wave operator $J=H_0-E$. One such basis which is compatible with χ^ℓ_{reg} (i.e., defined in the same range $r\in[0,\infty]$, behaves at the origin as $r^{\ell+1}$, and square integrable) is [1]

$$\phi^\ell_n(r)=(\lambda r)^{\ell+1}e^{-\lambda r/2}L^\nu_n(\lambda r), \tag{2.4}$$

where $L^\nu_n(x)$ is the associated Laguerre polynomial of order n, $\nu>-1$, and λ is a positive basis scale parameter. Using the differential equation of the Laguerre polynomials [8] and their differential formula, $x\frac{d}{dx}L^\nu_n=nL^\nu_n-(n+\nu)L^\nu_{n-1}$, we can write

$$\begin{aligned}(H_0-E)\left|\phi^\ell_n\right\rangle=&\left[\frac{n}{2r}\left(\lambda+\frac{\nu-2\ell-1}{r}\right)\right.\\&\left.+\lambda\frac{\ell+1}{2r}-\frac{\lambda^2}{8}-E\right]\left|\phi^\ell_n\right\rangle\\&+\frac{n+\nu}{2r^2}(2\ell+1-\nu)\left|\phi^\ell_{n-1}\right\rangle.\end{aligned} \tag{2.5}$$

If we project on the left by $\langle\phi^\ell_m|$ then the orthogonality relation for the Laguerre polynomials [8] dictates that a tridiagonal representation is obtained only if $\nu=2\ell+1$. Moreover, using the recursion relation of the Laguerre polynomials and their orthogonality property we obtain the following tridiagonal representation of the reference wave operator

$$\begin{aligned}J^\ell_{nm}(E)=&\left\langle\phi^\ell_n\middle|H_0-E\middle|\phi^\ell_m\right\rangle\\=&\frac{\Gamma(n+2\ell+2)}{\lambda\Gamma(n+1)}\left(E+\lambda^2/8\right)\\&\times\left[-2(n+\ell+1)\frac{E-\lambda^2/8}{E+\lambda^2/8}\delta_{n,m}+n\delta_{n,m+1}\right.\\&\left.+(n+2\ell+2)\delta_{n,m-1}\right].\end{aligned} \tag{2.6}$$

Therefore, if we write

$$\chi_{\sin}^{\ell}(r,E) \equiv \chi_{\mathrm{reg}}^{\ell}(r,E) = \sum_{n=0}^{\infty} s_n^{\ell}(E)\phi_n^{\ell}(r). \tag{2.7}$$

Then the sine-like expansion coefficients, $\{s_n^\ell\}_{n=0}^\infty$, satisfy a three term recursion relation obtained from (2.6) as $\sum_m J_{nm}^\ell s_m^\ell = 0$, which reads

$$2(n+\ell+1)ys_n^\ell = ns_{n-1}^\ell + (n+2\ell+2)s_{n+1}^\ell, \tag{2.8}$$

where $y = \frac{E-\lambda^2/8}{E+\lambda^2/8} = \frac{\mu^2-1/4}{\mu^2+1/4} = \cos\theta$, $\mu = k/\lambda$, and $0 < \theta \leqslant \pi$. To transform (2.8) to the three term recursion relation of a familiar orthogonal polynomial we rewrite this recursion relation in terms of the polynomials $P_n^\ell(E) = [\Gamma(n+2\ell+2)/\Gamma(n+1)]s_n^\ell(E)$, we then obtain the more familiar recursion relation

$$2(n+\ell+1)yP_n^\ell = (n+2\ell+1)P_{n-1}^\ell + (n+1)P_{n+1}^\ell, \quad n = 1,2,\ldots, \tag{2.9a}$$

$$2(\ell+1)yP_0^\ell = P_1^\ell. \tag{2.9b}$$

The solutions of this recursion relation are unique modulo an arbitrary function of y which is independent of n. If we fix this arbitrariness by choosing the normalization $P_0(y) = 1$ then these will be the Gegenbauer polynomial $C_n^{\ell+1}(y)$ [8]. Thus, $\{s_n^\ell\}$ can now be determined modulo an arbitrary real function of the energy. At this point we divert from the traditional J-matrix approach which uses the recursion relation to derive the second order differential equation obeyed by $\{s_n^\ell\}$. Instead, we evaluate $\{s_n^\ell\}$ using the orthogonality property of the Laguerre polynomials in the integration of (2.7) giving

$$s_n^\ell(E) = \frac{\Gamma(n+1)}{\Gamma(n+2\ell+2)} \int_0^\infty x^\ell e^{-x/2} L_n^{2\ell+1}(x) \times \chi_{\mathrm{reg}}^\ell(x/\lambda, E)\,dx, \tag{2.10}$$

where $x = \lambda r$. Rewriting the wavefunction (2.3a) in terms of the Bessel function $J_{\ell+\frac{1}{2}}(z) = \sqrt{\frac{2z}{\pi}}\,j_\ell(z)$ and substituting in (2.10) we obtain

$$s_n^\ell(E) = \sqrt{2\mu}\frac{\Gamma(n+1)}{\Gamma(n+2\ell+2)} \int_0^\infty x^{\ell+\frac{1}{2}} e^{-x/2} L_n^{2\ell+1}(x) \times J_{\ell+\frac{1}{2}}(\mu x)\,dx. \tag{2.11}$$

This integral is not found in mathematical tables but has recently been evaluated by one of the authors in [6]. The result is

$$s_n^\ell(E) = \frac{1}{\sqrt{\pi}} 2^{\ell+1} \frac{\Gamma(n+1)\Gamma(\ell+1)}{\Gamma(n+2\ell+2)} (\sin\theta)^{\ell+1} C_n^{\ell+1}(\cos\theta). \tag{2.12}$$

Now, at this stage we would like to derive the differential equation obeyed by $\{s_n^\ell\}$. For this purpose we use the differential equation for the Gegenbauer polynomials, $C_n^\nu(y)$, and show that $s_n^\ell(E)$ satisfies the following second order differential equation

$$\left[(1-y^2)\frac{d^2}{dy^2} - y\frac{d}{dy} - \frac{\ell(\ell+1)}{1-y^2} + (n+\ell+1)^2\right]s_n^\ell(E) = 0. \tag{2.13}$$

Now, this differential equation is also obeyed by the cosine-like expansion coefficient, $c_n^\ell(E)$, of the second independent solution of the J-matrix problem. Thus we are led to seek a second independent solution for this equation. Therefore, this approach differs from the construction of the cosine-like solution in the original J-matrix approach, which is given in Appendix A. Now, using the fact that $y = \pm 1$ are regular singular points then Frobenius method dictates that the solution has the following form [9]

$$c_n^\ell(E) = (1-y)^\alpha (1+y)^\beta f_n^\ell(\alpha,\beta;y), \tag{2.14}$$

where α and β are real parameters such that $\beta > 0$ to prevent infrared divergence (at $E = 0$ where $y = -1$). It should be noted that the solution that simultaneously satisfies the recursion relation (2.8) and the differential equation (2.13) will be unique modulo an arbitrary factor which is independent of E and n. That is, it will only depend on the angular momentum ℓ and we refer to it as A_ℓ. Substituting (2.14) in place of $s_n^\ell(E)$ in Eq. (2.13) shows that $f_n^\ell(\alpha,\beta;y)$ satisfies the following differential equation

$$\begin{aligned}&(1-y^2)\frac{d^2 f_n^\ell}{dy^2} + 2\left[(\beta-\alpha) - y\left(\alpha+\beta+\frac{1}{2}\right)\right]\frac{df_n^\ell}{dy}\\ &\quad + \left\{\frac{2y}{1-y^2}\left[\left(\alpha-\frac{1}{4}\right)^2 - \left(\beta-\frac{1}{4}\right)^2\right]\right.\\ &\quad + \frac{2}{1-y^2}\left[\left(\alpha-\frac{1}{4}\right)^2 + \left(\beta-\frac{1}{4}\right)^2 - \frac{1}{2}\left(\ell+\frac{1}{2}\right)^2\right]\\ &\quad \left. + (n+\ell+1)^2 - (\alpha+\beta)^2\right\} f_n^\ell = 0\end{aligned} \tag{2.15a}$$

which can be identified with that of the hyper-geometric function ${}_2F_1(a,b;c;\frac{1-y}{2})$ [8]

$$(1-y^2)\frac{d^2F}{dy^2} + \left[-2c + (a+b+1)(1-y)\right]\frac{dF}{dy} - abF = 0, \tag{2.15b}$$

where F is the hypergeometric function. This identification will be valid provided that

$$\begin{aligned}c &= 2\alpha + \frac{1}{2},\\ a &= \alpha+\beta \pm (n+\ell+1),\\ b &= \alpha+\beta \mp (n+\ell+1),\end{aligned} \tag{2.16a}$$

$$(\ell+1/2)^2 = 2(\alpha-1/4)^2 + 2(\beta-1/4)^2. \tag{2.16b}$$

Additionally, we must impose the condition that either $\alpha = \beta$ or $\alpha+\beta = \frac{1}{2}$. Next, we will investigate these two cases separately. We refer to the resulting expansion coefficients that satisfy the recursion relation (2.8) for all n by $s_n^\ell(E)$. Others that also do, but only for $n \neq 0$, will be referred to as $c_n^\ell(E)$. Thus, the wavefunction (2.7) with the expansion coefficients $\{s_n^\ell\}$ satisfy the reference wave equation $(H_0 - E)|\chi\rangle = 0$ whereas that with $\{c_n^\ell\}$ does not. Nonetheless, the latter will be considered as the regularized version of the irregular solution in the sense of regularization defined in the introduction.

2.1. The case $\alpha=\beta$

Maintaining positivity of β, this case produces two solutions. One is valid only for S-wave ($\ell=0$) whereas the other is true for all values of the angular momentum ℓ. Hence, there will be two inequivalent solutions for $\ell=0$. For general ℓ, Eqs. (2.16a) and (2.16b) give

$$\alpha=\beta=\frac{1}{2}(\ell+1),\qquad a=-n,\qquad b=n+2\ell+2,\qquad c=\ell+\frac{3}{2}. \tag{2.17}$$

This is the regular solution (2.3a) which we have already found in (2.7) and (2.12) and called it $s_n^\ell(E)$. This can easily be seen by noting that ${}_2F_1(-n,n+2\ell+2;\ell+\frac{3}{2};\frac{1-y}{2})$ is proportional to $C_n^{\ell+1}(y)$ [10] whereas $(1-y)^\alpha(1+y)^\beta=(1-y^2)^{\frac{\ell+1}{2}}=(\sin\theta)^{\ell+1}$. However, for S-wave ($\ell=0$) there exists another independent special solution where,

$$\alpha=\beta=-\frac{1}{2}\ell=0,\qquad a=-b=-n-1,\qquad c=\frac{1}{2}, \tag{2.18}$$

corresponding to ${}_2F_1(-n-1,n+1;\frac{1}{2};\frac{1-y}{2})$, which is the Chebyshev polynomial of the first kind, $T_{n+1}(y)$ [8]. Therefore, the expansion coefficients of the reference wavefunction are

$$c_n^0(E)=\frac{A}{n+1}T_{n+1}(\cos\theta)=\frac{A}{n+1}\cos(n+1)\theta, \tag{2.19}$$

where A is an overall factor, which is independent of E and n. Now, this solution satisfies the three term recursion relation (2.8) with $\ell=0$, but not the initial relation (i.e., for $n=0$). That is why we called it $c_n^0(E)$ and not $s_n^0(E)$. In fact, one can easily show that it satisfies an inhomogeneous initial relation which reads as follows

$$2yc_0^0=2c_1^0+A. \tag{2.20}$$

This is a crucial point. As stated in the Introduction, it means that the associated regularized wave function, $\chi_{\cos}^\ell(r,E)=\sum_n c_n^\ell(E)\phi_n^\ell(r)$, with these expansion coefficients does not solve the reference wave equation $(H_0-E)|\chi\rangle=0$ since $\sum_m J_{nm}^\ell c_m^\ell\neq 0$. However due to the physical requirement that $\chi_{\cos}^\ell(r,E)$ should behave asymptotically in the same way as $\chi_{\text{irr}}^\ell(r,E)$, the initial relation is changed as expressed in Eq. (2.20) which implies that $\sum_m J_{nm}^0 c_m^0=-\frac{\lambda A}{2}(\mu^2+\frac{1}{4})\delta_{n0}$. This means that $\chi_{\cos}^\ell$ solves the following regularized inhomogeneous wave equation

$$(H_0-E)\big|\chi_{\cos}^0\big\rangle=-\frac{kA}{2\sin\theta}\big|\tilde{\phi}_0^0\big\rangle, \tag{2.21}$$

where $\tilde{\phi}_0^0(r)=\lambda e^{-\lambda r/2}$ and $\langle\phi_n^\ell|\tilde{\phi}_0^\ell\rangle=\delta_{n0}$. One can easily find the value of A to be $-2/\sqrt{\pi}$ by equating the asymptotic behavior of $\chi_{\cos}^\ell(r,E)$ with that of $\chi_{\text{irr}}^\ell(r,E)$.

2.2. The case $\alpha+\beta=\frac{1}{2}$

Again, maintaining positivity of β, this case gives two solutions as well. One is valid for all ℓ where Eqs. (2.16a) and (2.16b) give

$$\alpha=-\frac{1}{2}\ell,\qquad \beta=\frac{1}{2}(\ell+1),\qquad a=-n-\ell-\frac{1}{2},\qquad b=n+\ell+\frac{3}{2},\qquad c=-\ell+\frac{1}{2}, \tag{2.22}$$

corresponding to

$$\left(\cos\frac{\theta}{2}\right)^{\ell+1}\left(\sin\frac{\theta}{2}\right)^{-\ell}\times{}_2F_1\left(-n-\ell-\frac{1}{2},n+\ell+\frac{3}{2};-\ell+\frac{1}{2};\sin^2\frac{\theta}{2}\right). \tag{2.23}$$

This hypergeometric function is a nonterminating series because none of the first two arguments will ever be a negative integer. However, we can use the transformation [8],

$${}_2F_1(a,b;c;z)=(1-z)^{c-a-b}{}_2F_1(c-a,c-b;c;z), \tag{2.24}$$

to write it in the following alternative, but equivalent, form

$$(\sin\theta)^{-\ell}{}_2F_1\left(-n-2\ell-1,n+1;-\ell+\frac{1}{2};\sin^2\frac{\theta}{2}\right). \tag{2.25}$$

Now, this hypergeometric series is a finite polynomial of order $n+2\ell+1$ in $\sin^2\frac{\theta}{2}$. Using the fact that $c_n^\ell(E)=A_\ell[\Gamma(n+1)/\Gamma(n+2\ell+2)]P_n^\ell(E)$ we can, therefore, write

$$c_n^\ell(E)=A_\ell\frac{\Gamma(n+1)}{\Gamma(n+2\ell+2)}(\sin\theta)^{-\ell}\times{}_2F_1\left(-n-2\ell-1,n+1;-\ell+\frac{1}{2};\sin^2\frac{\theta}{2}\right), \tag{2.26}$$

where A_ℓ is an overall factor, which is independent of the energy E and the index n. One can verify that this solution satisfies the three-term recursion relation (2.8) for all ℓ but not the initial relation (when $n=0$). Instead, it satisfies the following inhomogeneous initial relation

$$2(\ell+1)yc_0^\ell=2(\ell+1)c_1^\ell+(2\ell+1)A_\ell/\big[\Gamma(2\ell+2)(\sin\theta)^\ell\big]. \tag{2.27}$$

The corresponding wavefunction does not satisfy the reference wave equation but, as expected, an inhomogeneous one that reads

$$(H_0-E)\big|\chi_{\cos}^\ell\big\rangle=-\left(\ell+\frac{1}{2}\right)A_\ell k(\sin\theta)^{-\ell-1}\big|\tilde{\phi}_0^\ell\big\rangle, \tag{2.28}$$

where now $\tilde{\phi}_0^\ell(r)=\frac{\lambda(\lambda r)^\ell}{\Gamma(2\ell+2)}e^{-\lambda r/2}$. There might be several ways to obtain the overall factor A_ℓ. A direct approach is to equate the asymptotic ($kr\to\infty$) expression of $\chi_{\text{irr}}^\ell(r,E)$ in Eq. (2.3b) to that of $\chi_{\cos}^\ell(r,E)$ with the expansion coefficients given by Eq. (2.26). In such an approach, one utilizes the asymptotic behavior of the Laguerre polynomials [8]. However, a simpler approach is to use the Green's function method shown in Appendix A. By comparing Eq. (A.1) to Eq. (2.28) we obtain $\gamma(E) = -(\ell + \frac{1}{2})A_\ell k(\sin\theta)^{-\ell-1}$ which when inserted in Eq. (A.4) gives $\gamma = -W/2\langle\chi_{\mathrm{reg}}|\tilde{\phi}_0\rangle$, where $W(E)$ is the Wronskian of the regular and irregular solutions [given by Eqs. (2.3a) and (2.3b)] of the reference wave equation. That is, $\gamma(E) = -W(E)/2s_0^\ell(E)$. Now, for our problem, which is defined by the reference wave equation (2.2) and solutions in (2.3), the Wronskian is $-\frac{4}{\pi}k$. Using this and the value of $s_0^\ell(E)$ given by Eq. (2.12) for $n = 0$ along with the fact that $\Gamma(2\ell + 2) = 2^{2\ell+1}\pi^{-\frac{1}{2}}\Gamma(\ell + \frac{3}{2})\Gamma(\ell + 1)$ we obtain $A_\ell = -\frac{1}{\pi}2^{\ell+1}\Gamma(\ell + \frac{1}{2})$. It is easy to verify that the S-wave solution obtained above in (2.19) is a special case of (2.26) with $\ell = 0$ and $A = A_0$. Now, similarly to the previous case, we also find another independent special solution for S-wave ($\ell = 0$) where,

$$\alpha = \frac{1}{2}, \qquad \beta = 0, \qquad a = -n - \frac{1}{2}, \qquad b = n + \frac{3}{2}, \qquad c = \frac{3}{2}, \tag{2.29}$$

corresponding to $(1 - y)^{\frac{1}{2}}{}_2F_1(-n - \frac{1}{2}, n + \frac{3}{2}; \frac{3}{2}; \frac{1-y}{2})$. Using the transformation (2.24) this could be rewritten as $(\sin\theta) \times {}_2F_1(-n, n + 2; \frac{3}{2}; \frac{1-y}{2})$. Alternatively, we could write it as $\frac{\sin\theta}{n+1}U_n(y)$, where $U_n(y)$ is the Chebyshev polynomial of the second kind [8]. Therefore, the expansion coefficients of the reference wavefunction in (2.7) are

$$s_n^0(E) = \frac{B\sin\theta}{n+1}U_n(\cos\theta) = \frac{B}{n+1}\sin(n+1)\theta, \tag{2.30}$$

where B is a factor, which is independent of E and n. Now, one can easily verify that this solution satisfies the three term recursion relation (2.8) with $\ell = 0$, as well as its initial relation. That is why it was referred to as $s_n^\ell(E)$. In fact, one can easily show that this solution is a special case of that in (2.12) with $\ell = 0$ and $B = 2/\sqrt{\pi}$.

3. Conclusion

Now, we collect our findings and give a brief summary of the results obtained above for the 3D spherically symmetric problem with finite range scattering potential, $\tilde{V}(r)$, and whose reference Hamiltonian, H_0, is the free kinetic energy operator. Two solutions were obtained as infinite expansion in the discrete square integrable basis (2.4). We identified one of them with the regular solution of the problem where the expansion coefficients are given by (2.12). The other is a regularized version of the irregular reference solution with expansion coefficients given by (2.26). These regularized reference wavefunctions are used in scattering calculations by writing the asymptotic solution to the full problem, $H = H_0 + \tilde{V}$, as

$$\lim_{r\to\infty}\psi(r,E) = \chi_-^\ell(r,E) + e^{2\mathrm{i}\delta^\ell(E)}\chi_+^\ell(r,E), \tag{3.1}$$

where $\chi_\pm^\ell(r,E) = \chi_{\cos}^\ell(r,E) \pm \mathrm{i}\chi_{\sin}^\ell(r,E)$ and $\delta^\ell(E)$ is the energy-dependent phase shift that contains the contribution of the short range scattering potential $\tilde{V}(r)$ for a given value of the angular momentum ℓ. One can calculate $\delta^\ell(E)$ using any convenient approach based on the chosen scattering method [1,3]. The above regularization scheme is to be compared with the usual J-matrix method of scattering (see Appendix A). It is believed that this alternative approach is more transparent but equivalent to the usual J-matrix method.

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Appendix A. Regularization in the J-matrix method

We have seen that one of the solutions of the wave equation (2.2) is regular $\chi_{\mathrm{reg}}(r,E)$ while the other one is irregular $\chi_{\mathrm{irr}}(r,E)$. In the original J-matrix approach [5] the solution to the reference Hamiltonian H_0 is accomplished as follows:

(1) We choose an L^2 basis set $\{\phi_n\}_{n=0}^\infty$ which ensures a tridiagonal representation for H_0.

(2) The sine-like solution is identified with the regular solution of the reference wave equation $(H_0 - E)\chi(r,E) = 0$. This solution $\chi_{\mathrm{reg}}(r,E)$ is then expanded in the L^2 basis functions whose coefficients $\{s_n(E)\}$ are shown to obey a three term recursion relation. A first order differential equation (in the energy) satisfied by $s_n(E)$ is obtained. This together with the three-term recursion relation gives a second order differential equation whose two independent solutions are $s_n(E)$ and $c_n(E)$.

(3) The irregular reference solution, $\chi_{\mathrm{irr}}(r,E)$, being singular at the origin cannot be expanded in an L^2 basis set. Thus a regularized cosine-like solution, $\chi_{\cos}$, is chosen so that it obeys an inhomogeneous differential equation $(H_0 - E)|\chi_{\cos}\rangle = \gamma(E)|\tilde{\phi}_0\rangle$, where $\gamma(E)$ is an energy dependent regularization parameter. With this requirement the constructed $\chi_{\cos}$ has the correct asymptotic behavior, is regular at the origin and its expansion coefficients $\{c_n(E)\}$ obey the same three term recursion relation as the $\{s_n(E)\}$ for $n > 0$ but not for $n = 0$. Thus, $\chi_{\cos}$ could be expanded in terms of the square integrable basis, $\{\phi_n\}_{n=0}^\infty$, as $|\chi_{\cos}\rangle = \sum_n c_n|\phi_n\rangle$.

Obviously, the above traditional approach could be generalized to make $\chi_{\cos}$ satisfy the following inhomogeneous equation

$$(H_0 - E)\chi_{\cos}(r,E) = \gamma(E)\tilde{\xi}(r), \tag{A.1}$$

where $\tilde{\xi}(r)$ is a regularizing function that belongs to the space spanned by $\{\tilde{\phi}_n\}$ such that $\lim_{r\to\infty}\tilde{\xi}(r) = 0$. For a given $\tilde{\xi}(r)$ the parameter γ is evaluated by matching $\chi_{\cos}$ and χ_{irr} at the boundary of configuration space. Applying the two-point Green function $G_0(r,r',E)$, which is formally defined as $G_0(r,r',E) = \langle r|(H_0 - E)^{-1}|r'\rangle$, on Eq. (A.1) one obtains [5]

$$\chi_{\cos}(r,E) = -\gamma\int_0^\infty G_0(r,r',E)\tilde{\xi}(r')\,dr' \tag{A.2}$$

with $G_0(r, r', E) = \frac{2}{W(E)} \chi_{reg}(r_<, E) \chi_{irr}(r_>, E)$, where $r_<$ ($r_>$) is the smaller (larger) of r and r' and $W(E)$ is the Wronskian of the two independent reference solutions χ_{reg} and χ_{irr} which is independent of r. Substituting this in Eq. (A.2) we get

$$\chi_{\cos}(r) = -\frac{2\gamma}{W(E)} \left[\chi_{irr}(r) \int_0^r \chi_{reg}(r') \tilde{\xi}(r')\, dr' + \chi_{reg}(r) \int_r^\infty \chi_{irr}(r') \tilde{\xi}(r')\, dr' \right]. \tag{A.3}$$

It is worth mentioning that (A.3) ensures the two boundary conditions imposed on the regularized solution $\chi_{\cos}$. That is, it is proportional to $\chi_{reg}(r)$ as $r \to 0$ and to $\chi_{irr}(r)$ as $r \to \infty$. Taking the limit as $r \to \infty$ (where $\chi_{\cos}$ equals χ_{irr}) we obtain

$$\gamma(E) = -W(E) \Big/ \left(2 \int_0^\infty \chi_{reg}(r', E) \tilde{\xi}(r')\, dr' \right). \tag{A.4}$$

For a given set of chosen regularization parameters, $\{b_n\}$, we can write $\tilde{\xi}(r) = \sum_n b_n \tilde{\phi}_n(r)$. Substituting this together with $\chi_{reg}(r, E) = \sum_n s_n(E) \phi_n(r)$ in Eq. (A.4) we obtain

$$\gamma(E) = -W(E) \Big/ \left(2 \sum_n b_n s_n(E) \right). \tag{A.5}$$

In the classic version of the J-matrix method [5], regularization is performed by choosing $b_n = \delta_{n0}$.

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