

## Time-dependent Born-series calculations of three-body scattering systems

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Time-dependent Born-series calculations are carried out for various short and long range three-body scattering systems. The long range system is a standard  $s$ -wave model for electron-atom scattering developed by Temkin [Phys. Rev. **126**, 130 (1962)] and Poet [J. Phys. B **11**, 3081 (1978)]. A direct solution of the time-dependent Schrödinger equation yields exact excitation and ionization cross sections for all the scattering systems. For short range forces the time-dependent Born-series calculations are found to converge more rapidly for weak binding potentials and high incident electron energies. For long range forces the time-dependent Born-series calculations do not converge, although the first-order excitation and ionization cross sections are quite reasonable.

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Formal convergence studies of the Born series have been made for two-body scattering systems involving central potentials [1,2]. Two well-known theorems are that the Born series converges at all energies for central potentials that do not support bound states, and that the Born series converges at sufficiently high scattering energies for central potentials that decrease faster than  $1/r^3$  asymptotically. Convergence studies of the Born series for three-body scattering systems, including inelastic collision processes, are much more difficult. A serious impediment to a convergence study has been the lack of exact solutions.

In this Brief Report, we carry out time-dependent Born series calculations for various short range and long range three-body scattering systems. The scattering systems are based on an  $s$ -wave model developed by Temkin [3] and Poet [4] to simulate the inelastic processes found in electron-atom scattering. A single cutoff parameter is used to adjust the range of the charged particle interactions. For all the scattering systems, the Born-series calculations are compared to exact cross sections obtained by direct solution of the time-dependent Schrödinger equation [5].

The time-dependent Schrödinger equation for the modified Temkin-Poet model is given by (in atomic units)

$$i \frac{\partial \Psi(r_1, r_2, t)}{\partial t} = [H_0(r_1, r_2) + V(r_1, r_2)] \Psi(r_1, r_2, t), \quad (1)$$

where the unperturbed Hamiltonian is given by

$$H_0(r_1, r_2) = -\frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} - \frac{e^{-\alpha r_1}}{r_1} - \frac{e^{-\alpha r_2}}{r_2}, \quad (2)$$

the perturbation is given by

$$V(r_1, r_2) = \frac{e^{-\alpha r_>}}{r_>}, \quad (3)$$

$r_> = \max(r_1, r_2)$ , and  $\alpha$  is an adjustable cutoff parameter. A set of time-dependent Born series equations may be easily derived:

$$i \frac{\partial \psi_0(r_1, r_2, t)}{\partial t} = H_0(r_1, r_2) \psi_0(r_1, r_2, t), \quad (4)$$

$$i \frac{\partial \psi_1(r_1, r_2, t)}{\partial t} = H_0(r_1, r_2) \psi_1(r_1, r_2, t) + V(r_1, r_2) \psi_0(r_1, r_2, t), \quad (5)$$

⋮

$$i \frac{\partial \psi_n(r_1, r_2, t)}{\partial t} = H_0(r_1, r_2) \psi_n(r_1, r_2, t) + V(r_1, r_2) \psi_{n-1}(r_1, r_2, t). \quad (6)$$

The time-dependent Schrödinger equation or the time-dependent Born-series equations may be solved by discretization of all radial wave functions and operators on a two-dimensional lattice. The initial condition for  $^1S$  scattering is that  $\Psi(r_1, r_2, t=0)$  equals a symmetrized product of the ground state solution of the single-particle Schrödinger equation:

$$\left( -\frac{1}{2} \frac{\partial^2}{\partial r^2} - \frac{e^{-\alpha r}}{r} \right) P(r) = \epsilon P(r) \quad (7)$$

TABLE I. Inelastic cross sections for an  $\alpha=1$  short-range three-body scattering system. Cross sections are given in Mb (1.0 Mb =  $1.0 \times 10^{-18}$  cm<sup>2</sup>).

Born-series order	30 (eV)		50 (eV)		100 (eV)	
	$1s \rightarrow ks$	Norm	$1s \rightarrow ks$	Norm	$1s \rightarrow ks$	Norm
1	2.012	1.16	0.817	1.10	0.224	1.06
2	2.315	1.02	0.938	1.01	0.255	1.01
3	1.480	0.98	0.648	0.99	0.192	1.00
4	1.526	1.00	0.658	1.00	0.193	1.00
5	1.591	1.00	0.676	1.00	0.196	1.00
Exact	1.573	1.00	0.672	1.00	0.195	1.00

TABLE II. Inelastic cross sections for an  $\alpha = \frac{1}{4}$  short range three-body scattering system. Cross sections are given in Mb ( $1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$ ).

Born-series order	30 (eV)			50 (eV)			100 (eV)		
	$1s \rightarrow 2s$	$1s \rightarrow ks$	Norm	$1s \rightarrow 2s$	$1s \rightarrow ks$	Norm	$1s \rightarrow 2s$	$1s \rightarrow ks$	Norm
1	0.491	4.61	4.48	0.175	2.40	3.43	0.045	0.78	2.44
2	1.999	20.70	5.60	0.547	9.05	3.32	0.099	2.27	1.84
3	1.770	19.28	2.83	0.389	7.15	1.49	0.060	1.51	1.02
4	0.425	4.67	0.78	0.110	1.85	0.78	0.031	0.59	0.92
5	0.161	1.48	0.83	0.102	1.38	0.96	0.034	0.63	1.00
6	0.370	3.69	1.09	0.142	2.11	1.04	0.037	0.73	1.01
7	0.393	3.93	1.05	0.141	2.12	1.01	0.037	0.72	1.00
8	0.358	3.56	0.99	0.136	2.03	0.98	0.036	0.71	1.00
Exact	0.356	3.55	1.00	0.136	2.03	1.00	0.036	0.71	1.00

and an incoming radial wave packet. The initial condition for the Born-series equations is that  $\psi_0(r_1, r_2, t=0)$  equals the same symmetrized product and  $\psi_n(r_1, r_2, t=0) = 0$  for all  $n > 0$ . Following the wave packet propagation, excitation and ionization probabilities and cross sections are extracted by projecting the exact wave function  $\Psi(r_1, r_2, t=T)$  or the  $n$ th-order approximate wave function  $\sum_{j=0}^n \psi_j(r_1, r_2, t=T)$  onto a complete set of bound and continuum solutions of the single-particle Schrödinger equation. Further computational details are found in previous work [5].

We begin by considering a short range three-body scattering system with  $\alpha = 1$ . For this choice of the cutoff parameter there is only one bound state solution of the single-particle Schrödinger equation, with a binding energy of  $-0.242$  eV. Thus, the only inelastic process is direct ionization of the ground state. The ionization cross section results at several different incident energies are presented in Table I. A  $200 \times 200$  point radial lattice with a mesh spacing of  $\Delta r_1 = \Delta r_2 = 0.2$  was found sufficient to calculate time converged collision probabilities. We also track the norm of the wave function,  $\langle \Psi | \Psi \rangle$ , which is always 1.0 for the exact results and should converge to 1.0 for the Born-series results. The Born-series calculations are found to converge for all the incident energies, although more quickly for the higher energies. The lowest incident energy of 30 eV is still relatively high since it is almost 124 times the ionization potential. We note that all the first-order Born results are in better agreement with the exact calculations than the second-order Born results.

We next considered a short range three-body scattering system with  $\alpha = \frac{1}{4}$ . For this choice of the cutoff parameter

there are two bound state solutions, the ground state with a binding energy of  $-7.790$  eV and an excited state with a binding energy of  $-0.088$  eV. Thus, we have  $1s \rightarrow 2s$  excitation and direct ionization of the ground state. The inelastic cross section results at several different incident energies are presented in Table II. A  $400 \times 400$  point radial lattice with a mesh spacing of  $\Delta r_1 = \Delta r_2 = 0.2$  was found to be needed in order to obtain time converged collision probabilities. The Born-series calculations are again found to converge for all the incident energies, although more quickly for the higher energies. The lowest incident energy of 30 eV is now only four times the ionization potential. We note that for an incident energy of 30 eV the first-order Born results are in better agreement with the exact calculations than the fifth-order Born results.

Finally, we considered a long range three-body scattering system with  $\alpha = 0$ , that is, the standard Temkin-Poet model. Using a  $400 \times 400$  point radial lattice with a mesh spacing of  $\Delta r_1 = \Delta r_2 = 0.2$ , there are seven bound state solutions, the ground state having a binding energy of  $-13.47$  eV. Of course in the continuum limit, as the mesh spacing goes to zero and the box size goes to infinity, we obtain an infinite number of bound states and a ground state with a binding energy of  $-13.61$  eV. The inelastic cross section results at several different incident energies are presented in Table III. Time converged collision probabilities can only be extracted for the first-order Born and the exact calculations. In the first-order Born calculations, the normalization of the wave function and the probability of remaining in the ground state continue to increase with time propagation of the equations. On the other hand, we do obtain time-converged inelastic

TABLE III. Inelastic cross sections for an  $\alpha = 0$  long range three-body scattering system. Cross sections are given in Mb ( $1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$ ).

Born-series order	30 (eV)			50 (eV)			100 (eV)		
	$1s \rightarrow 2s$	$1s \rightarrow ks$	Norm	$1s \rightarrow 2s$	$1s \rightarrow ks$	Norm	$1s \rightarrow 2s$	$1s \rightarrow ks$	norm
1	1.682	2.65		0.620	1.69		0.160	0.62	
Exact	1.301	1.97	1.00	0.509	1.50	1.00	0.137	0.60	1.00

collision probabilities. In the second-order Born calculations, all the collision probabilities continue to increase with time propagation of the equations. Thus, the Born-series calculations are found to diverge for all the incident energies. We note that the inelastic first-order Born results are in fair agreement with the exact calculations, becoming even better for higher incident energies.

Our first-order time-dependent Born calculations for the Temkin-Poet model are closely related to first-order time-independent Coulomb-Born calculations for inelastic cross sections. Unfortunately, we have difficulty in adapting the present time-dependent Born-series calculations for the Temkin-Poet model to correspond to first-order time-independent distorted-wave calculations for inelastic cross sections. The problem lies with the two-electron wave function initial condition. If we let  $\bar{H}_0(r_1, r_2) = H_0(r_1, r_2) + U(r_2)$  and  $\bar{V}(r_1, r_2) = V(r_1, r_2) - U(r_2)$ , then a symmetrized product of the ground state solution and an incoming radial wave packet is not a solution of Eq. (4) with  $H_0 \rightarrow \bar{H}_0$ . Thus, we are not able to ascertain with the present time-dependent method which first-order distorted-wave theory is best.

As first pointed out by H. P. Kelly in his many-body perturbation theory calculations for inelastic electron-atom scattering [6], long range Coulomb field divergences appear in the higher-order terms for the optical potential for any choice of Coulomb or distorted wave. A possible course of action, as suggested by Pan and Kelly [7], is to choose a mixed basis of Coulomb and distorted-wave continuum states such that strong cancellations occur among the higher-order divergent terms for the optical potential. Then this mixed basis is used to calculate only the finite lower-order optical potential terms to obtain inelastic scattering cross sections. On the other hand, our study of time-dependent Born-series calculations for model three-body scattering systems suggests another approach. To wit, high-order optical potential calculations for a set of short range many-body Hamiltonians that gradually approach (as  $\alpha \rightarrow 0$ ) the exact many-body Hamiltonian. Of course, exact time-dependent solutions of the full many-body Hamiltonian may prove to be easier.

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