Modified J-Matrix Method for Scattering

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(Received 24 May 2001; published 19 December 2001)

We modify the J-matrix technique for scattering so that problems with long-range interactions are easily solved. This is done by introducing additional terms in the asymptotic three-term recurrence relation that take into account asymptotic effects of the potential. The solutions of this modified recurrence relation are a very good approximation of the exact scattering solution. Only a small number of residual coefficients need to be calculated. As a result, the numerical effort to solve the scattering problem is seriously reduced. The technique is illustrated with a Yukawa potential.

DOI: 10.1103/PhysRevLett.88.010404 PACS numbers: 03.65.Nk

Introduction.—In quantum scattering calculations, it is the aim to find for a given positive energy E the scattering solution that fits the Schrödinger equation with interaction $V(r)$. The goal of the calculations is to compare theoretical results for the cross section with the experimental values. Therefore, we need to determine, in the energy range of interest, the phase shift $\delta(E)$ of the scattering solutions.

Several methods in quantum scattering theory reduce the problem to a set of algebraic equations by an introduction of a square integrable (L^2) basis [1,2]. In this Letter, we consider the *J-matrix method,* developed in a series of papers [1,3,4], with applications in atomic and molecular physics [5]. A similar approach, referred to as the *algebraic method* by its authors, was applied in nuclear physics [6–9]. Recently, it was shown that a relativistic formulation is also possible [10,11]. These calculations used a Laguerre or harmonic oscillator basis.

We introduce modifications to the J-matrix method in oscillator formulation that significantly improve the convergence. That is to say, only very small interaction matrices are needed to calculate converged phase shifts. The approach is based on asymptotic approximations for matrix elements in the oscillator basis. It leads to a simplification of the matrix equations, whereby diagonalization is effectively replaced by the solution of the recursion relations. Some numerical examples will be given. The results are useful for scattering calculations of many-body systems where a harmonic potential is important, for example, a system contained in a harmonic trap.

In this Letter, we limit ourselves to discuss a single channel problem. The results are, however, easily generalized to multiple channels. We use the radial eigenfunctions of a three-dimensional harmonic oscillator as a L^2 basis. These eigenfunctions are

$$\phi_{nl}(r) = (-1)N_{n,l}\left(\frac{r}{b}\right)^l \exp\left\{-\frac{1}{2}\left(\frac{r}{b}\right)^2\right\} \times L_n^{l+1/2}\left[\left(\frac{r}{b}\right)^2\right], \quad (1)$$

with

$$N_{nl} = b^{-3/2}\sqrt{\frac{2n!}{\Gamma(n+l+3/2)}}, \quad (2)$$

and oscillator length $b = \sqrt{\hbar/m\omega}$.

The J-matrix method,—In one way or another, a scattering calculation usually involves matching a solution of the internal region—determined by the range of $V(r)$—to a combination of asymptotic free-space or reference solutions. For a spherically symmetric, non-Coulombic potential, the solution of

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)}{\hbar^2 r^2} + V(r) - E\right]\psi_l(r) = 0 \quad (3)$$

needs to be matched with

$$\psi_l(r \to \infty) \to j_l(kr) + \tan\delta_l(k)\eta_l(kr), \quad (4)$$

the free-space Bessel and Neumann function, where $E = \hbar^2k^2/2m$. This matching of the internal with the asymptotic solution determines the phase shift δ_l.

In [1], it was shown that the same general approach can be taken when the scattering equations are expressed in basis states. The Schrödinger equation is now a matrix equation:

$$\sum_{m=0}^{\infty}\langle\phi_{nl}|T + V - E|\phi_{ml}\rangle c_{m,l} = 0, \quad (5)$$

and its solution is a vector of expansion coefficients $\{c_{n,l}\}_{n\epsilon IN}$. As previously, the solution becomes asymptotically a combination of two reference states,

$$c_{n\to\infty,l} \to b_{n,l} + \tan\delta_l n_{n,l}, \quad (6)$$

where $\{b_{n,l}\}_{n\epsilon IN}$ and $\{n_{n,l}\}_{n\epsilon IN}$, are the regular and the irregular solution of the free-space equation (the irregular solution should be regularized as explained in [1]):

$$\sum_{m=0}^{\infty}\langle\phi_{nl}|T - E|\phi_{ml}\rangle c_{m,l} = 0. \quad (7)$$

This free-space matrix equation is in fact a three-term recurrence relation,

$$T_{nl,n-1l}c_{n-1,l} + (T_{nl,nl} - E)c_{nl} + T_{nl,n+1l}c_{n+1,l} = 0, \tag{8}$$

since the matrix elements of the kinetic energy $T_{nl,ml} = \langle\phi_{nl}|T|\phi_{ml}\rangle$ are tridiagonal in oscillator representation. The solutions $\{b_{n,l}\}_{n\in\mathbb{N}}$ and $\{n_{n,l}\}_{n\in\mathbb{N}}$ can be found analytically [1,9] or numerically using the asymptotic behavior outlined in the next sections. The J-matrix method then proposes to solve Eq. (5) by truncating the potential matrix $\langle\phi_{nl}|V|\phi_{nl}\rangle$ at some large index N. This approximation allows one to seek a solution of the form

$$c_{nl} = \begin{cases} c^0_{nl} + b_{nl} + \tan\delta_l n_{nl} & n < N \\ b_{nl} + \tan\delta_l n_{nl} & n \geq N, \end{cases} \tag{9}$$

where only N residual coefficients c^0_{nl} and the phase shift δ_l are needed to fit the truncated equation.

The matrix equation (5) is now reduced to a linear system of $N+1$ equations in the $N+1$ unknowns $\{c^0_{0l}, c^0_{1,l}, \ldots, c^0_{N-1l}, \tan\delta_l\}$:

$$\sum_{m=0}^{N-1}\langle\phi_{nl}|T + V - E|\phi_{ml}\rangle c^0_{ml} + \tan\delta_l(E)\left(\sum_{m=0}^{N+1}\langle\phi_{nl}|T + V - E|\phi_{ml}\rangle n_{ml}\right) = -\sum_{m=0}^{N+1}\langle\phi_{nl}|T + V - E|\phi_{ml}\rangle b_{ml}. \tag{10}$$

Convergence of the phase shift and the scattering wave function is achieved by extending the interaction region, i.e., making the N larger. The drawback is, however, that the number of matrix elements scales with N^2 and that the computation of the potential matrix elements is often the most time consuming step in the calculation.

The modified J-matrix method.—We address this problem by distinguishing three regions in the oscillator representation space. In each region, the expansion coefficients fit different equations. In the *near interaction region,* $0 \leq n < M$, the exact equations apply. In the *far interaction region,* $M \leq n < M_a$, we use asymptotic expressions for the matrix elements. In the *asymptotic region,* $M_a \leq n$, the exact free-space situation applies.

New in this approach is the introduction of the far interaction region. In this region, we use approximate expressions for the matrix elements. This leads to excellent convergence properties and lightens significantly the computational burden.

Asymptotic matrix elements.—Let us start with the expansion coefficient. Suppose ψ_l is an arbitrary solution of the Schrödinger equation. It can be a bound or a scattering state. The expansion coefficients c_{nl} are then determined by the projection integral,

$$c_{n,l} = \int_0^\infty dr\, r^2 \phi_{n,l}(r)\psi_l(r). \tag{11}$$

Since ϕ_{nl} has n nodes, the number of oscillations increases with n. We are interested in the value of the integral when $n \to \infty$.

This integral reminds us of the integral,

$$I(\lambda) = \int_a^b e^{i\lambda\phi(x)} f(x)\, dx, \tag{12}$$

discussed in books on asymptotic expansions [12–14]. These books conclude that the value of the integral for $\lambda \to \infty$ is determined by (i) the behavior of $f(x)$ near stationary points of the phase $\phi(x)$ and (ii) by behavior near the integration boundaries a and b.

Applied to our projection integral (11), this means that its value is determined by the behavior of $\psi_l(r)$ near the classical turning point $R_{nl} = b\sqrt{4n + 2l + 3}$, the stationary point of the radial oscillator wave function ϕ_{nl}, and the behavior of $\psi_l(r)$ near $r \to 0$, the integration boundary. Note that the upper integration boundary, $r \to \infty$, does not contribute, since $\phi_{nl}(r \to \infty) = 0$.

Since the behavior near the origin and the classical turning point determine the value of the integral, further simplifications can be made. We approximate the oscillator states in these two points. The oscillator state ϕ_{nl} near $r = 0$ is easily approximated by a spherical Bessel function (see Fig. 1),

$$r\phi_{n,l} \approx (-1)^n \frac{\sqrt{2}}{b}\sqrt{\frac{2K_{n,l}}{\pi}}\, r j_l(K_{n,l}r), \tag{13}$$

since the oscillator potential is negligible when $r \to 0$. Near the classical turning point, we use an approximation with an Airy function (see Fig. 1)

$$r\phi_{n,l}(r) \approx \frac{2}{b}\left(\frac{b^4}{2R_{n,l}}\right)^{1/6} \mathrm{Ai}[(r - R_{n,l})(2R_{n,l}/b^4)^{1/3}], \tag{14}$$

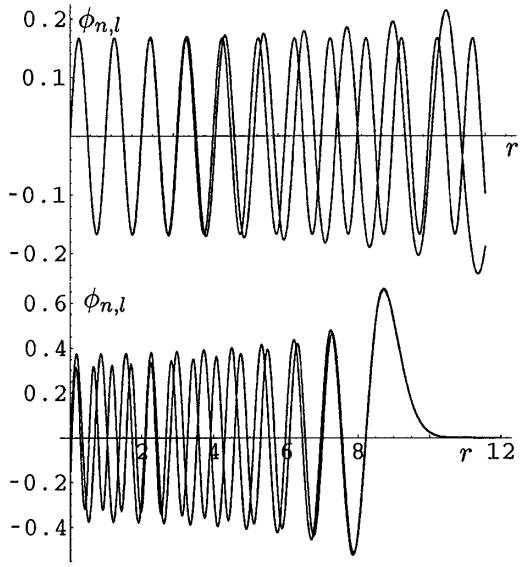

FIG. 1. We approximate the oscillator function near the origin by a Bessel function and near the turning point by the Airy function ($n = 20, b = 1$).

which is the solution of the harmonic oscillator equation, where the oscillator potential is linearized near the turning point.

The integral (11) is now split into two parts:

$$c_{n,l} = \int_0^a dr\, r^2 \psi_l(r) \phi_{n,l}(r) + \int_a^\infty dr\, r^2 \psi_l(r) \phi_{n,l}(r). \tag{15}$$

In the first integral, we use the Bessel function to approximate the oscillator function; in the second integral, we use the Airy function,

$$\begin{aligned} c_{n\to\infty} = & \int_0^a dr\, r \psi_l(r)\, (-1)^n \frac{\sqrt{2}}{b} \sqrt{\frac{2K_{n,l}}{\pi}}\, r j_l(K_{n,l} r) \\ & + \int_a^\infty dr\, r \psi_l(r)\, \frac{2}{b} \left(\frac{b^4}{2R_{n,l}}\right)^{1/6} \\ & \times \mathrm{Ai}[(r - R_{n,l})\, (2R_{n,l}/b^4)^{1/3}]. \end{aligned} \tag{16}$$

Because the Bessel function j_l does not have any stationary points, we can raise the integration boundary of the first integral to $a \to \infty$ without changing the integral. It then becomes a Fourier integral.

The second integral is calculated by replacing the Airy function by its integral representation and then applying the stationary phase approximation.

The end result is an approximate formula for the asymptotic expansion coefficients at large n:

$$\begin{aligned} c_{n,l} \approx & (-1)^n \sqrt{2}\, b^{-1} \sqrt{K_{n,l}}\, \tilde{\psi}_l(K_{n,l}) \\ & + \sqrt{2}\, b \sqrt{R_{n,l}}\, \psi_l(R_{n,l}). \end{aligned} \tag{17}$$

The two parts are determined by the wave function sampled at the turning points. Indeed, $\tilde{\psi}_l(k)$ is sampled at the point $K_{n,l} = \sqrt{4n + 2l + 3}/b$, the turning point of the oscillator state $\phi_{n,l}$ in Fourier space, and the second term is ψ_l sampled at $R_{n,l}$, the turning point in coordinate space.

Depending on the support of ψ_l in coordinate and Fourier space, one of the two terms will dominate the asymptotic expansion coefficient. The asympotic c_{nl} of a scattering function, for example, will be determined only by the coordinate term $\sqrt{2}\, b \sqrt{R_{n,l}}\, \psi_l(R_{n,l})$, since from a certain n on, all $K_{n,l}$ will lie beyond the maximal momentum $k_{\max}$ present in the scattering function. The Fourier term will then be zero.

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

$$\langle \phi_{nl} | V(r) | \phi_{ml} \rangle = \int_0^\infty dr\, r^2 \phi_{nl}(r) V(r) \phi_{ml}(r) \tag{18}$$

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 behavior near $r = 0$. For this reason, it can be approximated by

$$\langle \phi_{nl} | V(r) | \phi_{ml} \rangle \approx (-1)^{n+m} \frac{\sqrt{K_{m,l} K_{n,l}}}{b^2} \tag{19}$$

$$\times \int_0^\infty dr\, r^2 j_l(K_{n,l} r) V(r) j_l(K_{m,l} r), \tag{20}$$

where $K_{m,l}$ and $K_{n,l}$ are the turning points in Fourier space.

We use these approximations to formulate an approximation to (5) in the far interaction region, i.e., the region of oscillator space with large n, but still having non-negligible matrix elements. We start by applying the asymptotic formula (17) to approximate the potential term in

$$\langle nl | T + V - E | \psi_l \rangle = 0. \tag{21}$$

The approximation is

$$\begin{aligned} \langle nl \,|\, V\psi_l \rangle \approx & \; b \sqrt{2R_{n,l}}\, (V\psi_l)\, (R_{n,l}) \\ & + (-1)^n b^{-1} \sqrt{2K_{n,l}}\, (\tilde{V}\psi_l)\, (K_{n,l}), \end{aligned} \tag{22}$$

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 $\tilde{V}$ and $\tilde{\psi}_l$ sampled in $K_{n,l}$.

When n is large enough such that $K_{n,l} \gg k_{\max}$, further simplifications can be made. Indeed, the asymptotic expansion coefficient of ψ_l is solely determined by the behavior of $\psi_l(r)$ in turning points $R_{n,l}$ in coordinate space. Consequently, we can replace $b\sqrt{2R_{n,l}}\, \psi_l(R_{nl})$ in the first term by $c_{n,l}$, and so it is approximated by $V(R_{nl}) c_{nl}$.

Because of the convolution product, the second term in (22) is more complicated. Nevertheless, by using smoothness and averaging arguments, the term is approximately the matrix element at the boundary of the potential matrix $\langle nl | V(r) | 0l \rangle$ multiplied with an unknown number W.

Using the split-up (22) and its subsequent approximations, the Schrödinger matrix equation for the scattering function becomes a recurrence relation with a source term,

$$T_{nn-1,l} c_{n-1,l} + [T_{nl,nl} + V(R_{nl}) - E] c_{n,l} + T_{nl,n+1l} c_{n+1,l} = -W \langle nl | V(r) | 0l \rangle, \tag{23}$$

The difference with Eq. (8) is the additional diagonal elements and the source. In many situations, the generic source term $W(-1)^n K_{n,l}^{-l+5/2}$ can be used. It is the leading order term of an expansion in $1/K_{n,l}$.

Numerical strategy.—We now propose a strategy to solve the Schrödinger matrix equation. It involves two steps: (i) the solution of the recurrence relation and (ii) the solution of the residual linear system.

In the first step, we solve the recurrence relation. We search for two independent solutions, $\{b_{nl}\}_{n \in \mathbb{N}}$ and $\{n_{nl}\}_{n \in \mathbb{N}}$, of the homogeneous version of the recurrence relation (23) that fit the boundary conditions,

$$b_{n\to\infty l} = \sqrt{2}\, b\sqrt{R_{n,l}}\sqrt{\frac{2}{\pi}}\, j_l(kR_{n,l})\,, \tag{24}$$

$$n_{n\to\infty l} = \sqrt{2}\, b\sqrt{R_{n,l}}\sqrt{\frac{2}{\pi}}\, \eta_l(kR_{n,l})\,. \tag{25}$$

This is easily done by starting a recurrence with the boundary condition in two successive points at large n. In addition, we have to do a third recurrence. This one uses the inhomogeneous equation and fits zero boundary conditions, and determines the vector $\{Ws_{nl}\}_{n\in IN}$.

The sum of the three vectors,

$$b_{nl} + \tan\delta_l n_{nl} + Ws_{nl}\,, \tag{26}$$

will fit the Schrödinger matrix equation in the asymptotic region $M_a \le n$ and in the far interaction region $M \le n < M_a$, but not in the near interaction region $n < M$.

The second step of our strategy involves the solution of the near interaction region, $n \le M$. In this region, no approximations are made and the exact matrix elements apply. The complete solution is then

$$c_{nl} = \begin{cases} c^0_{nl} + b_{nl} + \tan\delta_l n_{nl} + Ws_{n,l} & n < M \\ b_{nl} + \tan\delta_l n_{nl} + Ws_{n,l} & n \ge M\,, \end{cases} \tag{27}$$

and the Schrödinger equation (5) is transformed into a system of equations,

$$\sum_{m=0}^{M-1} \langle\phi_{nl}|T + V - E|\phi_{ml}\rangle c^0_{ml} + \sum_{m=0}^{\infty} \langle\phi_{nl}|T + V - E|\phi_{ml}\rangle (b_{nl} + \tan\delta_l n_{nl} + Ws_{n,l}) = 0\,, \tag{28}$$

for the M residual coefficients $\{c_{0l}, c_{1l}, \ldots, c_{M-1,l}\}$, $\tan\delta_l$, and W. The second term in the equation is small (if we were to assume the semiclassical approximation for the matrix elements, it would be zero by construction) and its sum converges rapidly. The examples we have investigated (see also [8]) lead us to the conclusion that the sum can be truncated at a $M < M' < N$.

Application.—We apply this new strategy to a simple one-dimensional problem with a Yukawa interaction. The potential is

$$V(r) = V_0 e^{-\mu r}/r\,, \tag{29}$$

where we choose $V_0 = -30$ MeV and $\mu = 0.3$ fm^{-1}. As illustrated in Fig. 2, the conventional J-matrix method has convergence difficulties, since the potential matrix elements decrease only very slowly. With the asymptotic behavior included in the recurrence relation, we need a minimal number of residual coefficients $M = 5$ and a summation of the nonresidual term up to $M' = 10$ to obtain a converged phase shift over a wide energy range.

Conclusions and outlook.—We have modified the J-matrix method for scattering. We have formulated a modified recurrence relation that is valid in the far interaction region, i.e., the region with large n but still important matrix elements. The main result is that fewer matrix elements need to be calculated to obtain a converged phase shift.

The results are useful in scattering calculations with multiple channels and Slater determinants as basis states. With the new insights, many-body scattering calculations can be solved with a minimal of computational burden.

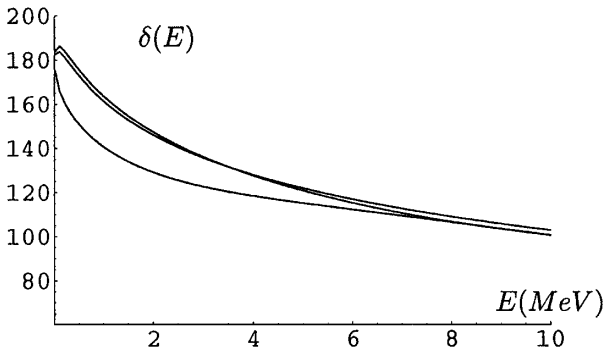

FIG. 2. Phase shift δ_l of the Yukawa potential ($\mu = 0.3$ fm^{-1} and $V_0 = 30$ MeV). The two upper curves are the "exact" results calculated with the variable phase method [15], and the modified J-matrix results obtained with $M = 5$ and $M' = 10$. The lower curve shows the original J-matrix results obtained with $N = 10$; at least $N = 80$ is needed to obtain a similar accuracy.

Note that a similar study of the far interaction can be done for other L^2 basis sets, for example, the Laguerre basis.

The authors acknowledge financial support from *Fonds voor Wetenschappelijk Onderzoek–Vlaanderen*.

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