APPLICATION OF THE FINITE ELEMENT METHOD TO ATOMIC AND MOLECULAR PHYSICS

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ABSTRACT

The finite element method (FEM) is a numerical algorithm for solving second order differential equations. It has been successfully used to solve many problems in atomic and molecular physics, including bound state and scattering calculations. To illustrate the diversity of the method, we present here details of two applications. First, we calculate the non-adiabatic dipole polarizability of H_2^+ by directly solving the first and second order equations of perturbation theory with FEM. In the second application, we calculate the scattering amplitude for e-H scattering (without partial wave analysis) by reducing the Schrödinger equation to set of integro-differential equations, which are then solved with FEM.

I. INTRODUCTION

The finite element method (FEM) is a powerful numerical tool for solving differential equations, including eigenvalue problems [1]. FEM utilizes a piecewise interpolation scheme, in which the unknown function is approximated locally by a simple polynomial. Although the method was originally developed to solve problems in structural mechanics, Frank Levin was one of the first to recognize that FEM could be used to study few-body systems [2]. For bound states, FEM has been used to calculate to high accuracy the energy and structure of three-body Coulomb systems with arbitrary masses [3]. Another important application is the study of atoms and molecules in strong external fields [4]; when the wave function is strongly distorted, the piecewise interpolation approach is often superior to standard hydrogenic or Gaussian basis set expansion. FEM can also be used to study collisions, where the complicated boundary conditions associated with scattering can be treated in a straightforward fashion. Accurate phase shifts and inelastic cross sections have been calculated for e-H collisions for $0 \le L \le 3$ [5]. For the Temkin-Drachman Retirement Symposium, I have selected two FEM examples which reflect the research interests of the honorees.

Richard Drachman has contributed greatly to our understanding of long-range interactions. In his series of papers on the Rydberg states of Helium [6] and Lithium [7], he has provided a rigorous theoretical description for Rydberg atoms based on an effective polarization potential. An important extension of this work has been the formulation of an effective polarization potential for the Rydberg electron of H_2; microwave spectroscopy of high Rydberg states provided a mechanism for determining the multipole moments of the ionic core, including the static dipole polarizability [8].

The measurement of α_s for H_2^+ motivated several groups (including Drachman and Bhatia [9]), to calculate the polarizability of H_2^+ without invoking the Born-Oppenheimer approximation. In section II, we present a description of a FEM calculation of the dipole polarizability of H_2^+.

Aaron Temkin's contributions to scattering theory have had a major and lasting impact on the field. With his method of polarized orbitals [10], he was the first to include the effects of polarization and exchange in the ansatz for the wavefunction. In 1962, he introduced the now famous Temkin-Poet model [11]. For the past eight years, I have had the privilege to collaborate with Aaron, pursuing a new approach to scattering that does not use partial wave analysis. The scattering amplitude is calculated directly by solving a set of coupled integro-differential equations. Section III summaries our progress to date and outlines our plans for the future. Atomic units are used throughout.

II. NONADIABATIC DIPOLE POLARIZABILITY OF H_2^+

In the late 90's, experiments on the Rydberg states of H_2 provided a mechanism for determining the static dipole polarizabiltiy of H_2^+ to high precision [8]. At that time, the only theoretical calculation for α_s employed the Born-Oppenheimer approximation [12]. Given the accuracy of the new results, it was not surprising that there was a discrepancy between the experimental value α_s =3.1681(7) and the theoretical value α_s^{BO}=3.1713 on the order of m_e / m_p. This breakdown of the Born-Oppenheimer approximation motivated several groups to attempt a non-adiabatic calculation of the dipole polarizability.

The static dipole polarizability α_s is defined in terms of the second order correction to the energy due to the presence of an external electric field $\vec{\varepsilon}$:

$$E^{(2)} = -\tfrac{1}{2}\alpha_s \varepsilon^2 = \left\langle \Psi^{(1)}(\vec{r},\vec{R}) \,|\, (1+\delta)\,\vec{\varepsilon}\cdot\vec{r} \,|\, \Psi^{(0)}(\vec{r},\vec{R}) \right\rangle \tag{1}$$

where $(1+\delta) = \frac{(2m_p+2)}{(2m_p+1)}$. In the variational approach, the first order correction to the wave function is expanded in a basis set that includes nuclear and electronic states. Using FEM, one can solve directly the first and second order equations of perturbation theory [13]. The first step is to carry out the frame transformation that reduces the number of variables in the problem.

Frame transformation

In the space-fixed laboratory frame (x', y', z'), the electric field is aligned with the z'-axis (see Fig. 1). After separating out the center-of mass motion, the (field-free) Hamiltonian for the relative motion is given by

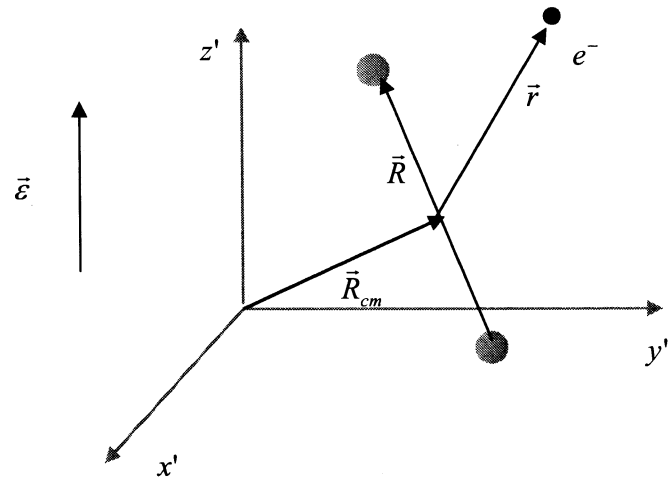

Figure 1. H_2^+ in the space-fixed (laboratory frame). $\vec{\varepsilon}$ indicates the direction of the external electric field.

$$H = -\frac{1}{2\mu}\nabla_R^2 - \left(\frac{1}{2}+\frac{1}{8\mu}\right)\nabla_r^2 + V(\vec{R},\vec{r}) \tag{2}$$

where

$$V(\vec{R},\vec{r}) = \frac{1}{R} - \frac{1}{|\vec{r}+\frac{\vec{R}}{2}|} - \frac{1}{|\vec{r}-\frac{\vec{R}}{2}|} \tag{3}$$

and $\mu = m_p/2$.

The vector $\vec{R}$ lies along the internuclear axis and $\vec{r}$ is the vector from the center of the internuclear axis to the electron. The Hamiltonian commutes with L^2 and $L_{z'}$ and in general, the non-adiabatic wave function $\Psi(L, M'; \vec{r}, \vec{R})$ depends on all six coordinates.

To simplify the problem, we perform a rotation $\Re(\Phi', \Theta', 0)$ which leaves the internuclear axis aligned with the new z-axis. It appears that we have eliminated two degrees of freedom, since the wave function is now a function of only $\vec{r}$ and R. But there is a price to pay for this frame transformation. The Hamiltonian does not commute with L_z; M is not a good quantum number and the Hamiltonian is not diagonal in the basis spanned by the eigenstates of L^2 and L_z. The electric field, which appears in the matrix element of Eq. (1), is now a function of the Euler angles

$$\vec{\varepsilon} = \varepsilon(-\sin\Theta'\,\hat{x} + \cos\Theta'\,\hat{z}). \tag{4}$$

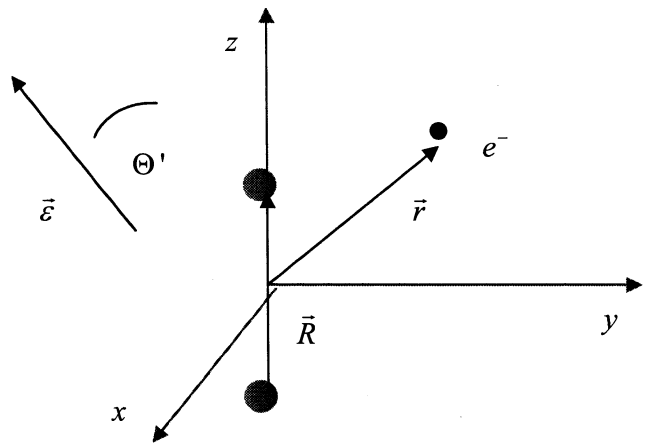

Figure 2. H_2^+ in the body-fixed frame. $\vec{\varepsilon}$ indicates the direction of the external electric field.

Despite these complications, it is still desirable to work in the body-fixed frame. Ultimately, we must reduce the problem to a solution of a set of differential equations in three variables if we are to apply the FEM.

The space-fixed wave function (with 'good' quantum numbers *L, M'*) is a linear combination of the body-fixed wave functions,

$$\Psi_{SF}(L, M'; \vec{r}, \vec{R}) = \sum_{M=-L}^{L} D^{L}_{MM'}(\Phi', \Theta', 0)\Psi_{BF}(L, M; \vec{r}, R) \tag{5}$$

where $D^{L}_{MM'}(\Phi', \Theta', 0)$ are the coefficients of the irreducible representation associated with the rotation $\Re(\Phi', \Theta', 0)$. The Hamiltonian in the body-fixed frame is given by

$$H = \frac{1}{2\mu}\left[p_R^2 + \frac{1}{R^2}\left(L^2 + L_e^2 - 2L_z^2 - L_{e-}L_+ - L_{e+}L_-\right)\right] + \left(\frac{1}{2} + \frac{1}{8\mu}\right)\left[p_r^2 + \frac{1}{r^2}L_e^2\right] + V(\vec{r}, R) \tag{6}$$

where

$$L_{\pm}\Psi_{BF}(L, M; \vec{r}, R) = \sqrt{L(L+1) - M(M \pm 1)}\,\Psi_{BF}(L, M \pm 1; \vec{r}, R). \tag{7}$$

Perturbation Theory

We now return to the evaluation of the matrix element in Eq. (1). It is clear that we must start in the space-fixed frame, where the 'good' quantum numbers associated with the unperturbed ground state are $L = 0$ and $M' = 0$; from the Wigner-Eckart theorem, we know that the first order correction to the wave function must be a state with $L = 1$ and $M' = 0$. Therefore, we re-express Eq. (1) more precisely as

$$E^{(2)} = -\tfrac{1}{2}\alpha_s \varepsilon^2 = \left\langle \Psi_{SF}^{(1)}(1,0;\vec{r},\vec{R}) \,|\, (1+\delta)\,\vec{\varepsilon}\cdot\vec{r} \,|\, \Psi_{SF}^{(0)}(0,0;\vec{r},\vec{R}) \right\rangle \tag{8}$$

where $\Psi_{SF}^{(0)}$ and $\Psi_{SF}^{(1)}$ are found by solving the zeroth and first order equations of perturbation theory:

$$H\,\Psi_{SF}^{(0)}(0,0;\vec{r},\vec{R}) = E^{(0)}\Psi_{SF}^{(0)}(0,0;\vec{r},\vec{R}) \tag{9a}$$

$$(H - E^{(0)})\Psi_{SF}^{(1)}(1,0;\vec{r},\vec{R}) = -(1+\delta)\,\vec{\varepsilon}\cdot\vec{r}\;\;\Psi_{SF}^{(0)}(1,0;\vec{r},\vec{R}). \tag{9b}$$

For the special case $L = 0$, $M' = 0$, there is a one-to-one correspondence between the space-fixed wave function and the body-fixed wave function

$$\Psi_{SF}^{(0)}(0,0;\vec{r},\vec{R}) = \Psi_{BF}^{(0)}(0,0;\vec{r},R). \tag{10}$$

The body-fixed Hamiltonian is diagonal since $L_{\pm}\Psi_{BF}^{(0)}(0,0;\vec{r},R)$=0. Furthermore, the wave function is independent of the electronic azimuthal angle ϕ, and the resultant differential equation (in three variables)

$$\left\{\frac{1}{2\mu}\left[p_R^2 + \frac{1}{R^2}L_e^2\right] + \left(\frac{1}{2} + \frac{1}{8\mu r^2}\right)\left[p_r^2 + \frac{1}{r^2}L_e^2\right] + V(\vec{r},R) - E^{(0)}\right\}\Psi_{\mathrm{BF}}^{(0)}(0,0;r,\theta,R) = 0 \tag{11}$$

can be solved with FEM for the ground state energy and wave function. We obtained $E^{(0)} = -0.597\,139\,055(8)$.

In order to obtain the first order correction to the wave function, we need to solve Eq. (9b) by transforming it to the body-fixed frame. The zeroth order wave function $\Psi_{SF}^{(0)}$ is given by Eq. (10) and the dipole interaction is given by

$$\vec{\varepsilon}\cdot\vec{r} = \varepsilon\, r(\cos\Theta'\cos\theta - \sin\Theta'\sin\theta\cos\phi). \tag{12}$$

Using Eq. (5), the first order correction to the wave function $\Psi_{SF}^{(1)}$ is re-expressed in the body-fixed frame as

$$\Psi_{SF}^{(1)}(1,0;\vec{r},\vec{R}) = \cos\Theta'\,\Psi_{BF}^{(1)}(1,0;\vec{r},R) + \tfrac{1}{\sqrt{2}}\sin\Theta'\,[\Psi_{BF}^{(1)}(1,1;\vec{r},R) - \Psi_{BF}^{(1)}(1,-1;\vec{r},R)]\,; \tag{13}$$

the (body-fixed) Hamiltonian is given by Eq. (6).

The resultant coupled equations depend on the five variables Θ', r, θ, ϕ and R. Equating terms that multiply $\cos\Theta'$ and $\sin\Theta'$, we can eliminate the dependence on the Euler angle Θ'. We are left with three coupled differential equations for the body-fixed wave functions $\Psi_{BF}^{(1)}(1, M;\vec{r},R)$, $M = 0,\pm 1$. The dependence on the electronic azimuthal angle ϕ can be obtained analytically; one can show that the wave functions must be of the form

$$\Psi_{BF}^{(1)}(1,0;\vec{r},R) = \varepsilon\, f(r,\theta,R) \tag{14a}$$

$$\Psi_{BF}^{(1)}(1,\pm 1;\vec{r},R) = \pm\tfrac{1}{\sqrt{2}}\,\varepsilon\, g(r,\theta,R)\,\mathrm{e}^{\pm i\phi}\,. \tag{14b}$$

Thus we have reduced the problem to a set of two coupled equations in three variables:

$$\left[H_{00} - E^{(0)}\right] f(r,\theta,R) + \frac{1}{\mu R^2}\left(\frac{\partial}{\partial\theta} + \cot\theta\right) g(r,\theta,R) = -r\cos\theta\,\Psi_{BF}^{(0)}(r,\theta,R) \tag{15a}$$

$$\left[H_{11} - E^{(0)} + \left(\frac{1}{2\mu R^2} + \frac{1}{2r^2} + \frac{1}{8\mu r^2}\right)\frac{1}{\sin^2\theta}\right] g(r,\theta,R) + \frac{1}{\mu R^2}\frac{\partial}{\partial\theta} f(r,\theta,R) = r\sin\theta\,\Psi_{BF}^{(0)}(r,\theta,R) \tag{15b}$$

where

$$H_{MM} = \frac{1}{2\mu}\left[p_R^2 + \frac{1}{R^2}(L_e^2 + 2\delta_{M,0})\right] + \left(\frac{1}{2} + \frac{1}{8\mu}\right)\left[p_r^2 + \frac{1}{r^2}L_e^2\right] + V(\vec{r},R)\,. \tag{16}$$

Eqs. (15a) and (15b) are solved with FEM. Once we know $f(r,\theta,\phi)$ and $g(r,\theta,\phi)$ we can construct the first order correction to the wave function and evaluate the matrix element of Eq. (8) to determiner α_s.

In Table I, we compare the FEM value of α_s with the experimental value and several variational calculations; also included is the Born-Oppenheimer result. It is interesting to note that there remains a discrepancy between the theoretical and experimental value of α_s, that cannot be accounted for by relativistic corrections.

TABLE I. Experimental and theoretical values for the dipole-polarizability of H_2^+.

Author (year)	Ref.	α_s
Bishop and Lamb (1988) *Born-Oppenheimer*	[12]	3.1713
Jacobson et. al (1997) *Experiment*	[8]	3.168 1(7)
Shertzer and Greene (1998)	[13]	3.168 2(4)
Bhatia and Drachman (1999)	[9]	$3.168\,0^{+.0018}_{-.0001}$
Taylor *et al.* (1999)	[14]	3.168 725 6(1)
Moss (1999)	[15]	3.168 726
Jacobson *et al.* (2000) *Experiment*	[16]	3.167 96(15)
Korobov (2001)	[17]	3.168 725 76
Hilico *et al.* (2001)	[18]	3.168 725 803(1)
Yan *et al.* (2003)	[19]	3.168 725 802 67(1)

DIRECT CALCULATION OF THE SCATTERING AMPLITUDE

We present here a new approach to scattering which does not use partial wave analysis [20]. The basic idea is to reduce the Schrödinger equation to a set of coupled integro-differential equations that can be solved with FEM for the scattering wave function. The wave function is then used in the integral expression for the scattering amplitude.

e-H Scattering (static approximation with exchange)

Our first application is electron-hydrogen scattering in the static approximation (with exchange). The trial wave function is given by

$$\Psi_k^{\pm}(\vec{r}_1,\vec{r}_2) = \psi_k^{\pm}(\vec{r}_1)\phi_{1s}(r_2) \pm \psi_k^{\pm}(\vec{r}_2)\phi_{1s}(r_1), \tag{17}$$

where $\psi_k^{\pm}(\vec{r})$ is an unknown function. We require that the wave function satisfy the Schrödinger equation for the two-electron system subject to the asymptotic boundary condition

$$\psi_k^{\pm}(\vec{r}) \to e^{ikr\cos\theta} + f_k^{\pm}(\theta)\frac{e^{ikr}}{r} \tag{18}$$

as $r \to \infty$. Projecting the Schrödinger equation onto $\phi_{1s}(r_2)$, we have

$$\left\langle \phi_{1s}(r_2) \middle| \nabla_1^2 + \nabla_2^2 + \frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}} + k^2 - 1 \middle| \Psi_k^{\pm}(\vec{r}_1,\vec{r}_2) \right\rangle = 0 \tag{19}$$

Carrying out the integration over the coordinates of the second electron, we are left with a integro-differential equation for the unknown function $\psi_k^{\pm}$:

$$\left[\nabla^2 + V(r) + k^2\right]\psi_k^{\pm}(\vec{r}) \;\; \pm (k^2+1)\phi_{1s}(r)\left\langle \phi_{1s} \mid \psi_k^{\pm}\right\rangle \pm \; \phi_{1s}(r)\left\langle \phi_{1s}\right| \tfrac{-2}{|\vec{r}-\vec{r}'|}\left|\psi_k^{\pm}\right\rangle = 0\,. \tag{20}$$

where $V(r) = 2e^{-2r}(1+\frac{1}{r})$.

Although FEM can be applied to integro-differential equations, the last term $\left\langle \phi_{1s}\right| \frac{-2}{|\vec{r}-\vec{r}'|}\left|\psi_k^{\pm}\right\rangle$ is problematic because it involves a numerical integration over d^3r' for *each* value of $\vec{r}$. This is computationally prohibitive. To eliminate this problem, we introduce a new function

$$\alpha_k^{\pm}(\vec{r}) = \left\langle \phi_{1s} \mid \tfrac{-2}{|\vec{r}-\vec{r}'|} \mid \psi_k^{\pm}\right\rangle \tag{21}$$

which satisfies

$$\nabla^2 \alpha_k^{\pm}(\vec{r}) = 8\pi\phi_{1s}(r)\psi_k^{\pm}(\vec{r}) \tag{22}$$

subject to the boundary condition

$$\alpha_k^{\pm}(\vec{r}) \to \frac{-2}{r}\left\langle \phi_{1s} \mid \psi_k^{\pm}\right\rangle \tag{23}$$

as $r \to \infty$. Eq. (20) is now replaced by *two* coupled integro-differential equations

$$\begin{aligned} \left[\nabla^2 + V(r) + k^2\right]\psi_k^{\pm}(\vec{r}) \pm \; \phi_{1s}(r)\alpha_k^{\pm}(\vec{r}) \pm (k^2+1)\,\phi_{1s}(r)\left\langle \phi_{1s} \mid \psi_k^{\pm}\right\rangle &= 0 \\ \nabla^2 \alpha_k^{\pm}(\vec{r}) - 8\pi\phi_{1s}(r)\psi_k^{\pm}(\vec{r}) &= 0 \end{aligned} \tag{24}$$

which are solved with FEM. The solution yields $\psi_k^{\pm}(r,\theta)$, $\alpha_k^{\pm}(r,\theta)$ and $f_k^{\pm}(\theta)$ (where we have assumed azimuthal symmetry).

In general, the scattering amplitude obtained directly from the FEM calculation is not accurate unless the FEM grid is very large ($r_{\max} \to \infty$). The results are sensitive to the accuracy of the wave function on the boundary, where it is highly oscillatory.

Integral formula for the scattering amplitude

In order to reduce the computational effort and improve the accuracy of the scattering amplitude, we employ the integral formula for $f_k^{\pm}(\theta)$ given by

$$f_k^{\pm}(\theta) = -\frac{1}{4\pi}\int e^{-i\vec{k}\cdot\vec{r}_1}\,\phi_{1s}(r_2)\left[-\frac{2}{r_1} + \frac{2}{r_{12}}\right]\Psi_k^{\pm}(\vec{r}_1,\vec{r}_2)\,d^3r_1\,d^3r_2\,. \tag{25}$$

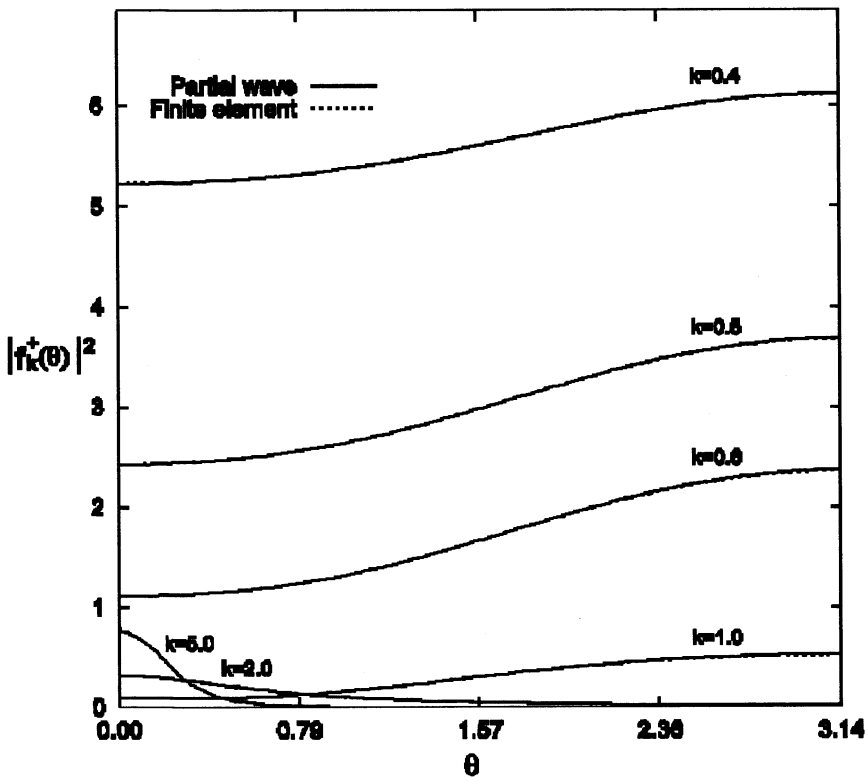

Figure 1. Results for $|f_k^+(\theta)|^2$ obtained with FEM are compared with fully converged partial wave results.

Using the ansatz of Eq. (17), we have

$$f_k^{\pm}(\theta) = -\frac{1}{4\pi}\int e^{-i\vec{k}\cdot\vec{r}_1}\phi_{1s}(r_2)\left[-\frac{2}{r_1}+\frac{2}{r_{12}}\right]\left[\psi_k^{\pm}(r_1,\theta_1)\,\phi_{1s}(r_2)\pm\psi_k^{\pm}(r_2,\theta_2)\,\phi_{1s}(r_1)\right]d^3r_1 d^3r_2 . \quad (26)$$

The accuracy of $f_k^{\pm}(\theta)$ now depends on how well the wave function $\psi_k^{\pm}(r,\theta)$ is represented in the interaction region. In general, the integral expression is not particularly useful because it involves a six dimensional integration. However, using our definition for $\alpha_k^{\pm}(r,\theta)$, we can analytically integrate over four of the six variable to obtain

$$f_k^{\pm}(\theta) = \frac{1}{2}\int J_o(kr'\sin\theta'\sin\theta)\, e^{-ikr'\cos\theta'\cos\theta}\left[V(r')\,\psi_k^{\pm}(r',\theta')\pm\phi_{1s}(r')\,\alpha_k^{\pm}(r',\theta')\right]\sin\theta' r'^2\, dr' d\theta'$$
$$\pm\frac{4}{k^2+1}\int\phi_{1s}(r)\,\psi_k^{\pm}(r',\theta')\sin\theta' r'^2\, dr' d\theta' . \quad (27)$$

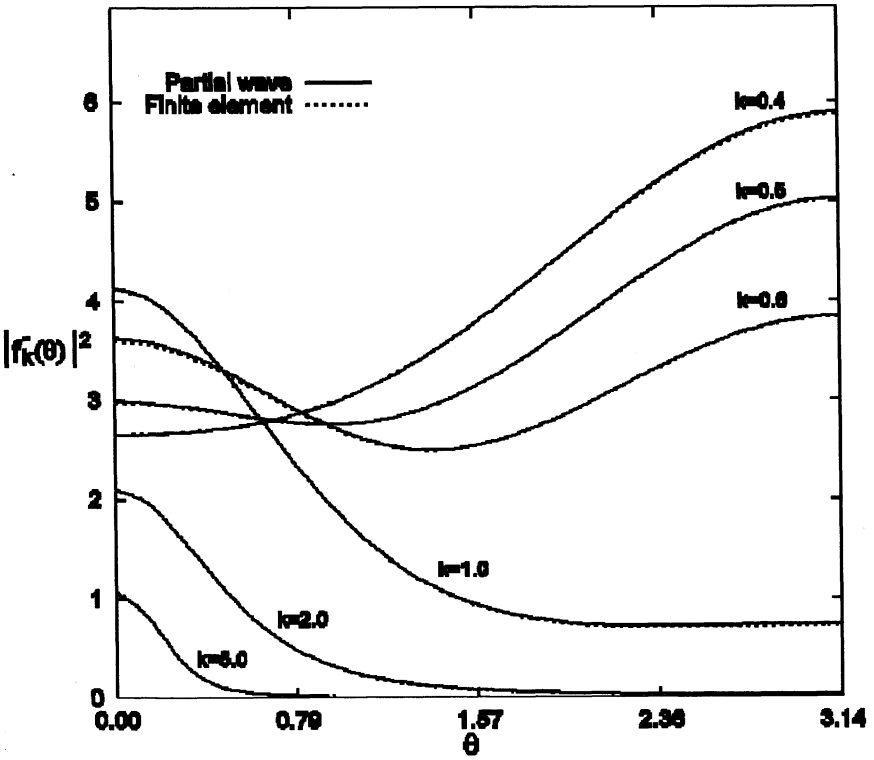

Figure 2. Results for $|f_k^-(\theta)|^2$ obtained with FEM are compared with fully converged partial wave results.

The final integration is done numerically.

Using the integral formula, we can obtain extremely accurate and stable results with relatively little computational effort. Unlike partial wave analysis, the computational effort is independent of energy. In Figs. (1) and (2), we compare our results with a fully converged partial wave calculation [21] for the elastic scattering amplitude for e-H in the static approximation (with exchange).

In order to extend this analysis beyond the static exchange approximation, we need to include correlation in the wave function, via an explicit dependence on $\cos\theta_{12}$. Eventually we plan to include excitation channels in order to obtain the inelastic cross sections.

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