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Convergence of an L^2 approach in the coupled-channel optical-potential method for e-H scattering

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An L^2 approach to the coupled-channel optical method is studied. The investigation is done for electron-hydrogen elastic scattering at projectile energies of 30, 50, 100, and 200 eV. Weak-coupling, free-particle Green's function, and no exchange in Q space are approximations used to calculate the polarization potential. This model problem is solved exactly using actual hydrogen discrete and continuum functions. The convergence of an L^2 approach with the Laguerre basis to the exact result is investigated. It is found that a basis of ten Laguerre functions is sufficient for convergence of approximately 5% in the polarization potential matrix elements, and 2% in the differential cross sections for nonlarge angles. The convergence is faster for smaller energies. In general, the convergence to the exact result is slow.

I. INTRODUCTION

The coupled-channel optical (CCO) method is widely used for calculations of electron-atom scattering, see Ref. 1, for example. This a nonperturbative method that involves the calculation of the first-order amplitudes together with the complex, nonlocal polarization potential to form the optical potential. The purpose of the polarization potential is to include all channels that are not treated explicitly in the coupled-channel calculation.

The problem of electron scattering on atomic hydrogen, which has not as yet been solved exactly, is often used in the investigation of various theoretical methods for electron-atom scattering. The CCO method has proven to be very successful for many aspects of this problem; see Ref. 2, for example.

There are a number of approaches for the calculation of the polarization potential for electron-hydrogen scattering. One is a fully microscopic method[2,3] that uses exact hydrogen discrete and continuum wave functions. Another is to use L^2 (square integrable) pseudostates instead.[4-6]

In this paper we are interested in comparing the two methods. In particular, we are interested in the convergence of an L^2 approach to the exact result in the CCO calculations.

In order to compare the two approaches we make some often used approximations[4,5] to the polarization potential that enable it to be calculated in both methods. We use the Laguerre basis to define our pseudostates. This basis is similar to a Slater basis, but has the advantage of being complete and orthogonal.

A similar investigation was done by Madison and Callaway,[7] where they compared second-order distorted-wave amplitudes calculated using a number of different pseudostates, with exact results.

In Sec. II we define the approximations used to calculate the polarization potentials. The exact (for this model) differential, integrated elastic, and reaction cross sections for elastic scattering at 30, 50, 100, and 200 eV are presented. In Sec. III the convergence of the L^2 method to the exact result is investigated.

II. DEFINITION OF THE MODEL

The complete description of the CCO method used in this paper has been given by McCarthy and Stelbovics[1] and Bray, Madison, and McCarthy.[2]

The polarization potential in the plane-wave representation without exchange is given by

$$\langle \mathbf{k}'i'|W^{(Q)}|i\mathbf{k}\rangle = \langle \mathbf{k}'i'|VQ\frac{1}{Q(E^{(+)}-H)Q}QV|i\mathbf{k}\rangle \ , \tag{1}$$

where i and i' denote target states in P space. The Hamiltonian of the system is given by

$$H = K + H_T + V \ , \tag{2}$$

where K is the kinetic-energy operator of the incident electron, H_T is the nonrelativistic target Hamiltonian, and V is the potential between the incident electron and the hydrogen atom.

The projection operators for target states in P and Q spaces are

$$P = \sum_{i\in P} |i\rangle\langle i| \ , \tag{3}$$

$$Q = I - P = \sum_{i \in Q} |i\rangle\langle i| \ , \tag{4}$$

where

$$H_T|i\rangle = \epsilon_i|i\rangle \ . \tag{5}$$

We use i as a discrete notation that includes the target continuum in Q space.

The model that we use for our investigations assumes weak-coupling, free-particle Green's function, and no exchange in Q space.[4,5] In this approximation (1) becomes

$$\langle \mathbf{k}'i'|W^{(Q)}|i\mathbf{k}\rangle = \sum_{i'' \in Q} \int d^3q \frac{\langle \mathbf{k}'i'|V|i''\mathbf{q}\rangle\langle \mathbf{q}i''|V|i\mathbf{k}\rangle}{(E^{(+)} - \epsilon_{i''} - q^2/2)} \ , \tag{6}$$

where $\mathbf{q}$ represents a plane wave.

A. Exact solution of the model for elastic scattering

In the present formulation we can solve (6) exactly.[2] The discrete notation i'' denotes a sum over the discrete states and an integral over the continuum states of the hydrogen atom. In coordinate space representation these states are

$$\langle \mathbf{r}|i\rangle = \langle \mathbf{r}|nlm\rangle = r^{-1}u_{nl}(r)Y_{lm}(\hat{\mathbf{r}}) \ \text{(discrete case)} \tag{7}$$

$$= \langle \mathbf{r}|\mathbf{p}lm\rangle = r^{-1}u_{pl}(r)Y_{lm}(\hat{\mathbf{r}})Y^{*}_{lm}(\hat{\mathbf{p}}) \ \text{(continuum case)}. \tag{8}$$

Equation (6) is then

$$\begin{aligned} \langle \mathbf{k}'i'|W^{(Q)}|i\mathbf{k}\rangle = &\sum_{n,l,m \in Q^-} \int d^3q \frac{\langle \mathbf{k}'i'|V|nlm\mathbf{q}\rangle\langle \mathbf{q}mln|V|i\mathbf{k}\rangle}{E^{(+)} - \epsilon_n - q^2/2} \\ &+ \sum_{l,m \in Q^+} \int_0^\infty dp\,p^2 \int d\hat{\mathbf{p}} \int d^3q \frac{\langle \mathbf{k}'i'|V|\mathbf{p}lm\mathbf{q}\rangle\langle \mathbf{q}ml\mathbf{p}|V|i\mathbf{k}\rangle}{E^{(+)} - p^2/2 - q^2/2} \ , \end{aligned} \tag{9}$$

where Q^- and Q^+ are the discrete and the continuum parts of Q space, respectively. The integral over p is divided into two parts, namely

$$\int_0^\infty dp\,p^2 = \int_0^{p_0} dp\,p^2 + \int_{p_0}^\infty dp\,p^2 \tag{10}$$

$$= \sum_{p_n < p_0} w_n p_n^2 + \sum_{p_n > p_0} w_n' p_n^2 \ , \tag{11}$$

where $p_0 = (2E)^{1/2}$ and w_n and w_n' are Gaussian-type weights. The interval of integration is divided in such a way that the Q^+ contribution to the imaginary part of the polarization potential comes only from the first interval.

For elastic scattering, both i and i' in (6) are the ground state of hydrogen. Convergence of the partial-wave polarization potential matrix elements to 0.1% is achieved by taking in the discrete case n=2 to 20, and 20 integration points p_n in the continuum case. The sum over l in (9) is done up to l=6. The calculations are at

TABLE I. Differential, integrated elastic (σ_e) and reaction (σ_r) cross sections (a_0^2) at 30, 50, 100, and 200 eV for elastic e-H scattering calculated by the one-channel CCO method. The polarization potential is calculated with the weak-coupling, free-particle Green's function and no exchange in Q space approximations. Square brackets denote powers of 10.

θ (deg)	30 eV	50 eV	100 eV	200 eV
0	1.321[1]	1.066[1]	7.174[0]	4.602[0]
10	8.150[0]	5.143[0]	2.258[0]	1.086[0]
20	4.311[0]	2.199[0]	8.700[−1]	3.980[−1]
30	2.243[0]	1.033[0]	3.920[−1]	1.518[−1]
40	1.214[0]	5.361[−1]	1.909[−1]	6.413[−2]
60	4.354[−1]	1.858[−1]	5.828[−2]	1.677[−2]
80	2.102[−1]	8.565[−2]	2.418[−2]	6.455[−3]
100	1.304[−1]	4.916[−2]	1.275[−2]	3.278[−3]
120	9.635[−2]	3.317[−2]	8.023[−3]	2.017[−3]
140	8.027[−2]	2.545[−2]	5.871[−3]	1.474[−3]
160	7.281[−2]	2.187[−2]	4.917[−3]	1.207[−3]
180	7.046[−2]	2.077[−2]	4.695[−3]	1.193[−3]
σ_e	7.738	3.839	1.494	6.243[−1]
σ_r	8.453	8.160	5.893	3.657

projectile energies of 30, 50, 100, and 200 eV. The resulting differential, integrated elastic, and reaction cross sections are in Table I. An accuracy of 1% requires only ten discrete and ten continuum states.

B. L^2 solution of the model

An L^2 approach in the CCO method[4–6] can be formulated using the above notation as

$$\bar{P} = \sum_{j \in \bar{P}} |j\rangle\langle j| \ , \tag{12}$$

$$\bar{Q} = \sum_{j \in \bar{Q}} |j\rangle\langle j| \ , \tag{13}$$

where j denotes eigenstates of the target Hamiltonian in the space of finite basis of square-integrable (L^2) functions. Denoting the basis set by ξ_{kl} we have

$$\langle j'|H_T|j\rangle = \bar{\epsilon}_j \delta_{j'j} \ , \tag{14}$$

$$\langle \mathbf{r}|j\rangle = \langle \mathbf{r}|\bar{n}lm\rangle = r^{-1}\phi_{\bar{n}l}(r)Y_{lm}(\hat{\mathbf{r}}) \ , \tag{15}$$

$$\langle j'|j\rangle = \delta_{j'j} = \delta_{\bar{n}'\bar{n}}\delta_{l'l}\delta_{m'm} \ , \tag{16}$$

and where

$$\phi_{\bar{n}l} = \sum_{k=1}^{N_l} C^l_{\bar{n}k}\xi_{kl}(r) \ . \tag{17}$$

The basis size N_l can in general depend on l, however, we take it to be the same for each l, $N_l = N$. The coefficients $C^l_{\bar{n}k}$ result from the diagonalization of the target Hamiltonian (14).

In order to compare exact and L^2 theories for the calculation of P-space phenomena we must have $\bar{P} = P$. This can be achieved by including exact bound states in (17), or by taking a sufficiently large N.

Using L^2 states, the polarization potential (6) is

$$\langle \mathbf{k}'i'|W^{(\bar{Q})}|i\mathbf{k}\rangle = \sum_{\bar{n},l,m \in \bar{Q}} \int d^3q \frac{\langle \mathbf{k}'i'|V|\bar{n}lm\mathbf{q}\rangle\langle \mathbf{q}ml\bar{n}|V|i\mathbf{k}\rangle}{(E^{(+)} - \bar{\epsilon}_{\bar{n}l} - q^2/2)} \ , \tag{18}$$

where the sum and integral over exact hydrogen states in (9) has now been replaced with a single sum over L^2 states. The sum over l in (18) is done up to l=6, as in the exact solution.

III. CONVERGENCE OF THE L^2 METHOD

Many authors[4–10] use a nonorthogonal Slater basis to create their L^2 states. This basis is not convenient for investigation of convergence as numerical linear dependence does not allow a set of arbitrarily large N. To avoid this problem we use the Laguerre basis

$$\xi_{kl}(r) = \left(\frac{\lambda(k-1)!}{(2l+1+k)!}\right)^{1/2} \times(\lambda r)^{l+1}\exp(-\lambda r/2)L^{2l+2}_{k-1}(\lambda r) \ , \tag{19}$$

which has the advantage of being orthogonal and has known analytical properties.[11] As we would like to get the 1s hydrogen wave function exactly, we take λ=2. In this basis, to achieve an accuracy of better than 10^{-2}% for the 2s and the 2p hydrogen states, we take $N \geq 7$. For more detail see Table II.

A. Convergence of the polarization potential matrix elements

We calculate one of the most sensitive polarization potential matrix elements, the partial wave expansion[2] J=0 element, to an accuracy better than 0.1% using (9). This result is compared with the result of (18), for N ranging from 7 to 100. In Fig. 1 we present the detailed results of comparison for 30 and 200 eV. The results for 50 and 100 eV are qualitatively similar to the presented results.

The convergence of the L^2 method to the exact result is not uniform, but is of an oscillatory nature. This result is consistent with the work of Stelbovics and Winata.[12] The rate of convergence is fast for small N, but is rather slow for large N. An accuracy of 5% can be achieved with $N \approx 10$ for all considered energies. Better convergence is achieved for smaller energies. An accuracy of 1% is achieved with $N \approx 20$ for 30 eV, $N \approx 35$ for 50 eV, $N \approx 45$ for 100 eV, and $N \approx 65$ for 200 eV.

B. Convergence of the cross sections

In terms of comparison of theory with experiment it is necessary to study convergence in the differential cross sections. To calculate a differential cross section one requires the polarization potential partial wave amplitudes from $J = 0$ up to convergence. We have taken the maximum J to be 80.

To study the convergence in the differential cross sections we have selected particular values, $N = 7, 10, 20$. Figure 2 shows the percentage relative error with the exact result for each L^2 calculation. The accuracy of the L^2

TABLE II. Percentage relative errors δ in eigenvalues of L^2 states at selected values N of the Laguerre basis. N_c is the number of pseudo-states with $\bar{\epsilon}_j > 0$ for l=0. The error columns contain the principal quantum number of the exact bound state of hydrogen that an L^2 state achieves with the prescribed error, for each possible l.

N	N_c	$\delta < 10^{-12}$%	$\delta < 10^{-5}$%	$\delta < 10^{-2}$%
7	4	1		2
10	7	1	2	
20	15	1,2	3	
100	88	1,...,6	7	8

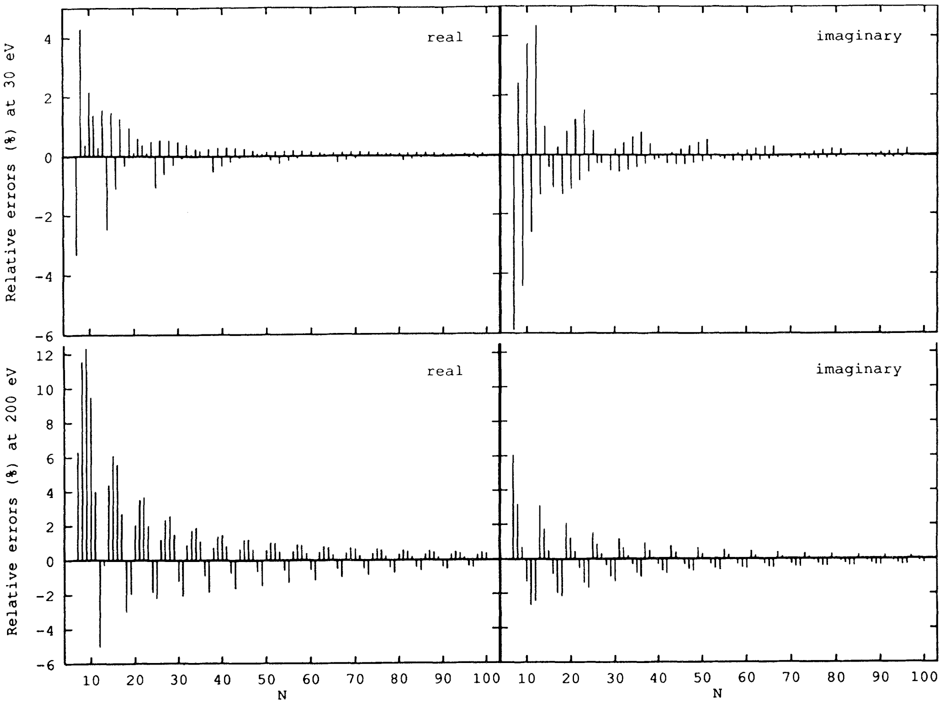

FIG. 1. Percentage relative errors for both the real and the imaginary parts of the elastic scattering polarization potential matrix element (partial wave $J=0$) at 30 and 200 eV, calculated using L^2 method. N is the size of the Laguerre basis.

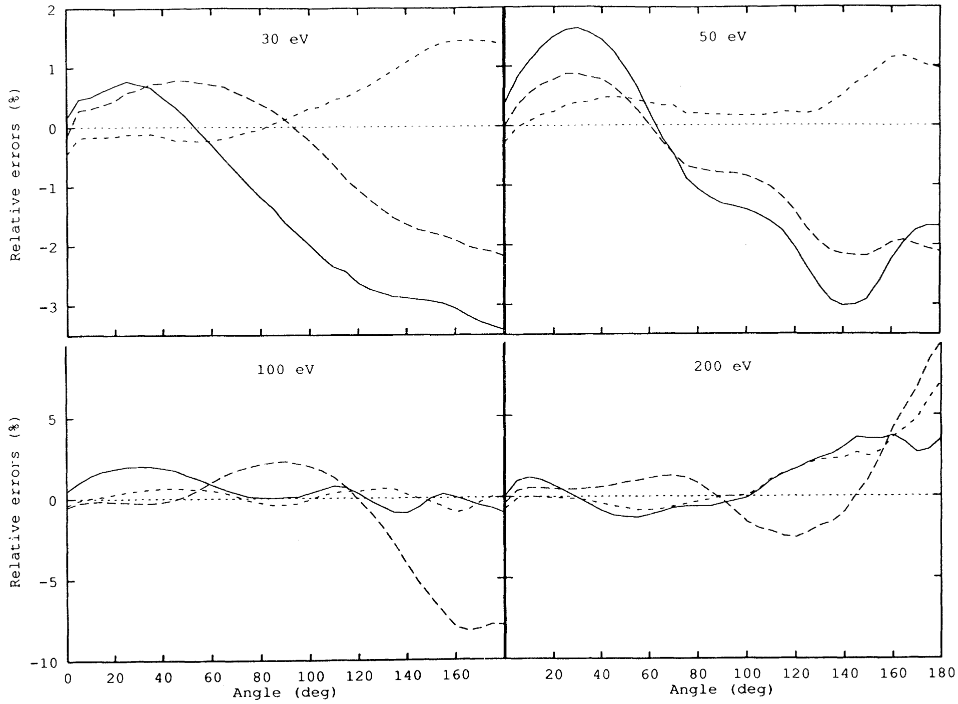

FIG. 2. Percentage relative errors for the elastic differential cross sections at 30, 50, 100, and 200 eV, calculated using L^2 method at selected values N of the Laguerre basis. The solid line is the L^2 calculation with $N=7$, the long-dashed line with $N=10$, and the short-dashed line with $N=20$.

method improves with increasing N. The bigger errors for large angles are due to lack of convergence of the L^2 polarization potential for small partial waves.

IV. CONCLUSIONS

We have shown that the L^2 approach with the Laguerre basis to the CCO method calculations is equivalent to using exact target states. The convergence as a function of basis size is slow and has an oscillatory behavior, different for each energy. Higher projectile energies require a larger number of L^2 states in order to achieve the same accuracy of calculation. A basis of ten Laguerre functions is sufficient for convergence of approximately 5% in the polarization potential matrix elements and 2% in the differential cross sections for nonlarge angles.

From the exact calculation for this range of energies we found that we required as many as 20 bound states to achieve an accuracy of 0.1%. This suggests that the slow convergence in the L^2 method may be due to a lack of accurate description of the higher bound states; see Table II. Because of this we are unable to study the convergence in the continuum part on its own. Using the results of Stelbovics and Winata[12] we believe that the convergence is slow for both the "discrete" and "continuum" contributions to the polarization potential. The convergence to the exact result as a function of the number of states is faster using actual target states than using the L^2 states.

As the model chosen is one of the simplest, we believe that if a more sophisticated model is chosen for the L^2 approach to atomic hydrogen or higher atoms,[8] then the difficulties will only increase. For example, some non-free-particle Green's functions may lead to pseudoresonances.

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