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Direct numerical solution of the Schrödinger equation for quantum scattering problems

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A direct numerical solution of the Schrödinger equation for quantum scattering problems is presented. The wave function for each partial wave is expanded in coupled spherical harmonics and the corresponding radial functions are expanded in a local basis set using finite-element analysis, with the appropriate scattering boundary conditions. The method is shown to give very accurate results for elastic phase shifts (S, P, D, and F) and resonance positions for electron-hydrogen scattering.

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Various formalisms have been developed over the years to treat electron-atom quantum scattering, including variational [1–3] close-coupling [4, 5] and R-matrix methods [6, 7]. Even though these methods have been used successfully to compute the scattering parameters in electron-atom scattering, their applicability has been limited both in the type of systems that can be treated and the energy range over which the calculated scattering parameters are accurate. These difficulties arise in part from the use of global basis functions, which must simulate the exact wave function over a large region of space. A different approach is to obtain a direct numerical solution of the Schrödinger equation. Until recently, such an approach has been limited by the availability of algorithms to solve the equations efficiently and the difficulty in applying the boundary conditions, which require matching the solution to the asymptotic limit that depends on unknown scattering parameters. We present here a method for treating electron-atom scattering that directly solves the Schrödinger equation using the finite-element method (FEM) [8]. The use of a local basis set has the advantage of providing greater flexibility in approximating the wave function over an extended region of space and facilitates the imposition of complicated boundary conditions.

In order to illustrate our method, we outline the procedure for obtaining elastic phase shifts for electron-hydrogen scattering. Unlike previous attempts at applying FEM to S-wave positron-hydrogen scattering [9, 10], the general scheme presented here is applicable to higher partial waves and can easily be extended to inelastic scattering. First, the total wave function is expanded in partial waves; each partial wave with definite parity is further expanded in coupled spherical harmonics $Y_{l_1 l_2}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)$,

$$\Psi^{LS}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{l_1,l_2}U_{l_1 l_2}^{LS}(r_1,r_2)Y_{l_1 l_2}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2). \quad (1)$$

Using Eq. (1) in the Schrödinger equation, and retaining ℓ terms in the expansion, one obtains a set of coupled differential equations for the unknown radial functions $U_{l_1 l_2}^{LS}$,

$$\sum_{l_1,l_2} H^{L}_{l_1' l_2',\, l_1 l_2} \; U_{l_1 l_2}^{LS}(r_1,r_2) = 0 \tag{2}$$

where

$$H^{L}_{l_1' l_2',\, l_1 l_2} = \sum_{i=1}^{2} \left[-\frac{1}{2}\frac{\partial^2}{\partial r_i^2} - \frac{1}{r_i}\frac{\partial}{\partial r_i} + \frac{l_i(l_i+1)}{2\, r_i^2} - \frac{1}{r_i} - \frac{E}{2} \right] \delta_{l_1',l_1}\delta_{l_2',l_2}$$
$$+ \sum_{k=0}^{\infty} \frac{r_<^k}{r_>^{k+1}} \langle\, Y_{l_1' l_2'}^{LM}(\hat{r}_1,\hat{r}_2) \mid P_k(\cos\theta_{12}) \mid Y_{l_1 l_2}^{LM}(\hat{r}_1,\hat{r}_2)\, \rangle. \tag{3}$$

The angle brackets indicate integration over the angular coordinates and $E = -1/2n^2 + k^2/2$ is the total energy, where k is the incident momentum of the electron and n is the principal quantum number of the hydrogen target. Atomic units are used throughout unless otherwise stated.

Equation (2) is solved using the finite-element method [8]. The coordinate space spanned by r_1 and r_2 is truncated and discretized into small regions called elements (see Fig. 1). In each element ϵ, the radial functions $U_{l_1 l_2}^{LS}$ are expanded in a local basis,

$$U_{l_1 l_2}^{LS\,(\epsilon)}(r_1,r_2) = \sum_{i=1}^{36} u_{l_1 l_2\, i}^{LS\,(\epsilon)} \;\; \phi_i^{(\epsilon)}(r_1,r_2). \tag{4}$$

The functions $\phi_i^{(\epsilon)}(r_1,r_2)$ are products of fifth-order polynomials in r_1 and r_2 and are nonzero only in element ϵ. These basis functions have the property that the 36 expansion coefficients $u_{l_1 l_2\, i}^{LS\,(\epsilon)}$ are the value of the function $U_{l_1 l_2}^{LS}$, and its derivatives $\partial U_{l_1 l_2}^{LS}/\partial r_1$, $\partial U_{l_1 l_2}^{LS}/\partial r_2$, and $\partial^2 U_{l_1 l_2}^{LS}/\partial r_1 \partial r_2$ at nine nodes in the element [8].

Substituting Eq. (4) into Eq. (2), we obtain a set of 36ℓ linear coupled equations for the expansion coefficients for element ϵ:

$$\underline{H}^{L(\epsilon)} \; u^{LS(\epsilon)} = 0, \tag{5}$$

where

$$H^{L(\epsilon)}_{i\, l_1' l_2',\, l_1 l_2\, j} = \langle\, \phi_i^{(\epsilon)}(r_1,r_2) \,| H^{L}_{l_1' l_2',\, l_1 l_2} |\, \phi_j^{(\epsilon)}(r_1,r_2)\, \rangle. \tag{6}$$

The brackets here indicate integration over the area of element ϵ. The local equations are *not* solved independently. The expansion coefficients for nodes that lie on the boundary between two or four elements (see Fig. 1) couple together the local equations for those elements. Therefore the local matrices for all the elements are mapped onto a single global matrix,

$$\underline{H}^{L} \; u^{LS} = 0. \tag{7}$$

The order of the global matrix is $N = 4\mathcal{N}\ell$, where $\mathcal{N}$ is the total number of nodes in the grid. The global matrix is banded and sparse. The unknown global vector components $u_{l_1 l_2\, j}^{LS}$ are the value of the radial functions and their derivatives at the $\mathcal{N}$ nodes in the grid.

The next step is to impose the scattering boundary conditions for elastic scattering from the ground state. On the boundary $r_1 = r_{\rm max}$, the radial functions are given by

$$U_{l_1 l_2}^{LS}(r_{max}, r_2)$$
$$= \delta_{l_1,L} \;\; \delta_{l_2,0} \;\; R_{10}(r_2) \times \sqrt{k} \left[j_L(k r_{\rm max}) + \tan\delta_L \; j_{-L-1}(k r_{\rm max}) \right], \tag{8}$$

where j_L is the spherical Bessel function, R_{nl} is the hydrogen radial function, and δ_L is the elastic phase shift for the Lth partial wave. On the boundary $r_2 = r_{\rm max}$, we have

$$U_{l_1 l_2}^{LS}(r_1, r_{\rm max}) = (-1)^S \; P_{12} \; U_{l_1 l_2}^{LS}(r_{\rm max}, r_2), \tag{9}$$

where P_{12} is the electron exchange operator.

The components that correspond to nodes on the boundary are completely determined by Eqs. (8) and (9) except for the common phase shift δ_L. One nonvanishing component of the vector u^{LS} on the boundary is left arbitrary; all other nonvanishing components of u^{LS} on the boundary are expressed as a constant plus a multiple of the single unknown component on the boundary, through the common phase shift. Fixing these values of the global vector in Eq. (7) and carrying out the matrix

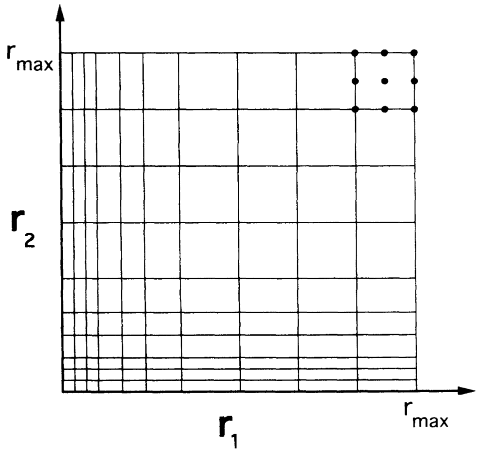

FIG. 1. Schematic diagram of the finite-element grid. The dots on the upper right corner show the distribution of the nodes in every element.

multiplication, one obtains a new global equation,

$$\underline{\tilde{H}}\,\tilde{u}^{LS} = c^{LS}. \qquad (10)$$

The dimension of $\underline{\tilde{H}}$ is $\tilde{N}$, where $N - \tilde{N}$ is the number of vector components fixed by imposing the boundary conditions. The solution of Eq. (10) yields the value of the radial functions and their derivatives at the interior grid points and the single component on the boundary, from which the phase shift is obtained.

Table I gives the elastic phase shifts for partial waves up to $L = 3$. We compare our results with those obtained using the variational method [1–3] and the intermediate energy R-matrix theory [6]. No attempt was made to optimize the grid at each energy; rather, our intention was to show that the accuracy and computational effort involved in obtaining accurate phase shifts is independent of the partial wave L and the incident momentum k. All the phase-shift calculations were done using a 10×10 grid with $r_{\max} = 24$ for $k \geq 0.3$ and $r_{\max} = 40$ for $k \leq 0.2$. Smaller elements were used near the origin as shown in Fig. 1. The FEM results agree with the best variational calculations to within ± 0.001 and were extremely stable with respect to minor variation in $r_{\max}$ and the element size.

Table II gives the position and widths of the lowest resonance for each partial wave below the n=2 threshold. These results are compared with those obtained by R-matrix theory [6], complex coordinate rotation calculation [11–13], Feshbach projection operator formalism [14], a recent hyperspherical calculation [15], and experimental results [16]. The resonant calculations were carried out using a 20×20 grid with $r_{\max} = 64$.

Notice that in a direct solution of the Schrödinger equation, only the asymptotically open channels are included when imposing the boundary conditions, if the matching radius $r_{\max}$ is large enough. For the elastic case, only the 1s channel is included, even in the resonant energy region. The drawback of this method is that the collision parameters that vary slowly with energy [7, 15, 17] are not extracted directly. The extension to multichannel scattering is straightforward in principle. If there are N_c open channels, then the boundary condition for a state in incident channel i contains the N_c unknown reactance matrix elements K_{ji}, instead of the single phase shift. In imposing these conditions, N_c values of the radial functions are left arbitrary on the boundary. After obtaining these values from the FEM calculation, they can be used to compute the ith column of the K matrix. This work is in progress and results will be reported elsewhere.

We have presented an alternative method for solving the Schrödinger equation for quantum scattering problems. We illustrated the validity and accuracy of this method for elastic scattering of electrons off atomic hydrogen. The advantages and applications of this approach are manyfold. It gives directly both the collision

TABLE I. Singlet and triplet elastic phase shifts.

	k	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$^1S^e$	R matrix[a]	2.550	2.062	1.691	1.410	1.196	1.035	0.925	
	Variational[b]	2.553	2.0673	1.6964	1.4146	1.202	1.041	0.930	0.886
	FEM[c]	2.553	2.066	1.695	1.414	1.200	1.040	0.930	0.887
$^3S^e$	R matrix[a]	2.939	2.717	2.500	2.294	2.105	1.933	1.780	
	Variational[b]	2.9388	2.7171	2.4996	2.2938	2.1046	1.9329	1.7797	1.643
	FEM[c]	2.938	2.717	2.500	2.294	2.104	1.933	1.780	1.645
$^1P^o$	R matrix[a]	0.006	0.015	0.016	0.009	-0.002	-0.012	-0.016	
	Variational[d]	0.007	0.0147	0.0170	0.0100	-0.0007	-0.009	-0.013	-0.004
	FEM[e]	0.0060	0.0148	0.0160	0.0090	-0.0020	-0.0117	-0.0149	-0.0068
$^3P^o$	R matrix[a]	0.010	0.045	0.107	0.187	0.270	0.341	0.392	
	Variational[d]	0.0114	0.0450	0.1063	0.1872	0.2705	0.3412	0.3927	0.427
	FEM[e]	0.0100	0.0452	0.1067	0.1873	0.2708	0.3417	0.3933	0.4283
$^1D^e$	R matrix[a]	0.0013	0.0051	0.0109	0.0183	0.0272	0.0379	0.0518	
	Variational[f]	0.0012	0.0052	0.0108	0.0183	0.0274	0.0383	0.0523	0.0745
	FEM[g]	0.0007	0.0048	0.0105	0.0182	0.0271	0.0379	0.0518	0.0745
$^3D^e$	R matrix[a]	0.0013	0.0052	0.0114	0.0197	0.0301	0.0421	0.0553	
	Variational[f]	0.0013	0.0052	0.0114	0.0198	0.0304	0.0424	0.0549	0.0697
	FEM[g]	0.0007	0.0049	0.0110	0.0196	0.0300	0.0422	0.0554	0.0699
$^1F^o$	FEM[h]	0.0000	0.0016	0.0037	0.0065	0.0101	0.0145	0.0199	0.0264
$^3F^o$	FEM[h]	0.0000	0.0016	0.0037	0.0065	0.0102	0.0148	0.0204	0.0271

[a] From Ref. [6].

[b] From Ref. [1].

[c] $|l_1l_2\rangle = |00\rangle, |11\rangle, |22\rangle, |33\rangle$.

[d] From Ref. [2].

[e] $|l_1l_2\rangle = |10\rangle, |01\rangle, |21\rangle, |12\rangle, |32\rangle, |23\rangle$.

[f] From Ref. [3].

[g] $|l_1l_2\rangle = |20\rangle, |02\rangle, |31\rangle, |13\rangle, |11\rangle, |22\rangle$.

[h] $|l_1l_2\rangle = |30\rangle, |03\rangle, |12\rangle, |21\rangle, |14\rangle, |41\rangle$.

TABLE II. Resonances below the $n = 2$ threshold.

		Position (eV)	Width (eV)
$^1S^e$	R matrix[a]	9.5572	0.0471
	CCR[b]	9.55737	0.04710
	FPO[c]	9.55735	0.04717
	Hyperspherical[d]	9.559	0.0475
	FEM	9.559	0.0481
	Experiment[e]	9.549	0.063
$^3P^o$	R matrix[a]	9.7382	0.00582
	CCR[b]	9.7381	0.00580
	Hyperspherical[d]	9.745	0.00765
	FEM	9.738	0.0057
	Experiment[e]	9.736	0.005
$^1D^e$	R matrix[a]	10.1253	0.00881
	CCR[b]	10.12436	0.00862
	Hyperspherical[d]	10.129	0.0101
	FEM	10.127	0.0075
	Experiment[e]	10.115	0.006

[a] From Ref. [6].

[b] Complex coordinate rotation, from Refs. [11–13].

[c] Feshbach projection operator, from Ref. [14].

[d] From Ref. [15].

[e] From Ref. [16].

parameters and the wave function over the entire space for each partial wave. Transition amplitudes may then be calculated without much effort. The method may be easily extended to electron scattering from H-like atoms by replacing the Coulomb potential in the Hamiltonian by an effective potential. The procedure presented here may also be applied easily to the study of bound and doubly excited states of two-electron atoms with arbitrary total angular momentum, by imposing the much simpler bound-state boundary conditions [18].

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[1] C. Schwartz, Phys. Rev. **124**, 1468 (1961).
[2] R. L. Armstead, Phys. Rev. A **171**, 91 (1968).
[3] D. Register and R. T. Poe, Phys. Lett. **51A**, 431 (1975).
[4] P. G. Burke, H. M. Schey and K. Smith, Phys Rev. **129**, 1258 (1963), and references therein.
[5] J. Callaway and J. W. Wooten, Phys. Rev. A **9**, 1924 (1974); J. Callaway, *ibid.* **26**, 199 (1982); **32**, 775 (1985).
[6] T. Scholz, P. Scott, and P. G. Burke, J. Phys B **21**, L139 (1988).
[7] H. R. Sadeghpour, C. H. Greene, and M. Cavagnero, Phys. Rev. A **45**, 1587 (1992).
[8] K. J. Bathe, *Finite Element Procedures in Engineering Analysis* (Prentice-Hall, Englewood Cliffs, NJ, 1982); K. J. Bathe and E. Wilson, *Numerical Methods in Finite Element Analysis* (Prentice Hall, Englewood Cliffs, NJ, 1976); L. R. Ram-Mohan, S. Saigal, D. Dossa, and J. Shertzer, Comput. Phys. **4**, 50 (1990).
[9] F. S. Levin and J. Shertzer, Phys. Rev. Lett. **61**, 1089 (1988).
[10] B. J. Archer, G. A. Parker, and R. T. Pack, Phys. Rev. A **41**, 1303 (1990).
[11] Y. K. Ho, Phys. Rev. A **23**, 2137 (1981).
[12] Y. K. Ho, J. Phys. B **23**, L71 (1990).
[13] A. K. Bhatia and Y. K. Ho, Phys. Rev. A **41**, 504 (1990).
[14] Y. K. Ho, A. K. Bhatia, and A. Temkin, Phys. Rev. A **15**, 1423 (1977).
[15] H. Sadeghpour, J. Phys. B **25**, L29 (1992).
[16] C. D. Warner, G. C. King, P. Hammond and J. Slevin, J. Phys. B **19**, 3297 (1986).
[17] U. Fano and A. R. P. Rau, *Atomic Collisions and Spectra* (Academic, Orlando, FL, 1986).
[18] J. Shertzer and F. S. Levin, Phys. Rev. A **43**, 2531 (1991).