The modified J-matrix method for short range potentials

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Abstract
We modify the J-matrix method for scattering to improve its convergence and
reduce the computational cost. Our method applies to the oscillator basis
J-matrix method. We distinguish three regions in the space of wavefunction
coefficients. In the asymptotic region the free-space boundary conditions
hold. In the far interaction region, semi-classical approximations to the
matrix elements reduce the Schrödinger equation to an inhomogeneous three-
term recurrence relation, and in the near-interaction region one has the full
Schrödinger matrix equation. We apply the modified J-matrix method to
scattering off a Yukawa potential. The examples show that the number of
matrix elements that need to be calculated is significantly smaller than that for
the J-matrix method.

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1. Introduction

When the partial wave expansion is used in quantum potential scattering, one solves the
Schrödinger equation with interaction $V(r)$ for positive energy E and angular momentum
l in order to derive the phase shifts $\delta_l(E)$ and determine the cross sections [1, 2]. A
number of methods reduce the calculation of phase shifts to a set of matrix equations by
introducing a square integrable basis [3–5]. In this paper we consider the J-matrix (JM) method,
developed in a series of papers [4, 6, 7], with applications in atomic and molecular physics
[8, 9]. A similar approach, referred to as the algebraic method by its authors, was developed in
nuclear physics [10–13] with applications to many-particle scattering and in particular cluster
systems [14–16].

As with any basis expansion method, convergence in terms of the size of the basis is
an essential aspect of the application of the method. Several approaches were suggested to
improve the convergence of the J-matrix method results [4, 14, 17]. All these approaches

are formulated on top of the J-matrix calculation, and thus require the computational cost of calculating the Hamiltonian matrix to a certain size.

We introduce modifications to the J-matrix method that significantly improve the convergence while reducing the size of the basis that is required. That is, only small Hamiltonian matrices are needed to calculate the phase shift. This is significant because usually the calculation of the interaction matrix elements constitutes most of the computational cost of the method. Our approach is to use semi-classical approximations for the matrix elements in the oscillator basis at large radial quantum number. This also simplifies the matrix equations and effectively reduces them to recurrence relations.

In the J-matrix method a basis must be chosen to express the expansion coefficients of the scattering functions and the Hamiltonian matrix. The basis has to have some specific properties for the J-matrix method to be applicable. The harmonic oscillator basis and the Coulomb basis are the well-known examples. In this paper we address only the oscillator basis J-matrix method. As it stands our approach cannot be extended to the Coulomb basis. We limit ourselves to a single-channel scattering problem. The extension to many-channel calculations is perhaps technically involved but straightforward in principle. We also limit ourselves to short range potentials in this paper. The extension to long range, Coulombic potentials is feasible, and is being studied at present.

In the final section of the paper we demonstrate the effectiveness of our approach with a number of examples. They are based on the Yukawa potential not only because it provides ample material for comparison, but also because it is a potential where convergence is an issue. We show that to achieve results at least as good or even better than those of the J-matrix method, the number of matrix elements needed in the modified J-matrix (MJM) method is at least an order of magnitude smaller. This implies a significant and worthwhile decrease in the size of the computations required to perform J-matrix scattering calculations.

2. The J-matrix method

A Schrödinger equation with a spherically symmetric, non-Coulombic potential,

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{l(l+1)}{r^2} \right] + V(r) - E \right\} \psi_l(r) = 0 \tag{1}$$

must have a solution that is matched asymptotically with the free-space Bessel and Neumann functions

$$\psi_l(r \to \infty) \to \sqrt{\frac{2}{\pi}} j_l(kr) - \tan \delta_l(k) \sqrt{\frac{2}{\pi}} n_l(kr). \tag{2}$$

This match of a solution in the interaction region, where the effect of the potential is felt, with the asymptotic reference states determines the phase shift at momentum $k = \sqrt{2mE/\hbar^2}$ corresponding to energy E. We use the traditional spherical Bessel and spherical Neumann function definitions [2, 18] with the delta-function normalization convention.

Many methods, such as the R-matrix method and most variational methods [3, 19], solve (1) by assuming that ψ_l can be expressed as

$$\psi_l(r) = \psi_l^I + \psi_l^B(kr) - \tan \delta_l(k) \psi_l^N(kr). \tag{3}$$

The component of the solution in the interaction region is expressed by an L_2 basis set expansion truncated at some large n

$$\psi_l^I(r) = \sum_n c_{nl}^I \phi_{nl} \qquad \psi_l^I(r \to \infty) \to 0 \tag{4}$$

while the asymptotic behaviour is built into the solution through the Bessel and Neumann terms

$$\psi_l^B(r \to \infty) \to \sqrt{\frac{2}{\pi}} j_l(kr) \qquad \psi_l^N(r \to \infty) \to \sqrt{\frac{2}{\pi}} n_l(kr). \tag{5}$$

The latter is regularized to remove the singular behaviour at the origin. This may be done with a straightforward cut-off or with more sophisticated procedures. The ansatz leads to an algebraic problem for the coefficients c_{nl}, involving 'bound–bound', 'bound–free' and 'free–free' matrix elements of the Hamiltonian. The calculation of these matrix elements constitutes the bulk of the computational effort.

The same approach can be used when the problem is expressed in basis states, in our case the radial oscillator eigenstates. The wavefunctions for these states, with oscillator length parameter b, are given by

$$\phi_{nl}(r) = (-1)^n N_{nl} \left(\frac{r}{b}\right)^l L_n^{l+1/2}\left(\left(\frac{r}{b}\right)^2\right) \exp\left\{-\frac{1}{2}\left(\frac{r}{b}\right)^2\right\}$$
$$N_{nl} = b^{-3/2}\sqrt{2n!/\Gamma(n+l+3/2)} \tag{6}$$

with $L_n^{l+1/2}$ the Laguerre polynomial, and N_{nl} the normalization coefficient.

The Schrödinger equation turns into a matrix equation

$$\sum_{m=0}^{\infty} \langle\phi_{nl}|T+V-E|\phi_{ml}\rangle c_{ml} = 0 \tag{7}$$

with a (non-square-summable) solution $(c_{nl})_n$ representing the (non-square-integrable) ψ_l. The coefficients must satisfy the condition, equivalent to (2),

$$c_{n\to\infty,l} \to a_{nl}^B - \tan\delta_l(k)a_{nl}^N. \tag{8}$$

The $\left(a_{nl}^B\right)_n$ are the basis coefficients of the Bessel free-space solution and solve the equation

$$\sum_{m=0}^{\infty} \langle\phi_{nl}|T-E|\phi_{ml}\rangle a_{ml}^B = 0. \tag{9}$$

The T operator is tridiagonal in the oscillator basis, so this equation is in effect a three-term recurrence relation. It can be solved explicitly [4, 7, 20] and one finds

$$a_{nl}^B(k,b) = N_{nl}b^{3/2}(kb)^l \exp\left(-\frac{1}{2}(kb)^2\right) L_n^{l+1/2}((kb)^2)$$
$$= \frac{2}{N_{nl}} \frac{b^{3/2}}{\Gamma\left(l+\frac{3}{2}\right)}(kb)^l \exp\left(-\frac{(kb)^2}{2}\right) {}_1F_1\left(-n, l+\frac{3}{2}; (kb)^2\right)$$
$$\to b\sqrt{2R_{nl}}j(kR_{nl}) \qquad \text{for} \quad n \to \infty \tag{10}$$

where the ${}_1F_1$ stands for the confluent hypergeometric function [21]. The $R_{nl} = b\sqrt{4n+2l+3}$ in the expression for the asymptotic behaviour are the oscillator turning points.

The Neumann solution cannot be directly expressed in the oscillator basis because of its singularity at the origin. A regularization procedure is required [7]. Instead of (9), one solves the equation

$$\sum_{m=0}^{\infty} \langle\phi_{nl}|T-E|\phi_{ml}\rangle a_{ml}^N = \beta\delta_{n,0} \tag{11}$$

subject to the condition that the asymptotic behaviour coincides with the Neumann function. The effect of the right-hand side is to remove the singularity, but this effect is localized near

the origin. For large r, and equivalently for large n, the regularized solution coincides with the Neumann function. The coefficient β fixes the normalization. The regularized solution can thus serve equally well as a reference state to determine the phase shift in formula (8). Again this is a three-term recurrence relation that can be solved analytically

$$
\begin{aligned}
a_{nl}^N(k, b) &= \frac{(-)^{l+1} N_{nl} b^{\frac{3}{2}}}{\Gamma\left(-l + \frac{1}{2}\right)} (kb)^{-l-1} \exp\left(-\frac{(kb)^2}{2}\right) {}_1F_1\left(-n - l - \frac{1}{2}, -l + \frac{1}{2}; (kb)^2\right) \\
&\rightarrow b\sqrt{2R_{nl}} n_l(kR_{nl}) \qquad \text{for} \quad n \rightarrow \infty.
\end{aligned} \tag{12}
$$

The R_{nl} in the asymptotic expression are as defined before. In the following section the asymptotic behaviour of the coefficients (10) and (12) will be exploited to compute the a coefficients numerically.

In the J-matrix method one assumes that some large N delimits the interaction region and that, in equation (7), potential matrix elements with basis states outside of this region may be neglected. In [4] it is shown that the corresponding scattering state has the structure

$$
c_{nl} = \begin{cases} c_{nl}^I + a_{nl}^B - \tan\delta_l(k) a_{nl}^N & n < N \\ a_{nl}^B - \tan\delta_l(k) a_{nl}^N & n \geqslant N \end{cases} \tag{13}
$$

i.e. with a (square integrable) interaction component $\left(c_{nl}^I\right)_n$ of only N coefficients. The boundary condition is incorporated directly into the solution. The resulting problem consists of $N + 1$ equations for $n = 0, 1, \ldots, N$ in the unknowns $\left\{c_{0l}^I, c_{1,l}^I, \ldots, c_{N-1l}^I, \tan\delta_l\right\}$

$$
\begin{aligned}
\sum_{m=0}^{N-1} \langle\phi_{nl}|T + V - E|\phi_{ml}\rangle c_{ml}^I &- \tan\delta_l(E)\left(\sum_{m=0}^{N+1} \langle\phi_{nl}|T + V - E|\phi_{ml}\rangle a_{ml}^N\right) \\
&= -\sum_{m=0}^{N+1} \langle\phi_{nl}|T + V - E|\phi_{ml}\rangle a_{ml}^B.
\end{aligned} \tag{14}
$$

Note that in (14) the coefficient in front of the $\tan\delta_l(E)$ and in the right-hand side does not really sum up to $N + 1$ in terms of the potential matrix elements. Indeed the J-matrix assumption is that $\langle n|V|m\rangle = 0$ for n or $m > N - 1$.

Convergence of the phase shift is achieved by extending the interaction region. This increases the computational cost of the calculation significantly because the number of potential matrix elements that is required is $N(N + 1)/2$. Also, the high-order matrix elements are harder to compute numerically because of the oscillatory behaviour in the high-order basis states.

3. The modified J-matrix method

We address the convergence problem by returning to the equation

$$
\langle\phi_{nl}|T + V - E|\psi_l\rangle = 0 \qquad \text{for all} \quad n \tag{15}
$$

for the scattering function ψ_l and distinguishing three regions in the oscillator representation space. In each region, the expansion coefficients c_{nl} of the scattering solution fit different equations. In the *near interaction region*, $0 \leqslant n < N_n$, the exact equations apply. In the *far interaction region*, $N_n \leqslant n < N_f$, we use semi-classical expressions for the expansion coefficients and potential matrix elements. And, as before, when $n \geqslant N_f$, the free-space situation applies. The use of semi-classical approximations for the oscillator matrix elements in the far interaction region is the new feature of our approach.

Consider for instance the expansion coefficients for a scattering state

$$\langle \phi_{nl} | \psi_l \rangle = \int_0^\infty r^2 \, \mathrm{d}r \, \phi_{nl}(r) \psi_l(r). \tag{16}$$

At large n, the oscillator state $\phi_{nl}(r)$ in the integrand is highly oscillatory. The value of such integrals is determined [22–24] by the contributions near the integration boundaries and around stationary phase points. In (16) this means that there are contributions near the origin, where the oscillator function can be approximated by

$$r\phi_{nl} \approx (-1)^n \frac{\sqrt{2}}{b} \sqrt{\frac{2K_{nl}}{\pi}} r j_l(K_{nl} r) \qquad \text{at} \quad r \approx 0 \tag{17}$$

with $K_{nl} = \sqrt{4n + 2l + 3}/b$. There are also contributions around the classical oscillator turning point $R_{nl} = b\sqrt{4n + 2l + 3}$, where the oscillator function is approximated by the airy function

$$r\phi_{nl}(r) \approx \frac{2}{b} \left(\frac{b^4}{2R_{nl}} \right)^{1/6} \mathrm{Ai}((r - R_{nl})(2R_{nl}/b^4)^{1/3}) \qquad \text{at} \quad r \approx R_{nl}. \tag{18}$$

Beyond the turning point the $\phi_{nl}(r)$ are negligible and do not contribute to the integral. These approximations can be derived from semi-classical arguments and a linearization of the oscillator potential near the origin and the turning point [25]. They can also be found directly in mathematical texts on the large n behaviour of the Laguerre functions [26]. Inserting the previous expressions in (16) leads to a two-term formula, for large n,

$$\langle \phi_{nl} | \psi_l \rangle \approx b\sqrt{2R_{nl}} \psi_l(R_{nl}) + (-1)^n b^{-1} \sqrt{2K_{nl}} \tilde{\psi}_l(K_{nl}). \tag{19}$$

The first term samples the wavefunction at the turning point R_{nl} in coordinate space; the second samples its Fourier–Bessel transform $\tilde{\psi}_l$ at the oscillator turning point in momentum space, K_{nl}. Depending on the support (i.e. the domain in which the function has non-negligible value) of ψ_l in coordinate space and in momentum space, one of the terms will dominate. For a scattering state the momentum support will be a limited area centred on the classical momentum k. At some n the K_{nl} will lie beyond that momentum range and the second term in (19) disappears. The expansion coefficients then coincide with the scattering function sampled at the oscillator turning point.

Similar asymptotic expansion arguments hold for the integrals that determine the potential matrix elements. When $n \neq m$ and n and m are large, the integrand in

$$\langle \phi_{nl} | V(r) | \phi_{ml} \rangle = \int_0^\infty \mathrm{d}r \, r^2 \phi_{nl}(r) V(r) \phi_{ml}(r) \tag{20}$$

oscillates very rapidly, because the product $\phi_{nl}(r)\phi_{ml}(r)$ has $n \times m$ nodes. In addition, the product of the oscillator functions does not have a stationary point. The most important contribution to the integral comes from the region near $r = 0$. For this reason it can be approximated using (17). One finds

$$\langle \phi_{nl} | V(r) | \phi_{ml} \rangle \approx (-1)^{n+m} \frac{\sqrt{K_{ml} K_{nl}}}{b^2} \int_0^\infty \mathrm{d}r \, r^2 j_l(K_{nl} r) V(r) j_l(K_{ml} r)$$

$$\approx (-1)^{n+m} V(K_{nl}, K_{ml}) \tag{21}$$

where K_{ml} and K_{nl} are the turning points in Fourier space, and $V(K_{nl}, K_{ml})$ denotes the integral and its prefactors.

We use these expressions to derive an approximation to (20) in the far interaction region, i.e. the region of oscillator space with large n, but where one still has non-negligible matrix elements. We start by applying the asymptotic formula (19) to the potential term in

$$\langle \phi_{nl} | T + V - E | \psi_l \rangle = 0 \tag{22}$$

and find

$$\langle \phi_{nl} | V \psi_l \rangle \approx b \sqrt{2R_{nl}} (V\psi_l)(R_{nl}) + (-1)^n b^{-1} \sqrt{2K_{nl}} (\widetilde{V\psi_l})(K_{nl}) \tag{23}$$

where ψ_l is an unknown scattering function with maximal momentum k_{max}. The first term is the product $V(r)\psi_l(r)$ sampled in the turning point R_{nl}. The second term is the convolution product of Fourier–Bessel transforms $\tilde{V}$ and $\tilde{\psi}_l$ sampled in K_{nl}.

In view of the arguments of the previous paragraph, further approximations can be made. The first term in expression (23) can be simplified, for large n, leading to

$$\langle \phi_{nl} | V \psi_l \rangle \approx V(R_{nl})c_{nl} + (-1)^n b^{-1} \sqrt{2K_{nl}} (\widetilde{V\psi_l})(K_{nl}). \tag{24}$$

Indeed, ψ_l is a scattering state and its asymptotic expansion coefficient is determined by the behaviour of $\psi_l(r)$ in turning point R_{nl} in coordinate space. Consequently, we can replace $b\sqrt{2R_{nl}}\psi_l(R_{nl})$ in the first term by c_{nl}. The transform of the product makes the second term more complicated. Using smoothing and averaging arguments [25], and taking into account that n is large and ψ_l is a scattering solution, the second term in (24) can be approximated by

$$(-1)^n b^{-1} \sqrt{2K_{nl}} (\widetilde{V\psi_l})(K_{nl}) \approx (-1)^n WV(K_{nl}, K_{0l}) \tag{25}$$

where W is an unknown depending on ψ_l only.

When we insert these approximations in (22) we obtain a modified recurrence relation

$$T_{nl,n-1l}c_{n-1l} + (T_{nl,nl} + V(R_{nl}) - E)c_{nl} + T_{nl,n+1l}c_{n+1l} = -(-1)^n WV(K_{nl}, K_{0l}) \tag{26}$$

with a source term. The source term can be constructed using the leading term of the $1/K_{nl}$ expansion

$$V(K_{nl}, K_{0l}) \sim K_{nl}^{-l+5/2}. \tag{27}$$

Because of the nature of the boundary conditions for (26), the full solution (see also (28)–(30)) is not sensitive to the precise form of the source term. Therefore in many situations the generic approximation above is sufficient.

To treat a scattering problem with the modified J-matrix method one must first solve the modified recurrence relation for the far interaction region and then solve the full matrix equation in the near interaction region. Equation (26) is a three-term recurrence relation with source term. A general solution can be found by combination of a solution $(b_{nl}^B)_n$ of the homogeneous equation with the Bessel boundary condition,

$$\begin{cases} T_{nl,n-1l}b_{n-1l}^B + (T_{nl,nl} + V(R_{nl}) - E)b_{nl}^B + T_{nl,n+1l}b_{n+1l}^B = 0 \\ b_{nl}^B \rightarrow a_{nl}^B \qquad \text{for} \quad n \rightarrow \infty \end{cases} \tag{28}$$

a solution $(b_{nl}^N)_n$ of the homogeneous equation with the Neumann boundary condition,

$$\begin{cases} T_{nl,n-1l}b_{n-1l}^N + (T_{nl,nl} + V(R_{nl}) - E)b_{nl}^N + T_{nl,n+1l}b_{n+1l}^N = 0 \\ b_{nl}^N \rightarrow a_{nl}^N \qquad \text{for} \quad n \rightarrow \infty \end{cases} \tag{29}$$

and a solution $(b_{nl}^S)_n$ of the inhomogeneous equation with the zero boundary condition

$$\begin{cases} T_{nl,n-1l}b_{n-1l}^S + (T_{nl,nl} + V(R_{nl}) - E)b_{nl}^S + T_{nl,n+1l}b_{n+1l}^S = -(-1)^n V(K_{nl}, K_{0l}) \\ b_{nl}^S \rightarrow 0 \qquad \text{for} \quad n \rightarrow \infty. \end{cases} \tag{30}$$

The full scattering state is represented by coefficients

$$c_{nl} = c_{nl}^I + b_{nl}^B - \tan \delta_l(k)b_{nl}^N + Wb_{nl}^S \tag{31}$$

where c_{nl}^I is limited to the near interaction region i.e. is zero when $n \geqslant N_n$. This state satisfies the equation in the far interaction region and asymptotic regions. The $N_n + 2$ unknowns of our

problem are $\left\{c_{0l}^I, c_{1,l}^I, \ldots, c_{N_n-1l}^I, \tan \delta_l, W\right\}$. They are determined by inserting (31) into the $N_n + 2$ linear equations derived from (22)

$$\sum_{m=0}^{N_n-1} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle c_{ml}^I - \tan \delta_l(E) \left(\sum_{m=0}^{\infty} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle b_{ml}^N\right)$$

$$+ W \left(\sum_{m=0}^{\infty} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle b_{ml}^S\right)$$

$$= -\sum_{m=0}^{\infty} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle b_{ml}^B. \tag{32}$$

The term in the right-hand side of (32) connected with the b_{ml}^B coefficients is essentially a bound–free matrix element for a modified Bessel wavefunction

$$\psi_l^B = \sum_{m=0}^{\infty} b_{ml}^B |\phi_{ml}\rangle. \tag{33}$$

Equation (28) defining this state expresses that

$$\langle \phi_{nl}|T + V - E|\psi_l^B\rangle \cong 0 \qquad \text{for} \quad n \quad \text{large.} \tag{34}$$

However, that does not hold for the small values of n that occur in (32). We need to evaluate the sum in (32) explicitly. Because the potential matrix elements decrease rapidly when $|n - m|$ gets large, we can truncate the sum at some M, provided we include at the very least the $n = m$ term. The same arguments hold for the b_{ml}^N and b_{ml}^S terms. This then leads to the final set of $N_n + 2$ equations for $n = 0, \ldots, N_n + 1$:

$$\sum_{m=0}^{N_n-1} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle c_{ml}^I - \tan \delta_l(E) \left(\sum_{m=0}^{M-1} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle b_{ml}^N\right)$$

$$+ W \left(\sum_{m=0}^{M-1} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle b_{ml}^S\right)$$

$$= -\sum_{m=0}^{M-1} \langle \phi_{nl}|T + V - E|\phi_{ml}\rangle b_{ml}^B. \tag{35}$$

To write down this set of equations, we need to calculate the $(N_n + 2) \times M$ matrix of $(T + V - E)$. Assuming that $M \geqslant N_n + 2$, and taking into account the symmetry of the square $(N_n + 2) \times (N_n + 2)$ submatrix, one finds that $(N_n + 2)(2M - N_n - 1)/2$ potential matrix elements have to be computed. The application of the method will be discussed in the following section.

4. Application of the method

In this section we consider the application of the modified J-matrix method, and how it differs from the J-matrix method. The discussion summarizes the experience gained in calculations with a number of potentials. The following section will present results of specific examples.

The JM computations consist of the following steps:

(1) Fix an oscillator basis by choosing a width parameter b. It should be of same order of magnitude as the range of the potential.

(2) Compute the coefficients a_{nl}^B and a_{nl}^N by solving equations (9) and (11), respectively. Use the asymptotic forms in (10) and (12), typically at $n = 10\,000$, to seed the backward recurrence in (9) and (11). This turns out to be more efficient than a direct evaluation of (10) and (12).

(3) Fix the size N of the interaction region and compute the $N(N + 1)/2$ potential matrix elements that occur in (14). In this paper we do this by direct numerical integration. For high n care must be taken to accommodate the oscillatory nature of the integrand.

(4) Solve equations (14) for the phase shift and derive the cross sections (partial, total, differential), one is interested in.

The key parameters in this scheme are the oscillator width b and the size of the interaction region N. One can increase the latter, and repeat steps 3 and 4 of the computation until no significant change is observed in the phase shift. This convergence is reached at different N when one uses different b-values. The b-value that achieves convergence for the smallest N is referred to as the optimum b. We always determine the optimum b for the $l = 0$ phase shift.

The MJM computations consist of the following steps:

(1) Fix the oscillator basis by choosing a width parameter b as before.

(2) Fix the size N_f of the far interaction region. Compute the coefficients b_{ml}^B, b_{ml}^N and b_{ml}^S by solving (28), (29) and (30), respectively. Again this is done by backward recurrence, seeding with the asymptotic expressions of (10) and (12) at $n = 10\,000$. Starting at $n = N_f$ the potential terms are included in the recurrence relations.

(3) Fix the size N_n of the near interaction region and the size M of the summation range of the bound–free matrix elements. Compute the $(N_n + 2)(2M - N_n - 1)/2$ potential matrix elements to set up equations (35).

(4) Solve equations (35) for the phase shift and derive the cross sections (partial, total, differential) of interest.

The parameters in the MJM scheme are b, N_f, N_n and M. Obviously the N_f is a key parameter. Calculations with successively larger N_f converge to a phase shift that may still depend on b, N_n and M. There is, however, a significant difference with the JM scheme. The computational cost of increasing N_f is negligible. Therefore, in step 2, we include the potential terms throughout the recurrence in (28), (29) and (30) (in effect $N_f = 10\,000$). Also, because we can extend the interaction region to such large N_f, the results become less sensitive to the choice of b, N_n and M. As a rule we try a few b-values, and that for which convergence is obtained with smallest M is referred to as the optimum b for the MJM scheme. We always determine the optimum b for the $l = 0$ phase shift.

The preceding exposition indicates that the relation between JM and MJM is not straightforward. The semi-classical approximation of oscillator matrix elements in MJM leads one to view MJM as an approximation to the JM method. However, precisely this approximation allows us to extend the interaction region in the MJM method way beyond the limit achievable in the JM, thereby improving on the convergence compared to the JM method.

5. Results

In this section we compare the scattering results, phase shifts and cross sections, for the JM and MJM methods. Our intention is to gauge the effectiveness of the modifications that we have introduced.

We have used the Yukawa potential

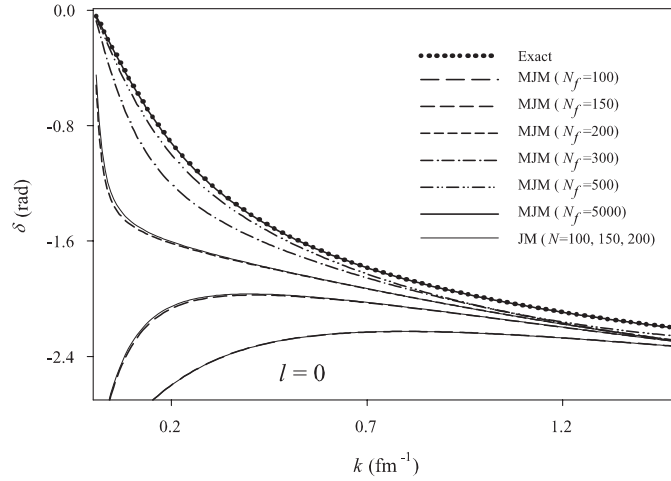$$V(r) = V_0 \frac{a}{r} \exp\left(-\frac{r}{a}\right)$$

Figure 1. Convergence of the MJM $l = 0$ phase shift for the Yukawa potential (36) of [28] in terms of the far interaction limit N_f; all calculations use $b = 0.051$ fm.

with depth V_0 and range a which is well known in quantum physical applications. We consider two different examples, both from a nuclear physics context. The first potential is taken from [28] corresponding to the ^3S neutron–proton interaction, that was considered to study variational methods for scattering. It has also been used to study the Born approximation [29]. The explicit form is

$$\begin{cases} V_0 = -53.8 \, \text{MeV} \\ a = 1.35 \times 10^{-13} \, \text{cm} = 1.35 \times \text{fm}. \end{cases} \quad (36)$$

The second Yukawa potential was used in [30] to fit phase shifts for nucleon–nucleon scattering and low-energy parameters, as well as some features of the deuteron. We consider only one specific case, the $^3P_2$ phase shift, that features very different parameters than those in the previous potential

$$\begin{cases} V_0 = -14\,250.0 \, \text{MeV} \\ a = 0.263\,157\,894 \, \text{fm}. \end{cases} \quad (37)$$

We also compare the JM and MJM results with the 'exact' phase shifts, obtained by the variable phase approximation of [27]. The latter are indistinguishable from those reported in [28, 30].

Figure 1 shows the $l = 0$ MJM phase shifts for the potential [28] at $b = 0.051$ fm, $N_n = 6$ and $M = 11$, for increasing size of the interaction region N_f. The progression towards the exact phase shift is evident. At $N_f = 5000$ the phase shift becomes indistinguishable from the exact.

Figure 1 also shows the JM phase shifts for $b = 0.051$ fm and $N = 100, 150, 200$. They are almost identical to the corresponding MJM phase shifts at $N_f = 100, 150, 200$. This indicates that the semi-classical approximation of oscillator matrix elements works well.

In figures 2 to 6 we compare MJM, JM and variable phase results for potential (36). For the JM method we have used the optimum $b = 0.28$ fm and usually show results for a number of N to give an idea of the convergence. For the MJM we have used its optimum $b = 0.051$ fm and $N_n = 6$, $M = 11$ and $N_f = 10\,000$. There is no issue of convergence here: even the smaller values for N_n and M yield phase shifts that are extremely close to the variable phase
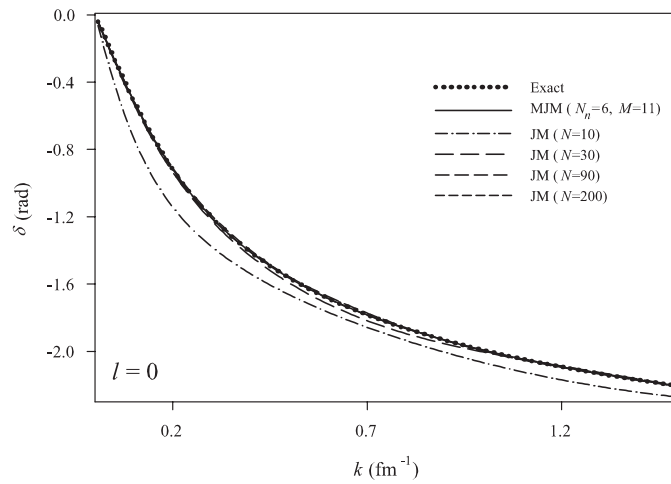
Figure 2. $l = 0$ phase shift for the Yukawa potential (36) of [28].
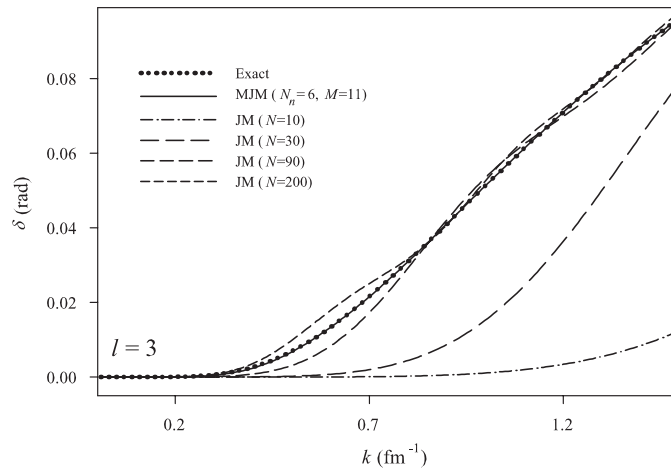

Figure 3. $l = 3$ phase shift for the Yukawa potential (36) of [28].

results. Figures 2 and 3 present the $l = 0$ and $l = 3$ phase shifts respectively, figures 4 and 5 the corresponding partial cross sections. Inspection reveals that for $l = 0$ the JM is nearing convergence at $N = 200$, but this is not the case for $l = 3$. Potentials that are singular at the origin have a matrix representation where the off-diagonal matrix elements drop to zero very slowly. This is the least favourable situation for the truncation to a square matrix. Therefore a Yukawa potential constitutes a stringent test case for the methods. The figures reveal that the MJM approach does achieve convergence, even though it requires the computation of only 60 potential matrix elements compared to 20 100 in the $N = 200$ JM calculation.

Figure 6 shows the differential cross section, calculated with all partial waves with $l = 0$ up to $l = 15$, for a selected, representative energy of $E = 45.0$ MeV taken from [28]. The figure demonstrates again that the MJM performs well, especially when one takes into account the number of matrix elements required. Even for small angles, the MJM, with a limited
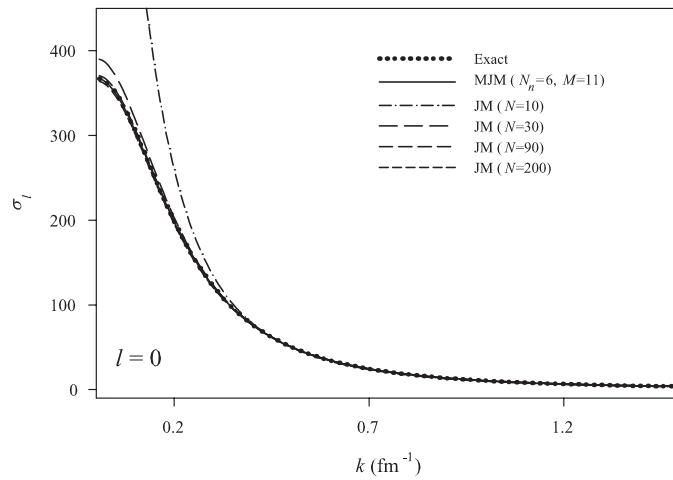
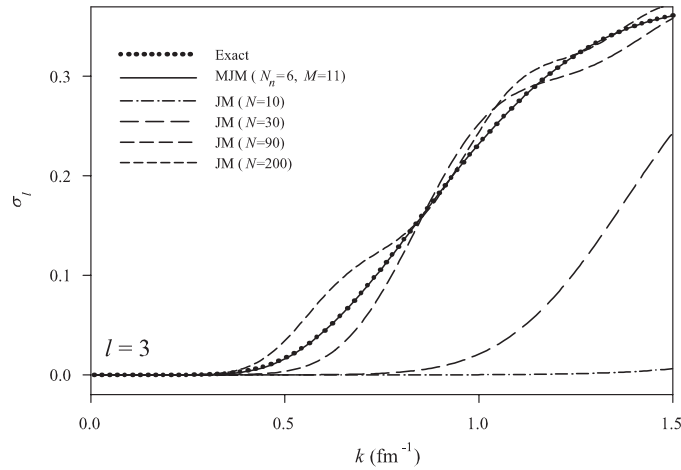**Figure 4.** $l = 0$ partial cross section for the Yukawa potential (36) of [28].

Figure 5. $l = 3$ partial cross section for the Yukawa potential (36) of [28].

dimension of the near interaction region, provides accurate results. The JM results on the other hand are not yet converged at $N = 200$.

In figure 7 we again compare exact, MJM and JM results, now for the Yukawa potential (37). The phase shift is for the partial wave with $l = 1$ corresponding to the $^3P_2$ case for which the potential was fitted. The exact, variable phase, results correspond to those of [30]. For the MJM method the optimum b-value is 0.02 fm, and we considered $N_n = 10$ for the near interaction, $M = 20$ for the truncation parameter and $N_f = 10\,000$ for the far interaction boundary. This amounts to the use of 174 potential matrix elements. For the original JM approach we limited the calculation to $N = 300$, i.e. 45 150 potential matrix elements. Due to the highly singular nature of this potential, convergence is not yet achieved. Figure 7 includes the results of two different J-matrix calculations with $b = 0.037$ fm and $b = 0.04$ fm.
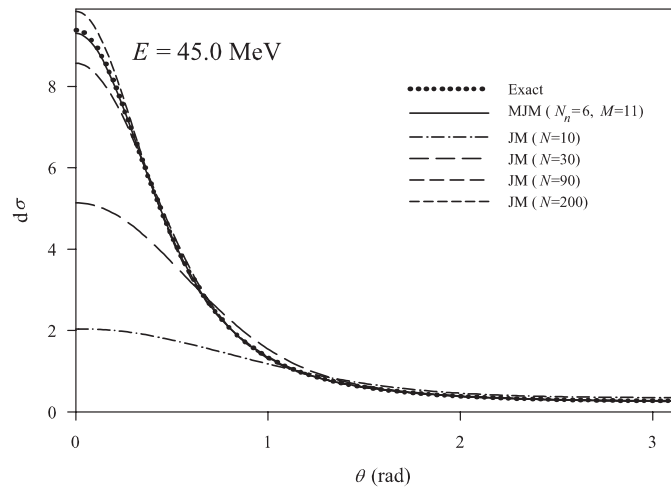
Figure 6. Differential cross section at 45.0 MeV for the Yukawa potential (36) of [28].
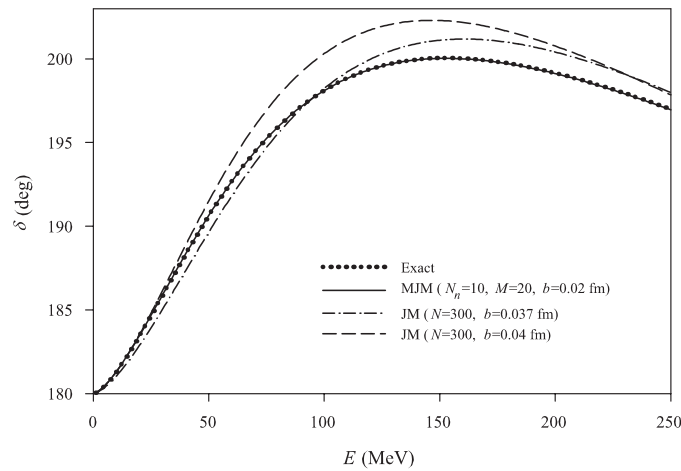

Figure 7. $l = 1$ phase shift for the Yukawa potential (37) of [30].

6. Conclusions

We have proposed a modified J-matrix method. It introduces three regions in the space of wavefunction coefficients for the oscillator basis: the asymptotic region where the asymptotic boundary conditions hold, the far interaction region where semi-classical approximations to the matrix elements reduce the Schrödinger matrix equations to three-term recurrence relations including the potential, and the near interaction region where the full matrix equation applies. Examples demonstrate that the method produces converged phase shifts with potential matrices that are at least an order of magnitude smaller than those required in the J-matrix method. They also show the importance of an extended far interaction region for the convergence of the results.

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