

# Collapsed close-coupling method: A systematic alternative to the multichannel optical potential for solutions of the Schrödinger equation in a truncated subspace

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We derive a new general method for reducing the number of coupled channels in scattering calculations, and we test it for electron-hydrogen-atom scattering in a truncated Hilbert space. The new method yields encouraging results.

## I. INTRODUCTION

The systematic approach to calculating scattering amplitudes for collisions of composite bodies is to expand the scattering wave function in a basis of internal states times functions of the relative scattering coordinate and to solve larger and larger sets of coupled equations for the variationally best scattering functions for the given basis.<sup>1-8</sup> This standard approach is called the close-coupling method. In most cases though the expansion requires many internal states for convergence, and the cost of solving the close-coupling equations, including the required number of internal states, may be prohibitive. In such cases it may be very useful to be able to include a large number of states but only approximately. In the present paper we propose an approximation to the close-coupling equations in which they are replaced by two coupled equations, one for the projection of the scattering wave function in the elastic channel and one for the scattering wave function in an artificial channel whose properties are calculated from all the nonelastic channels. This channel will be called a collapsed channel and the method will be called the collapsed close-coupling method. This name is meant to signify that a large number or infinite number of higher channels are collapsed into one. In the version considered here, this reduces the number of close-coupling equations to two. Generalizations in which one keeps two or more real channels plus one or more effective channels are possible and are of great interest as subjects for later study, but will not be developed in detail in the present paper.

After presenting the theory, the two-channel collapsed close-coupling approximation will be tested by application to electron-hydrogen-atom scattering without exchange. We must emphasize, however, that the goal of the computational part of the present study is not to improve on the best existing electron-hydrogen-atom calculations, which are very sophisticated,<sup>7</sup> but to provide a test of the new general approach to coupled-channels problems. If successful, this approach may be applied to a variety of collisional systems because it is very general.

In Sec. IV we will compare the collapsed close-coupling method to related methods including perturbation theory,<sup>9-14</sup> the Feshbach optical potential approach,<sup>15-18</sup> a smoothing procedure for obtaining local optical poten-

tials,<sup>19</sup> the pseudostate expansion method,<sup>4,7</sup> optical model potentials,<sup>20-28</sup> and—the technique most closely related to the new one presented here—the matrix effective potential method.<sup>29-31</sup> We also briefly discuss the possible extension of the present approach to larger collapsed close-coupling expansions based on two or more real channels plus one effective channel.

The close-coupling method is quite general and may be applied to any scattering problem in which two particles collide and two emerge. In Sec. II we will use a general notation for the case of a structureless particle scattering from an unspecified target with internal coordinates  $\mathbf{x}$  where the basis functions diagonalize the target Hamiltonian, the scattering particle's orbital angular momentum, and the total angular momentum. For the numerical example this will be specialized to electron-hydrogen-atom scattering without exchange. The extension to more complicated cases involving local potentials is straightforward. For rearrangements or other problems involving nonlocal potentials,<sup>1,3,4,6-8,18,24</sup> the method presented here can be applied if the nonlocal potentials are first replaced by approximations that are local in the coordinate representation. For problems involving derivative coupling operators, it is first necessary to transform to a diabatic representation, either accurately<sup>32</sup> or approximately.<sup>33</sup>

## II. THEORY

The Hamiltonian is given by

$$H = T_{\mathbf{x}} + T_{\mathbf{r}} + V(\mathbf{x}, \mathbf{r}) \quad (1a)$$

$$= H_{\text{int}} + T_{\mathbf{r}} + V_{\text{inter}}(\mathbf{x}, \mathbf{r}), \quad (1b)$$

where  $T_{\mathbf{x}}$  and  $T_{\mathbf{r}}$  denote the kinetic energy of the bound and scattering particles, respectively,  $V(\mathbf{x}, \mathbf{r})$  is the potential energy,  $H_{\text{int}}$  is the internal Hamiltonian of the target, and  $V_{\text{inter}}$  is the interaction potential of the scattering particle with the target. Thus

$$T_{\mathbf{r}} = -(\hbar^2/2\mu)\nabla_{\mathbf{r}}^2, \quad (2)$$

where  $\mu$  is the scattering reduced mass and  $\mathbf{r}$  is the scattering coordinate. Also,

$$V_{\text{inter}}(\mathbf{x}, \mathbf{r}) \xrightarrow{r \rightarrow \infty} 0. \quad (3)$$

The close-coupling expansion is

$$\Psi(\mathbf{x}, \mathbf{r}) = r^{-1} \sum_{i=1}^N f_i(r) \psi_i(\mathbf{x}, \hat{\mathbf{r}}), \quad (4)$$

where  $\psi_i(\mathbf{x}, \hat{\mathbf{r}})$  is a basis function corresponding to orbital angular momentum quantum number  $l_i$  for the scattering particle and total angular momentum  $L$ , and  $f_i(r)$  is a function to be determined. The close-coupling equations are block diagonal in  $L$  and have the following form for each block:

$$\frac{d^2}{dr^2} f_i(r) = \sum_{j=1}^N U_{ij}(r) f_j(r), \quad i=1, 2, \dots, N, \quad (5)$$

where

$$U_{ij}(r) = -(2\mu/\hbar^2) \int d\mathbf{x} d\hat{\mathbf{r}} \psi_i^*(\mathbf{x}, \hat{\mathbf{r}}) V_{\text{inter}}(\mathbf{x}, \mathbf{r}) \psi_j(\mathbf{x}, \hat{\mathbf{r}}) - \delta_{ij} \left[ \frac{l_i(l_i+1)}{r^2} - k_i^2 \right]. \quad (6)$$

Note that  $k_i$  is the scattering particle wave number defined by

$$k_i^2 = (2\mu/\hbar^2) [E - \int d\mathbf{x} d\hat{\mathbf{r}} \psi_i^*(\mathbf{x}, \hat{\mathbf{r}}) H_{\text{int}} \psi_j(\mathbf{x}, \hat{\mathbf{r}})]. \quad (7)$$

As mentioned in the last paragraph of the Introduction we have assumed here that

$$\int d\mathbf{x} d\hat{\mathbf{r}} \psi_i^*(\mathbf{x}, \hat{\mathbf{r}}) H_{\text{int}} \psi_j(\mathbf{x}, \hat{\mathbf{r}}) = 0, \quad i \neq j. \quad (8)$$

Note also that the  $U$  matrix is Hermitian.

We assume that the target ground state is nondegenerate and the target is initially in this state. Then  $l_1=L$  and the boundary conditions for open channels (those with  $k_i^2$  positive) are

$$f_1(r) \sim \exp[-i(k_1 r - \frac{1}{2}L\pi)] - \exp[2i\eta_L + i(k_1 r - \frac{1}{2}L\pi)], \quad \text{as } r \rightarrow \infty, \quad (9)$$

$$f_i(r) \sim \text{const} \times \exp(ik_i r), \quad r \rightarrow \infty, \quad i \neq 1. \quad (10)$$

The phase shift is  $\eta_L$ , and if more than one channel in the block is open it is complex. The boundary condition for closed channels is that  $f_i(r)$  must vanish at  $r = \infty$ . In addition, for all channels (open or closed) it is required that

$$f_i(r=0) = 0. \quad (11)$$

In the collapsed close-coupling method we seek to replace Eqs. (5) by

$$\frac{d^2}{dr^2} f_1(r) = U_{11}(r) f_1(r) + W_{12}(r) g(r) \quad (12a)$$

and

$$\frac{d^2}{dr^2} g(r) = W_{21}(r) f_1(r) + W_{22}(r) g(r), \quad (12b)$$

such that

$$W_{12}(r) = W_{21}(r). \quad (13)$$

In particular, since  $f_1(r)$  appears unchanged from Eq. (5), the phase shift  $\eta_L$  of Eq. (9) is also the same as obtained from Eq. (5). Next we show that such a construction is possible, although  $W_{12}(r)$  and  $W_{22}(r)$  depend on the  $f_i(r)$ . Since we would have to solve Eq. (5) to obtain these functions, the formally exact construction does not save any effort, but it does motivate the next step in which we approximate  $W_{12}(r)$  and  $W_{22}(r)$  in such a way that they do not depend on unknown functions. This yields an approximate  $f_1(r)$  and hence an approximate  $\eta_L$ . This is called the collapsed close-coupling method.

First we write

$$g(r) = a(r) \sum_{j=2}^N U_{1j}(r) f_j(r), \quad (14)$$

where  $a(r)$  is a new unknown function. Comparing Eqs. (5), (12), and (14) shows that

$$W_{12}(r) = 1/a(r), \quad (15)$$

which, when we obtain  $a(r)$ , will specify Eq. (12a). Equation (12b) is obtained in the following way. Multiply the  $s$ th equation of the set (5), for  $s=2, 3, \dots, N$ , by  $a(r)U_{1s}(r)$  and rearrange to obtain

$$\begin{aligned} & \frac{d^2}{dr^2} a(r) U_{1s}(r) f_s(r) \\ &= \sum_{j=1}^N a(r) U_{1s}(r) U_{sj}(r) f_j(r) \\ &+ 2 \left[ \frac{d}{dr} a(r) U_{1s}(r) \right] \frac{d}{dr} f_s(r) \\ &+ f_s(r) \frac{d^2}{dr^2} a(r) U_{1s}(r), \quad s=2, 3, \dots, N. \end{aligned} \quad (16)$$

Now, defining

$$S_{1j}(r) = \sum_{s=2}^N U_{1s}(r) U_{sj}(r) \quad (17)$$

and summing the  $(N-1)$  equations from (16) yields [using Eq. (14) and the Hermiticity of the  $U$  matrix],

$$\begin{aligned} \frac{d^2}{dr^2} g(r) &= f_1(r) a(r) S_{11}(r) + \sum_{j=2}^N f_j(r) a(r) S_{1j}(r) \\ &+ \sum_{s=2}^N \left[ 2 \frac{d}{dr} [a(r) U_{1s}(r)] \frac{d}{dr} f_s(r) \right. \\ &\left. + f_s(r) \frac{d^2}{dr^2} [a(r) U_{1s}(r)] \right]. \end{aligned} \quad (18)$$

Comparison to Eqs. (12) yields

$$W_{21}(r) = a(r) S_{11}(r) \quad (19)$$

and

$$\begin{aligned}
W_{22}(r) = & \left[ a(r) \sum_{j=2}^N U_{1j}(r) f_j(r) \right]^{-1} \\
& \times \sum_{j=2}^N \left[ a(r) f_j(r) S_{1j}(r) \right. \\
& \quad + 2 \left[ \frac{d}{dr} a(r) U_{1j}(r) \right] \frac{d}{dr} f_j(r) \\
& \quad \left. + f_j(r) \frac{d^2}{dr^2} a(r) U_{1j}(r) \right]. \quad (20)
\end{aligned}$$

The function  $a(r)$  can now be obtained from Eqs. (13), (15), and (19) which yield

$$a(r) = [S_{11}(r)]^{-1/2}. \quad (21)$$

Equations (13) and (15) and the Hermiticity of the  $U$  matrix then yield

$$W_{12}(r) = W_{21}(r) = \left[ \sum_{j=2}^N |U_{1j}(r)|^2 \right]^{1/2}. \quad (22)$$

Equation (22) for the coupling potential is a practical formula involving only known functions, namely the first row of the original potential matrix, exclusive of the diagonal element. Equation (20), however, involves the unknown functions  $f_j(r)$ . Since  $W_{12}(r)$  has a direct effect on  $f_1(r)$  in Eq. (12a), but  $W_{22}(r)$  has only an indirect effect through its effect on  $g(r)$  in Eq. (12b), it seems that we might obtain a reasonable approximation to  $f_1(r)$  by retaining Eq. (22) but approximating Eq. (20). We will use the approximation

$$W_{22}(r) = U_{11}(r) + k_2^2 - k_1^2, \quad (23)$$

i.e., we use the same averaged interaction potential and centrifugal potential in the collapsed channel as in the ground-state channel, and we set the threshold energy equal to the true threshold energy.

### III. EXAMPLE

The example we consider is electron-hydrogen-atom scattering without exchange. We use a six-state basis consisting of three hydrogenic eigenfunctions,  $1s$ ,  $2s$ , and  $2p$ ,

and three pseudostates, denoted  $\overline{3s}$ ,  $\overline{3p}$ , and  $\overline{3d}$ . The basis is specified in detail in Table I. The  $\overline{3s}$  function is taken from Burke and Mitchell,<sup>34</sup> and it accounts for short-range radial correlation effects. The  $\overline{3d}$  function is the same as used by Damburg and Karule,<sup>35</sup> and it accounts for the full quadrupole polarizability of the ground state. The  $\overline{3p}$  function is obtained by orthogonalizing the  $2p$  function of Temkin,<sup>36</sup> which accounts for the full dipole polarizability of the ground state, to the  $2p$  eigenfunction. Counting only channels with the right parity to couple to the ground-state channel, the number of channels corresponding to this six-state basis increases from 6 at  $L=0$ , to 9 for  $L=1$ , to 10 for  $L \geq 2$ . The close-coupling results for the six-state basis are considered as the exact solutions to a model problem, and the new collapsed close-coupling method is judged in terms of its agreement or disagreement with this reference calculation.

The close-coupling equations were solved by the Numerov method.<sup>37-39</sup> Phase shifts  $\eta_L$ , elastic integral cross sections  $\sigma_{el}$  and differential cross sections  $d\sigma_{el}/d\Omega$  as a function of scattering angle  $\theta$ , and elastic momentum transfer cross sections  $\sigma_{el}^m$  were extracted by standard formulas. Absorption cross sections  $\sigma_{abs}$  were defined as the sum of all inelastic cross sections for the close-coupling calculations and are set to the cross section for exciting the one collapsed channel in the collapsed close-coupling calculations. The total cross section is given by

$$\sigma_{tot} = \sigma_{el} + \sigma_{abs}. \quad (24)$$

All calculations are for an impact energy of  $2E_h$  ( $1E_h = 1$  hartree;  $2E_h = 54.4232$  eV). Phase shifts were calculated from the coupled-channels equations for  $L=0-50$ , and elastic cross sections were converged by adding polarized Born phase shifts for  $L=51-300$ , as calculated by the approximate formula of O'Malley *et al.*<sup>40</sup> (The magnitude of the elastic transition matrix element from the collapsed close-coupling calculation agrees with the value calculated from this approximate formula within 18% at  $L=50$ .)

Some of the complex phase shifts are given in Table II, and the cross sections are given in Table III. Table II shows that the real part of the phase shift obtained from the contracted close-coupling calculation agrees with the accurate value within 16% for  $L=0$ , disagrees more for  $L=1-10$ , then agrees within 14-10% for  $L=15-20$ .

TABLE I. Radical functions and excitation energies for the six-state target basis (in a.u.).

State	$R_\alpha(r)^a$	$\Delta E_\alpha^b$
$1s$	$2e^{-r}$	0.000 000
$2s$	$(\frac{1}{2})^{1/2}(1 - \frac{1}{2}r)e^{-r/2}$	0.375 000
$2p$	$\frac{1}{2}(6)^{-1/2}re^{-r/2}$	0.375 000
$\overline{3s}$	$[(\frac{300}{152})^{1/2} - (\frac{529}{456})^{1/2}r + (\frac{3}{132})^{1/2}r^2]e^{-r/2}$	0.489 040
$\overline{3p}^c$	$(1 - A^2)^{-1/2}r[\frac{1}{2}(6)^{-1/2}A - (\frac{32}{129})^{1/2}(1 + \frac{1}{2}r)e^{-r/2}]e^{-r/2}$	0.539 032
$\overline{3d}$	$(\frac{32}{535})^{1/2}r^2(\frac{1}{2} + r/3)e^{-r}$	0.560 750

<sup>a</sup>Radial function. The normalization is  $\int_0^\infty dr r^2 |R_\alpha(r)|^2 = 1$ .

<sup>b</sup>In a.u., the excitation energy  $\Delta E_\alpha$  equals  $(k_1^2 - k_\alpha^2)/2$ .

<sup>c</sup> $A = (\frac{2}{3})^6(43)^{-1/2}$ .

TABLE II. Phase shifts (in radians, modulo  $\pi$  in the real part) for  $e^-$ -H scattering at  $2E_h$ .

$L$	$1s-2s-2p-\overline{3s}-\overline{3p}-\overline{3d}$	Contracted close coupling
0	0.6958 + 0.0641 <i>i</i>	0.8044 + 0.1219 <i>i</i>
1	0.2401 + 0.0402 <i>i</i>	0.3334 + 0.1093 <i>i</i>
3	0.0472 + 0.0407 <i>i</i>	0.0962 + 0.0548 <i>i</i>
5	0.0222 + 0.0222 <i>i</i>	0.0406 + 0.0238 <i>i</i>
7	0.0127 + 0.0104 <i>i</i>	0.0200 + 0.0098 <i>i</i>
10	0.0061 + 0.0035 <i>i</i>	0.0082 + 0.0028 <i>i</i>
15	0.0022 + 0.0007 <i>i</i>	0.0026 + 0.0004 <i>i</i>
20	0.0010 + 0.0002 <i>i</i>	0.0011 + 0.0001 <i>i</i>

Interestingly, the error for the imaginary part of the phase shift is already only 35% at  $L=3$  and is only 20% or less for  $L=5-10$ . Table III shows that the momentum transfer and absorption cross sections predicted by the contracted close-coupling calculation are remarkably accurate, and the major error in  $\sigma_{el}$ ,  $d\sigma_{el}/d\Omega$ , and  $\sigma_{tot}$  is due to a systematic overestimate of the small-angle elastic differential cross section.

#### IV. COMPARISON TO OTHER METHODS

There are several other techniques available for obtaining the effect of missing channels on the scattering in a selected subset of one or more explicitly included channels. We will now contrast a few of these, with representative references, to the present approach.

The most straightforward way is to include the effects of missing channels by second- or higher-order perturbation theory. This may be applied to the transition matrix elements (or scattering amplitude) directly,<sup>9,10</sup> or it may be applied to calculate an effective potential.<sup>11-14</sup> The second approach is more similar to the collapsed close-coupling method, and both methods have the advantage that the dynamics in the explicit channels can be treated with great flexibility, e.g., close coupling, the distorted-wave approximation, or variational methods. When second-order perturbation theory is applied directly to cal-

culate the transition matrix, a complete calculation is difficult and it may be inaccurate if it is oversimplified for computational convenience.

The Feshbach optical potential<sup>15-18</sup> is a rigorous method to account for the effects of channels not included explicitly. Computation and use of the exact Feshbach optical potential suffers from several practical difficulties, especially nonuniqueness, nonlocality, and the fact that converging the calculation of the optical potential is in general as difficult as converging a close-coupling calculation in which all channels are included explicitly. The nonlocality can be overcome by exploiting the nonuniqueness to specify a local potential<sup>41,42</sup> (as suggested, e.g., by Wolken<sup>41</sup>); unfortunately this leads to a highly singular result. Recently a practical algorithm has been prepared for smoothing the singularities, but at the cost of losing the exactness.<sup>19</sup> The optical potential approach replaces the original  $N$ -channel problem with local potentials by a single-channel problem with nonlocal, exact, energy-dependent potentials, and the Wolken and smoothing procedures convert these to local, singular, energy-dependent and local, nonexact, energy-dependent potentials, respectively. Generalized optical potentials replace the original  $N$ -channel problem by two-or-more-channel problems with nonlocal, exact, energy-dependent potentials.<sup>17</sup> The present procedure, in contrast, attempts to replace the original  $N$ -channel problem with a two-channel problem with local, nonexact, energy-independent potentials. The closest analog is the matrix effective potential method,<sup>29-31</sup> which also involves multichannel, local, nonexact, energy-independent potentials. The coupling potentials in the matrix effective potential method have been computed by first solving the scattering equations for the adiabatic limit, and then embedding this limit exactly in a two-channel version of the equations. In contrast the collapsed close-coupling method obtains the coupling potentials without invoking the adiabatic limit.

An alternative way to reduce the order of the coupled-channels equations is the pseudostate method.<sup>4,7,34-36</sup> This is a variational method in which one uses a linear combination of target eigenstates as a single basis function. The collapsed close-coupling method, like the ma-

TABLE III. Cross sections (in  $a_0^2$  and  $a_0^2/\text{sr}$ ) for  $e^-$ -H scattering at  $2E_h$ .

Cross section	$1s-2s-2p-\overline{3s}-\overline{3p}-\overline{3d}$	Contracted close coupling
$\sigma_{el}$	2.02	3.22
$\sigma_{el}^m$	0.64	0.60
$\sigma_{abs}$	6.39	7.40
$\sigma_{tot}$	8.42	10.62
$d\sigma_{el}(\theta=0^\circ)/d\Omega$	6.85	12.43
$d\sigma_{el}(\theta=20^\circ)/d\Omega$	0.930	1.98
$d\sigma_{el}(\theta=40^\circ)/d\Omega$	0.263	0.365
$d\sigma_{el}(\theta=60^\circ)/d\Omega$	0.124	0.116
$d\sigma_{el}(\theta=80^\circ)/d\Omega$	0.068	0.053
$d\sigma_{el}(\theta=100^\circ)/d\Omega$	0.040	0.030
$d\sigma_{el}(\theta=120^\circ)/d\Omega$	0.028	0.020
$d\sigma_{el}(\theta=140^\circ)/d\Omega$	0.022	0.015
$d\sigma_{el}(\theta=160^\circ)/d\Omega$	0.018	0.013
$d\sigma_{el}(\theta=180^\circ)/d\Omega$	0.017	0.012

trix effective potential method, does not involve an actual pseudostate, and hence it is nonvariational. These methods directly approximate the potential matrix in a nonvariational close-coupling context.

The single-channel optical potential method has served as a formal foundation for a number of more approximate approaches. Approximate single-channel optical potentials are often called optical model potentials. Such potentials have been obtained many ways, e.g., by combining a charge polarization model with dispersion relations,<sup>25</sup> by frequency-dependent-susceptibility analyses of the second-order approximation to the exact optical potential,<sup>27</sup> by binary-collision models,<sup>22,28</sup> and by phenomenological fitting.<sup>26</sup> Equations (20) and (22) could presumably serve as prototype foundations for similar investigations of multichannel optical model potentials.

As mentioned in the Introduction, it would be interesting to extend the present method to three or more channels. Extension of the derivation in Sec. II to this case shows that the unknown functions  $f_i(r)$  do not cancel out of either the coupling potentials or the diagonal potentials

in this case; thus a three-channel contracted close-coupling scheme would be more arbitrary than a two-channel one. However, the three-or-more-channel format allows for much greater flexibility in modeling the full problem, and it would be very interesting to see how much additional accuracy could be gained by such an approach.

## V. CONCLUSION

We have derived a new general method for approximating the solution of coupled-channels scattering equations. This method, which we call the collapsed close-coupling method, is tested in its two-channel formulation for a model problem of electron-hydrogen-atom scattering, replacing between six and ten channels by two. The results are very encouraging, and this method should provide a useful alternative to existing approximation methods.

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