# The *J*-Matrix Method

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Editors

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## Recent Developments and Selected Applications

Foreword by H.A. Yamani and Eric J. Heller



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# Foreword

Although introduced 30 years ago, the $J$-matrix method has witnessed a resurgence of interest in the last few years. In fact, the interest never ceased, as some authors have found in this method an effective way of handling the continuous spectrum of scattering operators, in addition to other operators. The motivation behind the introduction of the $J$-matrix method will be presented in brief.

The introduction of fast computing machines enabled theorists to perform calculations, although approximate, in a conveniently short period of time. This made it possible to study varied scenarios and models, and the effects that different possible parameters have on the final results of such calculations. The first area of research that benefited from this opportunity was the structural calculation of atomic and nuclear systems. The Hamiltonian element of the system was set up as a matrix in a convenient, finite, bound-state-like basis. A matrix of larger size resulted in a better configuration interaction matrix that was subsequently diagonalized. The discrete energy eigenvalues thus obtained approximated the spectrum of the system, while the eigenfunctions approximated the wave function of the resulting discrete state. Structural theorists were delighted because they were able to obtain very accurate values for the lowest energy states of interest.

Of course, the result of diagonalization also gives information on the remaining discrete states, including those that lie in the energy continuum. The fact that the approximation yields 'discrete' scattering states could not be helped, since the Hamiltonian is represented by a finite matrix. The situation is worsened by the fact that the eigenfunctions of these "discrete" continuum states are bound-state-like, as all members of the basis set used in constructing the Hamiltonian have this property. This was deemed unnatural, and led theorists to believe that this data did not constitute information that was useful for the calculation of scattering. This belief almost put a stop to the application of basis-set techniques for the solving of scattering problems. However, a major turnaround occurred as a result of the work by Hazi and Taylor [1].

Hazi and Taylor took the natural step of asking whether a use could be made of the bound-state-like basis to describe resonances, which resemble bound states even though they are actually scattering states. This led to the "Stabilization method": real discrete energy eigenvalues closest to the resonance energy become stable as the parameters of the calculation are varied. This development rekindled confidence

among theorists for the belief that the discrete energy eigenvalues and eigenfunctions may indeed contain useful information about the continuous spectrum of the Hamiltonian.

The Reinhardt group at Harvard was in the meantime developing a computational scheme to extract scattering information from the Fredholm determinant [2]. For a given short range potential $V$, the Fredholm determinant $\mathcal{D}(z)$ is defined as:

$$\mathcal{D}(z) = \det\left(\frac{z - H}{z - H_0}\right),$$

with the phase of $\mathcal{D}(z)$ being the negative of the phase shift $\delta(E)$ in the limit $z \to E + i\varepsilon$. It also satisfies the dispersion relation

$$\mathcal{D}(z) = 1 + \int_0^\infty \frac{A(E)}{z - E} dE$$

where $\mathcal{D}(E + i\varepsilon) = d(E) - i\pi A(E)$, and the functions $d(E)$ and $A(E)$ are both real and analytic. Encouraged by the stabilization results, the group worked with the matrix representation of $H$ and $H_0$ in a finite $L^2$-basis set, $\{\phi_n\}_{n=0}^{N-1}$. Therefore, the Fredholm determinant has the approximate value

$$\mathcal{D}^{\text{approx}}(z) = \prod_{i=0}^{N-1}\left(\frac{z - E_i}{z - E_i^0}\right),$$

where $\{E_i\}_{i=0}^{N-1}$ and $\left\{E_i^0\right\}_{i=0}^{N-1}$ are the eigenvalues of the finite matrices $\tilde{H}$ and $\tilde{H}_0$, respectively. The above equation can be cast in the form

$$\mathcal{D}^{\text{approx}}(z) = 1 + \sum_{i=0}^{N-1} \frac{\Gamma_i}{z - E_i^0},$$

which resembles a quadrature approximation to the above dispersion relation with the set $\left\{E_i^0\right\}_{i=0}^{N-1}$ containing the abscissas. Furthermore, Schwartz observed that if the basis $\{\phi_n\}_{n=0}^{N-1}$ is a certain Laguerre functions, then the abscissas fall as the transformed zeros of an orthogonal polynomial with known properties [3]. These facts enabled the group to calculate $\mathcal{D}^{\text{approx}}(E + i\varepsilon)$ and obtain accurate scattering results.

This development added some analytical tools to the predominant numerical tools available for use in the $L^2$-Fredholm method. For instance, the discrete eigenfunction of the finite $N \times N$ Hamiltonian $H_0$ may now be written as a finite sum of $L^2$-basis, with the orthogonal polynomials as Fourier-like expansion coefficients:

$$|\psi_N(E)\rangle = B_N(E) \sum_{n=0}^{N-1} P_n(E)\,|\phi_n\rangle$$

where $P_n(E)$ is the orthogonal polynomial such that $P_N(E_i^0) = 0$.

Heller of the Reinhardt group, who was also studying ways of enhancing the $R$-matrix method of scattering, proposed a way to improve the accuracy of the $L^2$-Fredholm calculation. He first proposed that the exact sine-like solution of the reference Hamiltonian $H_0$ be expanded in the complete $L^2$-basis. This could formally be done since the Fourier-like expansion coefficients were obtainable, even analytically. Similar to the $R$-matrix method, but unlike the $L^2$ Fredholm method, this approach made it possible to take full account of the reference Hamiltonian $H_0$ by giving a full solution of the reference problem in the complete basis. Furthermore, in the spirit of the $R$-matrix method, Heller and Yamani proposed that the potential representation be limited to a finite subset of the complete basis. This is the basic idea behind the $J$-matrix method [4], so called because the matrix representation of the operator $J = H_0 - E$ in certain Laguerre or oscillator basis functions is tridiagonal (Jacobi).

The analogy with the $R$-matrix method [5] is strong. The language of the $R$-matrix in configuration space is translated for the $J$-matrix into the language of function space. The full model Hamiltonian and wavefunction are written for the $R$-matrix method and $J$-matrix method as follows, in their respective languages:

$$\tilde{H} = \begin{cases} H_0 + V(r) & r \le R \\ H_0 & r > R \end{cases} \quad \rightarrow \quad \tilde{H}_{nm} = \begin{cases} (H_0)_{nm} + V_{nm} & n, m \le N-1 \\ (H_0)_{nm} & n, m > N-1 \end{cases}$$

whereas in a pictorial representation it looks as follows

$$\tilde{H} - E \sim \left(\begin{array}{ccccc|ccccc} \times & \times & \times & \cdots & \times & 0 & & & & \\ \times & \times & \times & \cdots & \times & 0 & & 0 & & \\ \vdots & \vdots & \vdots & & \vdots & \vdots & & & & \\ \times & \times & \times & \cdots & \times & J_{N-1,N} & 0 & 0 & 0 & \cdots\ \cdots \\ \hline 0 & 0 & 0 & \cdots & J_{N,N-1} & J_{N,N} & J_{N+1,N+1} & & & \\ & & & 0 & & J_{N+1,N} & J_{N+1,N+1} & J_{N+1,N+2} & & 0 \\ & & 0 & & 0 & & J_{N+2,N+1} & J_{N+2,N+2} & J_{N+2,N+3} & \\ & & & & \vdots & & & \cdots & \cdots & \cdots \\ & & & & \vdots & & 0 & & \cdots & \cdots\ \cdots \end{array}\right)$$

If we expand the solution $\psi(E, r)$ in the complete basis as $\psi(E, r) = \sum_{n=0}^{\infty} f_n(E)\,\phi_n(r)$, then

$$\psi(E,r) = \begin{cases} \psi(E,r) & r \le R \\ \frac{1}{\sqrt{k}}\left[e^{-ikr} - S(E)e^{ikr}\right] & r > R \end{cases} \rightarrow$$
$$f_n = \begin{cases} f_n & n,m \le N-1 \\ \frac{1}{\sqrt{k}}\left[(c_n - is_n) - S(E)(c_n + is_n)\right] & n,m > N-1 \end{cases}$$

where $s_n$ and $c_n$ are the expansion coefficients of the sine-like and cosine-like solutions of the reference Hamiltonian in the complete $L^2$ basis. In both methods, the resulting scattering matrix $S(E)$ is exact for the approximate model Hamiltonian $\tilde{H}$. This contrasts with the use of variational schemes to solve the scattering problem, which basically seek an approximate solution to the exact Hamiltonian $H$. The latter methods sometimes lead to the existence of anomalous pseudo-resonance behavior of the calculated cross sections. This phenomenon is not present in $J$-matrix calculations [6].

An example of a closed form solution provided by the $J$-matrix method is the explicit result for the exact $S$-matrix of a truncated potential:

$$S(E) = \frac{(c_{N-1} - is_{N-1}) + g_{N-1,N-1}(E)J_{N-1,N}(E)(c_N - is_N)}{(c_{N-1} + is_{N-1}) + g_{N-1,N-1}(E)J_{N-1,N}(E)(c_N + is_N)}$$

Here $g_{N-1,N-1}(E)$ is the $(N-1,N-1)$ element of the inverse of the matrix representation of $(H-E)$ in the finite basis, and $J_{nm}(E) \equiv (H_0 - E)_{nm}$. Results show that $S(E)$ is a highly accurate approximation of the $S$-matrix of the exact Hamiltonian. Most notably, $S(E)$ has the following two desirable properties:

(a) $S(E)$ is a smooth function of $E$, even as it assumes the values of the eigenvalues $\{E_i\}_{i=0}^{N-1}$ or $\left\{E_i^0\right\}_{i=0}^{N-1}$. In fact, at the points $\{E_i\}_{i=0}^{N-1}$, $S(E)$ has the special value

$$S(E_i) = \left.\frac{c_N - is_N}{c_N + is_N}\right|_{E=E_i}$$

This is a noteworthy result, which states that the $S$-matrix (cross section, or phase shift) for the approximate Hamiltonian $\tilde{H}$ could be calculated exactly, at positive discrete energies, by knowing only the coefficients of the wavefunction of the reference Hamiltonian $H_0$ in the basis. Yamani and Abdelmonem took the set $\{S(E_i)\}_{i=0}^{N-1}$, representing the value of $S(E)$ on the real (scattering) energy axis, and analytically continued it to the lower complex energy plane to search for shallow resonances [7]. These are characterized by poles of $S(z)$ in the second sheet of the complex energy plane. The same authors showed that a similar, and slightly more complicated result, holds in the multi-channel case [7].

(b) The diagonalization of $H$ in the finite $L^2$ basis needs to be done only once to enable the calculation of $S(z)$ over the entire continuum range of energy.

The first application of the $J$-matrix method was in the Tempkin-Poet model of an S-wave e-H scattering analysis [8]. The target and incoming projectile are described on the same basis, resulting in a finite number of target channels. A six-state calculation was able to reproduce previous results using different theoretical methods, and the calculation improved when the finite basis was enlarged. Implicit in this model is the approximation of the target by a finite number of channels; some, if any, represent the bound states, while the rest represent the continuum of scattering states. This naturally leads to anomalous behavior of the scattering cross section when the scattering energy is increased, so that more discrete channels become "open." Of course, this should not be the case. The correction of this anomalous behavior is still an outstanding problem for the $J$-matrix method and for similar methods that approximate the target ionization region by a finite number of channels. Bray and Stelbovics showed that the anomalous behavior tends to disappear as the number of target channels is increased [9].

Another early application of the $J$-matrix method of scattering was carried out by Broad and Reinhardt, who calculated e-H$^-$ scattering cross-sections and accurately reproduced resonance positions [10].

Further developments in the $J$-matrix method ensued:

(1) The matrix elements of Green's function associated with the reference Hamiltonian $H_0$ were evaluated by Heller, showing the analogy to the configuration space result [6]:

$$G^0(r, r') = \tfrac{2}{k}\sin(kr_<)e^{ikr_>} \;\rightarrow\; G^0_{nm} = \langle\phi_n|\, G\,|\phi_m\rangle = \tfrac{2}{k}s_{n_<}(c_{n_>} + is_{n_>})$$

where $n_<$ ($n_>$) is the smaller (larger) of $n$ and $m$. Heller also showed that if the regular and irregular $J$-matrix solutions are written, respectively, as

$$|\psi_R(E)\rangle = \sum_n R_n(E)\,|\phi_n\rangle, \qquad |\psi_I(E)\rangle = \sum_n I_n(E)\,|\phi_n\rangle,$$

Green's function is then given as

$$G_{nm}(E) = \tfrac{2}{k}R_{n_<}(I_{n_>} + iR_{n_>})$$

(2) Yamani and Abdelmonem generalized these results to the multi-channel case. However, they adopted a different approach that cast the results in terms of the finite Green's function $g_{N-1,N-1}(E)$ and only considered quantities associated with $G^0(E)$ [11]. In so doing, they showed that the Lippman-Schwinger equation $T = V - VGV$ could be solved over a continuous range of energies, without re-diagonalization of matrices every time the energy is varied.

(3) Horodecki achieved a relativistic generalization of the $J$-matrix method [12]. This generalization was refined by Alhaidari et al. [13].

(4) Yamani et al. made an important generalization of the $J$-matrix method to any convenient $L^2$-basis, without any significant loss of the advantages provided by the method [14].
(5) Vanroose et al. [15] enhanced the method, especially in the treatment of long range potentials, by introducing additional terms in the three-term recursion relation that takes into account the asymptotic behavior of the potential.
(6) Alhaidari et al. [16] present an alternative, but equivalent, approach to the regularization of the reference problem in the $J$-matrix method. It is an integration approach, which was found to be more direct and transparent than the classical differential approach. They also developed the relativistic $J$-matrix method of scattering for spin $\frac{1}{2}$ Dirac projectile with position-dependent mass [17].

The contributions in the present volume are aimed at giving a brief account of recent developments, and some selected applications, of the method in atomic and nuclear physics:

In Part II, convergence issues are revisited by Igashove who makes a comprehensive study of the convergence of the Fourier expansion of the wavefunction in the oscillator basis. After investigating the effects of the regularization procedure on convergence, Broeckhove et al. propose an alternative regularization approach in the $J$-matrix method and demonstrate the resulting improvements. On the other hand, a method for the accurate evaluation of the $S$-matrix for multi-channel analytic and non-analytic potentials in complex $L^2$ bases is presented in the same Section by Yamani and Abdelmonem. Using the tools of the relativistic $J$-matrix, Alhaidari obtains analytic expressions for the scattering phase shift of separable potentials with Laguerre-type form factors. Shirokov and Zaytsev study an interesting problem that is best addressed in the language of the $J$-matrix. They show that non-local interaction models could result in "isolated bound states" embedded in the continuum with positive as well as negative energy.

In Part III, Knyr et al. use the $J$-matrix method as a universal approach for the description of the process involving the ionization of atoms. They succeed in addressing the difficult problem of correctly describing the continuous spectrum eigenfunctions in the scattering of three charged particles using the $J$-matrix method. Papp exploits the $J$-matrix structure of the Coulomb Green's matrix to solve the Faddeev-type integral equations of the three-body Coulomb problem. In the article by Yamani and Abdelmonem, three approximation methods are proposed that endow the complex scaling method with the ability to compute resonance partial widths for multi-channel problems.

In Part IV, Lurie and Shirokov give a review of their recent work on the three-body loosely-bound nuclear systems within the $J$-matrix approach with an extended oscillator basis. They apply their investigation to $^{11}$Li and $^{6}$He nuclei. Furthermore, Shirokov et al. construct the nucleon–nucleon interaction by means of the $J$-matrix version pertaining to inverse scattering theory, where they eliminate the problem of ambiguity of the interaction by postulating tridiagonal and quasi-tridiagonal forms of the potential matrix. In the same Section, Arickx et al. use their proposal of modifying the $J$-matrix method (to account for coupling to long range interactions)

to cluster descriptions of light nuclei. The method is applied to $^6$He and $^6$Be nuclei for scattering and reaction problems. Finally, in Part V, Johnson and Holder present a generalization of the density functional theory, which is widely used in chemical physics applications, using a theoretical framework whose structure parallels that of the $J$-matrix method.

It is the hope of the editors that this volume will provide the interested reader with enough material for him or her to appreciate the advantages of the $J$-matrix method, and to encourage its use and development into a viable method for theoretical calculation of nuclear and atomic systems.

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