Finite-Element Analysis of Low-Energy e^+-H Scattering

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Accurate S-wave phase shifts for low-energy ($0.1 \leq k \leq 0.7$) positron-hydrogen scattering have been calculated by use of the finite-element method. Simple criteria are developed for which the truncation of the relevant configuration space and its subsequent discretization appear to be optimized. These criteria are expected to be independent of the details of the collision system.

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In this article we describe some details of a successful calculation of the S-wave phase shifts for low-energy, positron-hydrogen scattering using the finite-element method.[1] This method has been applied to a variety of physical problems over the past years.[2-7] Its use here is the first time that the e^+-H scattering problem has been solved without the use of Hylleraas functions. Since the accuracy of the phase shifts obtained via the finite-element method (FE) is comparable to that obtained in previous calculations, the FE method is thus shown to be a feasible numerical alternative for solving few-particle atomic scattering problems.

Because it is simple and direct, there are several advantages to our using the FE method: First, the Schrödinger equation is solved numerically, subject to the appropriate scattering boundary conditions; second, no globally defined expansion basis is required; and third, electron-positron correlation is automatically incorporated into the wave function. In addition, there is no difficulty, in theory, in extending this approach to many-particle systems.

In the past, the application of the FE method to even the simplest systems has been limited because of the long central processing unit (CPU) times required for the generation and inversion of the large FE matrices. However, the FE algorithm is well suited for vectorization, and the use of array processors has typically led to greatly reduced CPU time. In the present case, a factor of 10 reduction was achieved with a STAR array processor to generate the FE matrices. Thus, problems previously deemed formidable are now within computational limits. The rapid advance in computer technology suggests that the FE approach will continue to be an attractive alternative for solving problems in atomic and molecular physics.

In the next section of the paper, the FE formulation of the e^+-H scattering problem is described. Since extensive literature exists on the subject of finite elements,[1] including applications to quantal bound-state and scattering problems,[2-7] only a brief outline of the algorithm is given. Results of the calculation are then presented and compared with the phase shifts obtained in seven previous calculations,[8-14] including the highly accurate bound calculations of Bhatia *et al.*[9]

The FE method is a numerical algorithm for solving operator equations via the use of piecewise interpolating polynomials. In the present case, we apply the method to the Schrödinger equation for S-wave elastic scattering of positrons from atomic hydrogen, viz.,

$$-\frac{1}{2r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial\psi}{\partial r}\right]-\frac{1}{2s^2}\frac{\partial}{\partial s}\left[s^2\frac{\partial\psi}{\partial s}\right]-\frac{1}{2}\left[\frac{1}{r^2}+\frac{1}{s^2}\right]\frac{\partial}{\partial\cos\theta}\left[(1-\cos^2\theta)\frac{\partial\psi}{\partial\cos\theta}\right]+\left[-\frac{1}{r}+\frac{1}{s}-\frac{1}{|\mathbf{r}-\mathbf{s}|}-E\right]\psi=0, \quad (1)$$

where r is the electron-proton distance, s is the positron-proton distance, and $\cos\theta=(\mathbf{r}\cdot\mathbf{s})/rs$. (Atomic units are used throughout.) The total energy is $E=(k^2-1)/2$, where k is the positron momentum. The asymptotic boundary conditions for E below the threshold for positronium formation are

$$\psi(r\to\infty,s,\cos\theta)\to 0 \quad (2a)$$

and

$$\psi(r,s\to\infty,\cos\theta)\to\exp(-r)\left[\frac{\sin(ks)}{s}+\tan\delta\frac{\cos(ks)}{s}\right], \quad (2b)$$

where δ is the unknown S-wave phase shift.

In our solving Eq. (1) by the FE approach, the coordinate space spanned by r, s, and $\cos\theta$ is truncated by choosing cutoff values for r and s, at which points it is assumed appropriate to impose the asymptotic boundary conditions. The truncated three-dimensional space is then discretized into small elements by the placement of nodes, which become the corners of the (three dimensional) elements.

In each element n, the global wave function ψ is approximated by a local wave function ψ^n, given as a linear combination of products of cubic Hermite polynomials[1]:

$$\psi^n(r,s,\cos\theta)=\sum_{i=1}^{4}\sum_{j=1}^{4}\sum_{k=1}^{4}\psi^n_{ijk}\phi_i(r)\phi_j(s)\phi_k(\cos\theta). \tag{3}$$

The polynomials ϕ are defined only within a particular element and have the unique property that the expansion coefficients ψ^n_{ijk} are the value of the unknown wave function (and seven partial derivatives) at the eight nodes of the element.[6] Substituting Eq. (3) into Eq. (1) and integrating over the volume of the element, one obtains a set of linear coupled equations for each of the ψ^n_{ijk}, which in vector form are

$$(\mathbf{H}^n-E\mathbf{U}^n)\boldsymbol{\psi}^n=0. \tag{4}$$

The local matrices $\mathbf{H}^n$ and $\mathbf{U}^n$ are symmetric and of order 64. Note that $\mathbf{U}^n$ is not the ordinary unit matrix, but involves the product of the Hermite polynomials integrated over the volume of the element. The integration is done numerically, with eight-point Gauss quadrature.

In order to guarantee the continuity of the global wave function, the locally defined functions ψ^n must be smoothly matched at the element boundaries. This is achieved by our mapping the local matrix $\mathbf{H}^n$ for each element onto a single global matrix $\mathbf{H}$, and similarly, mapping $\mathbf{U}^n$ for each element onto a global matrix $\mathbf{U}$. The global matrices are symmetric and sparse. The local vector $\boldsymbol{\psi}^n$ for each element is mapped onto a single global vector $\boldsymbol{\psi}$ of order $8N$, where N is the total number of nodes in the three-dimensional grid.

Boundary conditions are imposed on the global equations by requiring that the components of $\boldsymbol{\psi}$ corresponding to a node at $r=r_c$ satisfy Eq. (2a); similarly, components of $\boldsymbol{\psi}$ corresponding to a node at $s=s_c$ are required to satisfy Eq. (2b). The linear coupled equations can be expressed as

$$(\mathbf{H}-E\mathbf{U})\boldsymbol{\psi}=\mathbf{A}+\tan\delta\,\mathbf{B}, \tag{5}$$

where $\mathbf{A}$ and $\mathbf{B}$ are the vectors obtained when $\mathbf{H}-E\mathbf{U}$ operates on the components of $\boldsymbol{\psi}$ which are determined from the boundary conditions. The order of the global matrices in Eq. (5) is $8(N-M)$, where M is the number of boundary nodes, i.e., nodes at $r=r_c$ or $s=s_c$. One can now solve Eq. (5) for the remaining unknown expansion coefficients corresponding to the value of the wave function (and its derivatives) at the nonboundary nodes. The global wave function $\psi(r,s,\cos\theta)$ is obtained by our multiplying the expansion coefficients by the locally defined basis set given in Eq. (3). Introducing the vector $\boldsymbol{\phi}$, whose components are the products of the Hermite polynomials for each global node, one can express the global function ψ as a scalar product of two vectors:

$$\psi(r,s,\cos\theta)=[(\mathbf{H}-E\mathbf{U})^{-1}(\mathbf{A}+\tan\delta\,\mathbf{B})]\cdot\boldsymbol{\phi}(r,s,\cos\theta). \tag{6}$$

Using Eq. (6) in the integral formula for the phase shift,[15] one obtains an expression for $\tan\delta$,

$$\tan\delta=\frac{2k^{-1}\int[(\mathbf{H}-E\mathbf{U})^{-1}\mathbf{A}]\cdot\boldsymbol{\phi}e^{-r}[\sin(ks)/s][-2s^{-1}+2/|\mathbf{r}-\mathbf{s}|]r^2s^2\,dr\,ds\,d\cos\theta}{1-2k^{-1}\int[(\mathbf{H}-E\mathbf{U})^{-1}\mathbf{B}]\cdot\boldsymbol{\phi}e^{-r}[\sin(ks)/s][-2s^{-1}+2/|\mathbf{r}-\mathbf{s}|]r^2s^2\,dr\,ds\,d\cos\theta}. \tag{7}$$

Although one can in principle extract the phase shift directly from the FE wave function, the results are so extremely sensitive to the accuracy of the wave function at s_c that it is difficult to obtain stable values for $\tan\delta$. On the other hand, phase shifts obtained via Eq. (7) are remarkably insensitive to the accuracy of the FE wave function near s_c. The integral-formula approach is also a better indicator of the overall accuracy of the calculated wave function, particularly in the region where the positron-hydrogen interaction is strong.

The accuracy of the FE solution depends on both the truncation and the discretization. It is evident that one must choose the cutoff values r_c and s_c large enough to guarantee that the appropriate asymptotic behavior can be imposed, yet small enough to avoid excessive CPU times. In the present case, r_c was set at $8a_0$, on the basis of previous FE calculations on atomic hydrogen.

Many test cases were required before criteria were determined for choosing s_c, since our initial studies led to unstable values of $\tan\delta$. Stability was fairly well achieved when s_c was made large enough to include a full de Broglie length λ, where $\lambda=2\pi/k$. (For $k=0.1$, keeping CPU time to a manageable amount meant that s_c was smaller than a full wavelength, thus leading to a slightly higher error in $\tan\delta$ than for other values of k; note also that this is the only case where the phase shift lies above the value obtained by Bhatia *et al.*) In addition, the error in $\tan\delta$ was significantly reduced if s_c was chosen such that $\tan(ks_c)=1$. This is accounted for by our noting that the asymptotic wave function, Eq. (2b), is a linear combination of $\sin(ks)/s$ and $\cos(ks)/s$, and in order to extract an accurate value of $\tan\delta$, the error in both terms should be minimized. Both of these functions and their derivatives are smooth when $\tan(ks)=1$ and the error in matching the FE solution to the asymptotic

TABLE I. Finite-element nodes for e^+-H scattering.

k	Nodes along s (and r, $r \leq 8a_0$)	Number of elements	δ
0.1	0 1 2 4 6 8 12 16 24 32 39.27	200	0.152
0.2	0 1 2 4 6 8 12 18 24 30 35.34	200	0.188
0.3	0 1 3 5 8 11 14 17 20 23.56	144	0.166
0.4	0 1 3 5 8 11 14 17 20 23 25.52	160	0.118
0.5	0 1 3 5 8 11 14 17 20.42	128	0.061
0.6	0 1 3 5 8 11 14 17 20 22.25	144	0.003
0.7	0 1 3 5 8 11 14 17 19.07	128	−0.053

wave function is therefore minimized, resulting in a more accurate value for the phase shift.

Ideally, one would like first to determine r_c and s_c and then experiment with the grid. In practice, the variation of both the cutoff values and the location of the nodes must be carried out simultaneously. One of the particular goals of this calculation was to determine a method for choosing an optimal grid that does not rely on a comparison of the FE phase shift with those determined by other means. No rigorous lower-bound principle is valid in this case; in addition, numerical error may arise from truncation, discretization, or the numerical integration of Eq. (7). It is important to note that a larger error in the wave function can be tolerated in regions of space where the contribution to the phase-shift integral is small, whereas the wave function must be reasonably accurate in the regions of space where the contribution to the integral of Eq. (7) is large.

An optimal discretization for $\cos\theta$ was relatively easy to establish and was independent of the incident positron momentum. All reported calculations were done with only five $\cos\theta$ nodes, placed at $\cos\theta = -1$, -0.2, 0.5, 0.94, and 1, a grid that reflects the strength of the potential as a function of the angular separation.

In order to obtain the best positron-electron correlation, an identical discretization in r and s was used for values less than r_c. The phase shift was most sensitive to the discretization in the region $s < r_c$, where the potential is strongest and the contribution to the phase-shift integral is the largest. For $k \geq 0.3$, the contribution to the phase-shift integral is extremely small beyond $s = 5a_0$. This is not true for smaller incident positron momentum. As a result, a slightly finer discretization is used for $k = 0.2$ and 0.1 in this region. For $k = 0.1$, there is a small but significant contribution to the phase-shift integral even beyond $s = 8a_0$; since the grid spacing is larger in the region $s > 8a_0$, this may contribute numerical error in the integration of Eq. (7) for this case.

For $r_c \leq s \leq s_c$, nodes were evenly spaced at intervals of $3a_0$ for $k \geq 0.3$. It is worth noting that for the case of $k = 0.7$, a mere three nodes per de Broglie wavelength was sufficient to approximate the wave function in this region. Since the de Broglie wavelength is much larger for $k = 0.2$ and $k = 0.1$, the interval size was increased to $6a_0$ and $8a_0$, respectively. All results were very stable with respect to variation of the nodes in this region, and in some cases, even larger intervals gave accurate results.

Table I lists the node sites for r and s and the values of the phase shift. It should be noted that in some cases, it is possible to improve individual phase shifts slightly by the adjustment of the location of the nodes in particular regions of space. However, the point of this calculation is to show that using the criteria for discretization and truncation that we have developed, one can obtain accurate results for elastic scattering without attempting to optimize the mesh at each energy. Furthermore, the phase shifts are stable to within 0.002 for small variations in the mesh. Therefore, we have chosen to quote the results using almost identical grids for each value of incident positron momentum. With a STAR array processor to generate the FE matrices, the total CPU time for each phase shift was less than 1 h. The FE results are compared with phase shifts obtained from other calculations in Table II.

In conclusion, we have shown that the FE method offers an alternative approach to solving few-body scattering problems. In implementing the FE method, we have developed a simple algorithm for truncation and discretization that is expected to be independent of the details of the system.

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TABLE II. Comparison of S-wave phase shifts for e^+-H scattering.

Reference \ k		0.1	0.2	0.3	0.4	0.5	0.6	0.7
Finite element		0.152	0.188	0.166	0.118	0.061	0.003	−0.053
Schwartz	8	0.151	0.188	0.168	0.120	0.062	0.007	−0.054
Bhatia *et al.*	9	0.1483	0.1877	0.1677	0.1201	0.0624	0.0039	−0.0512
Houston and Drachman	10	0.149	0.189	0.169	0.123	0.065	0.008	−0.049
Stein and Sternlicht	12	0.148	0.187	0.167	0.120	0.062	0.003	−0.052
Register and Poe	13	0.146	0.185	0.165	0.117	0.059	0.000	−0.057
Doolen *et al.*	11	0.146	0.183	0.164	0.119	0.062	0.003	−0.052
Winick and Reinhardt	14	0.149	0.177	0.155	0.119	0.064	0.003	−0.051

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