Direct calculation of the scattering amplitude without partial-wave analysis

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Two developments in scattering theory are reported. We show, in a practical way, how one can calculate the scattering amplitude without invoking a partial-wave expansion. First, the integral expression for the scattering amplitude $f(\theta)$ is simplified by an analytic integration over the azimuthal angle. Second, the full scattering wave function that appears in the integral expression for $f(\theta)$ is obtained by solving the Schrödinger equation with the finite element method. As an example, we calculate electron scattering from static hydrogen (the Hartree potential). With minimal computational effort, we obtain accurate and stable results for the scattering amplitude.

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I. INTRODUCTION

For the past decades, the standard approach to obtaining scattering solutions for central potentials has been via partial-wave analysis [1,2]. For increasing projectile energy, the number of partial waves that must be included to obtain converged results increases. In the case of angular dependent potentials, the Schrödinger equation is not separable in spherical coordinates and the resulting equations for the partial waves are coupled. We propose an alternative to partial-wave analysis, that also permits the treatment of noncentral potentials.

We begin with the integral expression for the scattering amplitude $f(\theta)$ that involves the full scattering wave function. We show that the integration over the azimuthal angle can be done analytically. The Schrödinger equation is then solved directly by the finite element (FE) method, yielding both the scattering wave function and the scattering amplitude. Once the wave function has been determined, the integral expression for $f(\theta)$ can be evaluated numerically. The scattering amplitude obtained from the integral expression is far more accurate and stable than that obtained from the solution of the Schrödinger equation.

The paper is organized as follows. In Sec. II, we show how the integral expression for the scattering amplitude can be simplified for azimuthal symmetry. In Sec. III, we discuss how the FE method can be used to solve the Schrödinger equation subject to the (complex) scattering boundary condition. For the sake of completeness, we review in Sec. IV the equations for partial-wave analysis. In Sec. V, we present results for electron scattering from static hydrogen and compare them to fully converged partial-wave calculations.

II. INTEGRAL EXPRESSION FOR THE SCATTERING AMPLITUDE

Our starting point is the well-known integral expression for the scattering amplitude for central potentials [1]

$$f(\theta_k) = -\frac{1}{4\pi}\int e^{-i\mathbf{k}\cdot\mathbf{r}} V(r)\Psi(\mathbf{r})d^3r, \tag{1}$$

where $\Psi(\mathbf{r})$ is the full scattering wave function. We consider the case where $\Psi(\mathbf{r})$ is independent of the azimuthal angle. Re-expressing Eq. (1) in spherical coordinates,

$$f(\theta_k) = -\frac{1}{4\pi}\int_0^\infty \int_0^\pi e^{ikr\cos\theta_r\cos\theta_k} V(r)\Psi(r,\theta_r) \times \sin\theta_r d\theta_r r^2 dr \int_0^{2\pi} e^{-ikr\sin\theta_r\sin\theta_k\cos(\phi_k-\phi_r)} d\phi_r, \tag{2}$$

the integral over ϕ_r can be done analytically. In the simplified expression for the scattering amplitude,

$$f(\theta_k) = -\frac{1}{2}\int_0^\infty \int_0^\pi e^{ikr\cos\theta_r\cos\theta_k} V(r) J_0(r\sin\theta_r\sin\theta_k) \times \Psi(r,\theta_r)\sin\theta_r d\theta_r r^2 dr, \tag{3}$$

$J_0(x)$ is the zeroth-order Bessel function. If $\Psi(r,\theta_r)$ is known, then the remaining integration over θ_r and r can be performed numerically.

III. DIRECT SOLUTION OF THE SCHRÖDINGER EQUATION

In this initial application, we treat electron-hydrogen scattering with no exchange. Using an ansatz

$$\Psi(\mathbf{r_1},\mathbf{r_2}) = \frac{\psi(\mathbf{r_1})}{r_1}\frac{\phi_0(r_2)}{r_2}Y_0^0(\Omega_2), \tag{4}$$

where $\phi_0(r_2)$ is the reduced radial wave function for the ground state of hydrogen, we require

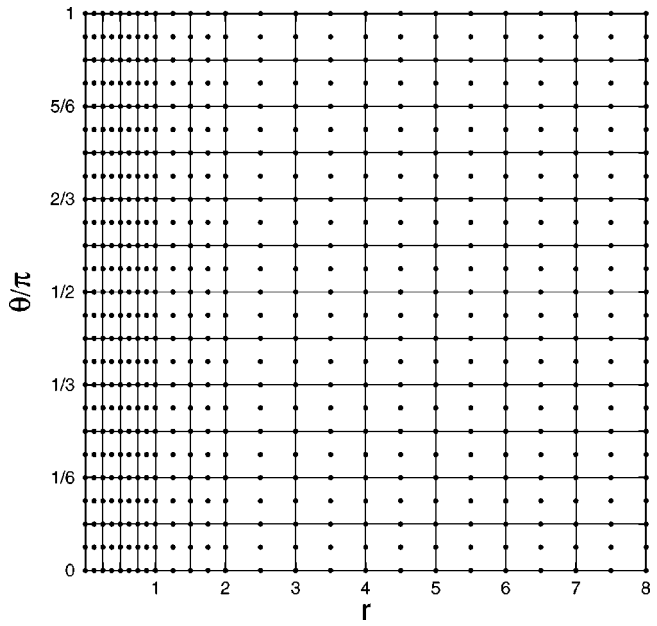

FIG. 1. Finite element grid with $R=8.0a_0$ and $N_r\times N_\theta=144$.

$$\int \frac{\phi_o(r_2)}{r_2}(H-E)\Psi(\mathbf{r_1},\mathbf{r_2})d^3r_2=0. \tag{5}$$

This leads to an effective Schrödinger equation for the unknown function $\psi(\mathbf{r_1})$:

$$\left[-\frac{\partial^2}{\partial r^2}-\frac{1}{r^2}\left(\frac{\partial}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}\right)+V(r)-k^2\right]\psi(r,\theta)=0, \tag{6}$$

where

$$V(r)=-2e^{-2r}\left(1+\frac{1}{r}\right), \tag{7}$$

is the well-known Hartree potential. We use Rydberg units throughout.

The boundary conditions require that $\psi(r,\theta)$ vanishes at the origin and, in the asymptotic region,

$$\psi(r,\theta)\sim re^{ikr\cos\theta}+f(\theta)e^{ikr}; \tag{8}$$

$f(\theta)$ is the unknown scattering amplitude that we wish to determine.

In the past, the FE method has been used successfully to solve the scattering problem within the framework of partial-wave analysis [3]. Here, we use the FE method to solve the multidimensional Schrödinger equation for the full scattering wave function $\psi(r,\theta)$ and the scattering amplitude $f(\theta)$.

In FE analysis [4], the coordinate space is discretized in the radial direction $(0\leqslant r\leqslant R)$ and in the angular direction $(0\leqslant\theta\leqslant\pi)$ into $N_r\times N_\theta$ as shown in Fig. 1. In each element n, the real and imaginary parts of the wave function are expanded in a locally defined basis:

$$\mathrm{Re}[\psi^n(r,\theta)]=\sum_{j=1}^{36}\alpha_j^n\phi_j^n(r,\theta), \tag{9}$$

$$\mathrm{Im}[\psi^n(r,\theta)]=\sum_{j=1}^{36}\beta_j^n\phi_j^n(r,\theta). \tag{10}$$

The basis functions $\phi_j^n(r,\theta)$ are products of quintic polynomials in r and θ; the functions are nonzero only in element n. The precise form of the basis functions is determined by the requirement that the unknown coefficients α_j^n and β_j^n are the value of the real and imaginary parts of the wave function ψ and derivatives $(\partial\psi/\partial r,\partial\psi/\partial\theta,\partial^2\psi/\partial\theta\partial r)$ at nine grid points in the element n. The grid points are located at the four corners, the midpoints of the four sides, and the center of the element, as shown in Fig. 1. Note that the expansion coefficients and the basis functions are real.

Using this expansion in Eq. (6) and projecting onto the basis set, we obtain a simple matrix equation for the real and imaginary parts of the wavefunction in element n:

$$\begin{bmatrix}\mathbf{H}^n-E\mathbf{U}^n & 0\\ 0 & \mathbf{H}^n-E\mathbf{U}^n\end{bmatrix}\begin{bmatrix}\alpha^n\\ \beta^n\end{bmatrix}=0. \tag{11}$$

The matrix elements $\mathbf{H}_{ij}^n=\langle\phi_i^n(r,\theta)|H|\phi_j^n(r,\theta)\rangle$ and $\mathbf{U}_{ij}^n=\langle\phi_i^n(r,\theta)|\phi_j^n(r,\theta)\rangle$ are integrated numerically with Gauss quadrature; with the exception of the term containing $V(r)$, the integrals are simple polynomials.

We then ''add'' the equations for the $N=N_r\times N_\theta$ elements. Since the grid points on the corners and sides of element n are shared by adjacent elements, continuity of the wave function and its derivative across the element boundary is guaranteed. In the final global matrix equation

$$\begin{bmatrix}\mathbf{H}-E\mathbf{U} & 0\\ 0 & \mathbf{H}-E\mathbf{U}\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix}=0, \tag{12}$$

the unknown vectors α and β contain the value of the real and imaginary parts of the wave function ψ and its derivatives $(\partial\psi/\partial r,\ \partial\psi/\partial\theta,$ and $\partial^2\psi/\partial r\partial\theta)$ at the $(2N_r+1)\times(2N_\theta+1)$ grid points in the coordinate space:

$$\psi(r,\theta)=\sum_{n=1}^{N}\sum_{j=1}^{36}[\alpha_j^n+i\,\beta_j^n]\phi_j^n(r,\theta). \tag{13}$$

Because the Hamiltonian is real, the real and imaginary parts of the wave function are still uncoupled in Eq. (12). The mixing between the components of α and β occurs when we impose the asymptotic complex boundary condition.

In order to satisfy the boundary condition at the origin, we set equal to zero the components of α and β that correspond to the value of ψ and $\partial\psi/\partial\theta$ at $(2N_\theta+1)$ grid points where $r=0$. This is equivalent to eliminating the corresponding rows and columns from the global matrix. The asymptotic boundary condition Eq. (8) is also straightforward to impose although the bookkeeping of the matrix elements is tedious. We identify the components of α and β that correspond to

TABLE I. Complex scattering amplitudes $(\mathrm{Re}[f(\theta)],\ \mathrm{Im}[f(\theta))$ at $k=0.5$ obtained from the integral formula $f_{int}(\theta)$ and partial-wave analysis $f_L(\theta)$; also included is the scattering amplitude obtained from the FE solution of the Schrödinger equation.

	$\theta=0$	$\theta=\pi/4$	$\theta=\pi/2$	$\theta=3\pi/4$	$\theta=\pi$
f_0	(0.869,1.495)	(0.869,1.495)	(0.869,1.495)	(0.869,1.495)	(0.869,1.495)
f_1	(1.025,1.500)	(0.979,1.498)	(0.869,1.495)	(0.758,1.493)	(0.713,1.491)
f_2	(1.039,1.500)	(0.982,1.498)	(0.862,1.495)	(0.762,1.493)	(0.726,1.491)
f_3	(1.040,1.500)	(0.982,1.498)	(0.862,1.495)	(0.762,1.493)	(0.725,1.491)
f_{int}	(1.040,1.500)	(0.982,1.499)	(0.862,1.496)	(0.762,1.493)	(0.725,1.491)
f_{FE}	(1.030,1.545)	(0.979,1.525)	(0.864,1.491)	(0.762,1.470)	(0.724,1.464)

the $(2N_\theta+1)$ grid points where $r=R$. Then, the values of the real and imaginary parts of ψ, $\partial\psi/\partial r$, $\partial\psi/\partial\theta$, and $\partial^2\psi/\partial r\partial\theta$ are completely determined by Eq. (8) *except* for the real and imaginary parts of $f(\theta)$ and $df/d\theta$. These unknowns are exactly the expansion coefficients for the FE representation of the scattering amplitude:

$$f(\theta)=\sum_{n=1}^{N}\sum_{j=1}^{36}[\gamma_j^n+i\,\delta_j^n]\phi_j^n(R,\theta). \tag{14}$$

$\phi_j^n(R,\theta)$ is zero in every element that does not include the boundary; in the boundary elements, only a few of the basis functions are nonzero at $r=R$. The unknown expansion coefficients that multiply these (nonzero) basis functions are the real and imaginary parts of $f(\theta)$ and $df/d\theta$ at the grid points on the boundary.

With certain components of the column vector α and β now expressed as real numbers and the unknowns γ_i^n and δ_i^n, we can carry out the matrix multiplication of these terms explicitly. Our goal is to rewrite Eq. (12) such that the unknown vector $[\alpha,\beta]$ is replaced by a new vector $[\alpha',\beta',\gamma,\delta]$; α' and β' differ from α and β only by the exclusion of the components that have been determined by the boundary conditions. The matrix-multiplied real constants are brought over to the right-hand side of the equation. The factors multiplying components of γ and δ are absorbed into off-diagonal matrix elements, which effectively couples together the equations for the remaining undetermined components of α' and β'.

The set of linear equations is then solved for the real and imaginary parts of the wave function (and derivatives) on the interior grid points and the scattering amplitude (and derivative) on the boundary grid points. These coefficients can then be used to construct piecewise analytic expressions for the full scattering wave-function Eq. (13) and the scattering amplitude Eq. (14).

The scattering wave function can now be used to evaluate the integral expression for $f(\theta)$ given in Eq. (3). The integrals are evaluated using Gauss quadrature, which converges very rapidly.

IV. PARTIAL-WAVE ANALYSIS

Since we want to compare our method with the conventional partial-wave approach, we shall review some of the partial-wave formulas [1,2]. The wave function is expanded in partial waves

$$\Psi(r,\theta)=\sum_{l=0}^{\infty}\frac{u_l(r)}{r}P_l(\cos\theta), \tag{15}$$

where the $u_l(r)$ satisfy

$$\left(-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+V(r)-k^2\right)u_l(r)=0. \tag{16}$$

The boundary conditions require that $u_l(r)$ vanishes at the origin and, for large r,

$$u_l(r)\sim kr[j_l(kr)-\tan\eta_l y_l(kr)]; \tag{17}$$

j_l and y_l are the spherical Bessel and Neumann functions, respectively. The point of writing the boundary condition on $u_l(r)$ in this way is that one can extract the phase-shift η_l at

TABLE II. Complex scattering amplitudes at $k=1.0$ obtained from the integral formula $f_{int}(\theta)$ and partial-wave analysis $f_L(\theta)$.

	$\theta=0$	$\theta=\pi/4$	$\theta=\pi/2$	$\theta=3\pi/4$	$\theta=\pi$
f_0	(0.486,0.619)	(0.486,0.619)	(0.486,0.619)	(0.486,0.619)	(0.486,0.619)
f_1	(0.817,0.656)	(0.720,0.645)	(0.486,0.619)	(0.251,0.593)	(0.154,0.582)
f_2	(0.906,0.658)	(0.742,0.646)	(0.441,0.618)	(0.273,0.593)	(0.243,0.583)
f_3	(0.928,0.658)	(0.739,0.646)	(0.441,0.618)	(0.277,0.593)	(0.221,0.583)
f_4	(0.933,0.658)	(0.737,0.646)	(0.443,0.618)	(0.275,0.593)	(0.226,0.583)
f_5	(0.934,0.658)	(0.736,0.646)	(0.443,0.618)	(0.276,0.593)	(0.225,0.583)
f_{int}	(0.934,0.658)	(0.736,0.646)	(0.443,0.618)	(0.276,0.593)	(0.226,0.583)

TABLE III. Complex scattering amplitudes at $k=2.0$ obtained from the integral formula $f_{int}(\theta)$ and partial-wave analysis $f_L(\theta)$.

	$\theta=0$	$\theta=\pi/4$	$\theta=\pi/2$	$\theta=3\pi/4$	$\theta=\pi$
f_0	(0.246,0.205)	(0.246,0.205)	(0.246,0.205)	(0.246,0.205)	(0.246,0.205)
f_1	(0.571,0.279)	(0.476.0.257)	(0.246,0.205)	(0.016,0.153)	(−0.079,0.131)
f_2	(0.771,0.295)	(0.526,0.261)	(0.146,0.197)	(0.066,0.157)	(0.122,0.147)
f_3	(0.878,0.298)	(0.507,0.261)	(0.146,0.197)	(0.085,0.157)	(0.015,0.144)
f_4	(0.931,0.299)	(0.485,0.260)	(0.166,0.197)	(0.064,0.157)	(0.068,0.145)
f_5	(0.957,0.299)	(0.475,0.260)	(0.166,0.197)	(0.073,0.157)	(0.043,0.145)
f_6	(0.969,0.299)	(0.474,0.260)	(0.162,0.197)	(0.072,0.157)	(0.055,0.145)
f_7	(0.974,0.299)	(0.474,0.260)	(0.162,0.197)	(0.071,0.157)	(0.049,0.145)
f_8	(0.977,0.299)	(0.475,0.260)	(0.163,0.197)	(0.072,0.157)	(0.052,0.145)
f_9	(0.978,0.299)	(0.475,0.260)	(0.163,0.197)	(0.071,0.157)	(0.051,0.145)
f_{int}	(0.979,0.300)	(0.476,0.261)	(0.164,0.197)	(0.072,0.157)	(0.051,0.145)

values of r where the potential $V(r)$ is negligible, but the centrifugal term is not. This is commonly referred to as the intermediate scattering region. [We are assuming that the potential $V(r)$ falls off faster than $1/r^2$.] If we then take the asymptotic limit of j_l and y_l as $r\rightarrow\infty$, it is clear that the scattering amplitude of Eq. (8) is related to the phase shifts of Eq. (17) by

$$f(\theta)=\frac{1}{k}\sum_{l=0}^{L}(2l+1)e^{i\eta_l}\sin\eta_l P_l(\cos\theta). \tag{18}$$

In practice, the number of partial waves that must be included in the sum to obtain convergence is finite and energy dependent.

V. RESULTS

We now present and discuss the results obtained by three methods: (i) $f_{FE}(\theta)$ of Eq. (14) is the scattering amplitude obtained from the direct solution of the Schrödinger equation by FE analysis; (ii) $f_{int}(\theta)$ of Eq. (3) is the scattering amplitude obtained from the integral expression using the scattering wave function obtained by FE analysis; and (iii) $f_L(\theta)$ of Eq. (18) is the scattering amplitude obtained by partial-wave analysis; L is the largest partial wave included in the sum.

If one wishes to obtain an accurate value of $f_{FE}(\theta)$ by direct solution of the Schrödinger equation, one must choose R sufficiently large that corrections to the asymptotic boundary condition of Eq. (8) are negligible. Any error in representing the FE wave function at $r=R$ by the asymptotic formula diminishes the accuracy of the scattering amplitude $f_{FE}(\theta)$ obtained from the solution of the linear equations. Although reasonable results can be obtained at low energies with small values of R (see Table I), the value of R must be increased dramatically with increasing energy. Likewise, the number of grid points in r and θ must be increased, resulting in prohibitively large grids. This limits the applicability of this direct approach.

In contrast, using the full FE scattering wave function in the integral expression for the scattering amplitude $f_{int}(\theta)$ yields stable and accurate results *as long as R is chosen such that* $V(R)\approx 0$. The main contribution to the integral comes from the region near the scattering center where the wave function is accurately represented by the local FE basis set. The contribution to $f_{int}(\theta)$ outside the intermediate scattering region is essentially zero. The error in the FE wave function in the vicinity of the boundary, where $V(r)$ is already small, does not appreciably effect the scattering amplitude. It is still necessary to impose the boundary condition of Eq. (8) exactly in order to obtain the scattering solution to the Schrödinger equation, but the value of R that is needed to obtain an accurate scattering amplitude with the integral formula is much smaller than one would expect and energy independent. This result is not one that could have been fully anticipated; it is an important finding of this calculation, which can be expected to be of even greater utility in further applications.

In Tables I–III, we present results for the scattering amplitude (Re$[f(\theta)]$,Im$[f(\theta)]$) obtained from the integral expression $f_{int}(\theta)$ of Eq. (3) and from a partial-wave calculation $f_L(\theta)$ [5] at $k=0.5$, 1.0, and 2.0. The number of partial waves that must be included in the sum to obtain convergence steadily increases. In contrast, the computational effort required to obtain converged results using the integral formula is independent of energy. We used the same FE grid for all three calculations, with $R=8a_0$ and $N_r\times N_\theta=144$. No attempt was made to optimize the FE grid. We used equal spacing in the θ direction; in the radial direction, smaller elements were used near the scattering center (see Fig. 1).

VI. CONCLUSION

We have presented an approach for obtaining the full scattering wave function by a direct solution of the Schrödinger equation. Combined with an integral expression for the scattering amplitude, one can obtain accurate and stable results with minimal computational effort. Having established the efficiency and accuracy of this approach, we plan to extend this calculation to multichannel processes and more complex systems.

The extension of this method to noncentral potentials $V(r,\theta)$ is straightforward. Since the FE solution of the

Schrödinger equation is carried out on a grid in r and θ, the dependence of the potential on the polar angle poses no additional computational effort. In the integral expression, we simply replace $V(r)$ with $V(r,\theta)$ and proceed with the numerical integration.

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