ELECTRONIC STRUCTURE OF MATERIALS CENTRE

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Abstract

The convergent close coupling approach developed by the authors is applied to positron scattering from atomic hydrogen below the first excitation threshold. In this approach the multi-channel expansion one-electron states are obtained by diagonalizing the target Hamiltonian in a large Laguerre basis. It is demonstrated that this expansion of the scattering wave function is sufficient to reproduce the very accurate low-energy variational results, provided target states with $l \leq 15$ are included in the expansions.

25.30.Hm,34.80.Bm

The general approach to electron-atom scattering, the Convergent Close-Coupling (CCC) method, has been recently applied to the problem of electron scattering from atomic hydrogen [1-3] and sodium [4]. The method uses a set of Laguerre functions to diagonalize the target Hamiltonian. It has the feature that the set is complete in Hilbert space and the basis functions can be chosen to be orthonormal. The details of the the theory are contained in Ref. [2]. The convergence properties of the scattering amplitudes have been investigated as a function of the basis set size for a given value of target orbital angular momentum quantum number l, and by increasing l in the target-state set. It has been shown that it is possible to get scattering ampltudes for low-lying excitations which are accurate to within a few percent over a wide range of energies. The method treats the full three-body problem to convergence. It's greatest success is that, unlike any other electron-atom scattering theory to date, it is able to achieve quantitative agreement with the measurements of the total ionization cross section and spin asymmetry [3] at the full range of projectile energies where measurements exist.

In this report we apply the above method to the problem of positron-hydrogen scattering below the first inelastic threshold for positronium formation. In this problem one only need modify the CCC theory for electron-hydrogen scattering by omitting the electron-exchange terms and changing the sign of the potentials in the three-particle Hamiltonian. In the elastic scattering region the boundary condition for both problems is the same. Thus, the interest in describing the scattering lies in seeing how large a basis set one needs to use to obtain convergent results. These may be tested by comparison with the very accurate variational calculations [5-7] which are available for the first few phase shifts. Since the CCC expansions of the three-body wave function depend on the coordinates of the positron ($\boldsymbol{r}_1$) and electron ($\boldsymbol{r}_2$) alone, and do not contain any correlation terms ($\boldsymbol{r}_1 - \boldsymbol{r}_2$), it is not *a priori* clear how quickly the expansions will converge.

We also apply the standard close-coupling (CC) formalism, where convergence in the expansion of the three-body wave function is obtained using just the exact discrete eigenstates of the atomic hydrogen target. Comparison of these results with those of the CCC method

allow for the examination of the effect of virtual excitation to the continuum. It is this effect that is left out in the CC formalism, but is fully treated to convergence in the CCC theory.

The existence of very accurate phaseshifts for the full $e^+ - H$ scattering problem is of great importance to the theorist. Any general positron-atom scattering theory must be able to reproduce these to a reasonable accuracy. Similarly, in the electron-hydrogen scattering problem there are very accurate solutions of the simplified Poet-Temkin model which contains most of the difficulties in the calculation associated with the full problem, see Ref. [1] and references therein. Successful application of the CCC method to the Poet-Temkin model verified the validity of the approach, and gave us the confidence to apply the method to the full problems of electron scattering on atomic hydrogen and sodium. We now use the accurate phaseshifts for positron scattering on atomic hydrogen to test, for the first time, the applicability of the CCC method to this problem.

The Laguerre basis $\xi_{kl}(r)$ we use is

$$\xi_{kl}(r) = \left(\frac{\lambda_l (k-1)!}{(2l+1+k)!}\right)^{1/2} (\lambda_l r)^{l+1} \exp(-\lambda_l r/2) L_{k-1}^{2l+2}(\lambda_l r), \qquad (1)$$

where the $L_{k-1}^{2l+2}(\lambda_l r)$ are the associated Laguerre polynomials, and k ranges from 1 to the basis size N_l. For a particular target partial-wave l the states and corresponding energies, resulting upon the diagonalization of the target Hamiltonian in this basis, depend on two parameters λ_l and N_l. In our earlier $e^- - H$ work [2] we found that convergence in the elastic and first inelastic channels was readily obtained at all energies by including target state expansions with orbital angular momentum up to $l = 3$. This is far from the case in positron-hydrogen scattering at the projectile momenta (a.u.) considered here of 0.1 to 0.7. We find that the behaviour of the convergence in the CCC results for electron or positron scattering on atomic hydrogen to be in stark contrast. For the first partial wave, $J = 0$, to obtain convergence of around one percent we require target states with $l \leq 15$. For the subsequent partial waves, $J = 1, 2, 3$, we require states with $l \leq 12$, $l \leq 10$, and $l \leq 6$, respectively. Typically, the higher the projectile momentum the larger target state l is required. Fortunately, the size of the Laguerre basis N_l, necessary for convergence, is

considerably smaller, and is typically $N_l \approx 6$. This is probably due to the fact that the projectile momentum under consideration is quite small. The choice of λ_l may be used to slightly speed up the rate of convergence as a function of N_l. We typically have $\lambda_l \approx 3$ for each l. A value of $\lambda_0 = 2$ would yield the exact $1s$ state with only $N_l = 1$. For $\lambda_0 = 3$ the $1s$ state is adequately reproduced with $N_l \geq 3$.

Convergence in the CC method is very easy to obtain. As this method uses only the discrete eigenstates of the hydrogen atom, the higher l states are all very long-ranged and do not contribute to the elastic channel. We achieve convergence for all partial-waves with target states having $l \leq 5$, and with around four states for each l.

The resulting elastic phaseshifts of our CCC and CC calculations are given in Table I. These are compared with variational calculations, as well as a calculation of Higgins *et al* [8] which is based on the Intermediate Energy R Matrix method (IERM) [9,10]. We see that the CCC results are in excellent agreement with the variational and IERM results. The IERM results [8] shown are those without extrapolation, because they are then directly comparable with our CCC numbers. It is not our intention here to provide phase shifts of four-figure accuracy, but merely to demonstrate the ability of the CCC theory to describe the features of positron scattering in the elastic region. On the other hand the CC theory is not even in qualitative agreement for the lower partial waves, indicating the importance of treating the virtual excitation of the continuum.

In conclusion, we have demonstrated that the CCC formalism of Bray and Stelbovics [2] is valid in describing positron scattering below the positronium formation threshold. The expansion of the method to treat target states with $l \leq 15$ has been achieved in order to treat the problem to an accuracy of order one percent. Higher accuracy can be obtained by extrapolation corrections. Phase shifts for partial waves higher than $J = 3$, or scattering amplitudes for the full problem may be obtained by correspondence with the first author.

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TABLES

TABLE I. Elastic phaseshifts for positron scattering on atomic hydrogen at projectile momenta (a.u.) of 0.1 to 0.7. The variational calculations for partial waves $J = 0, 1, 2$ denoted by indices a, b, and c are from Refs. [5-7], respectively. The IERM results are from Ref. [8].

J	method	0.1	0.2	0.3	0.4	0.5	0.6	0.7
0	variational[a]	0.1483	0.1877	0.1677	0.1201	0.0624	0.0039	-0.0512
	variational[c]	0.1460	0.1849	0.1649	0.1172	0.0593	0.0000	-0.0569
	CCC	0.145	0.183	0.163	0.119	0.062	0.0034	-0.0531
	IERM	0.142	0.180	0.159	0.111	0.055	-0.002	
	CC	0.015	0.015	0.064	0.118	0.172	0.221	0.265
1	variational[b]	0.0094	0.0338	0.0665	0.1016	0.1309	0.1547	0.1799
	variational[c]		0.030	0.063	0.097	0.128	0.146	0.169
	CCC	0.0088	0.0325	0.0649	0.0986	0.128	0.151	0.171
	IERM	0.009	0.032	0.064	0.096	0.123	0.144	0.163
	CC	0.006	0.018	0.029	0.035	0.034	0.028	0.017
2	variational[c]	0.0013	0.0054	0.0125	0.0235	0.0389	0.0593	0.0863
	CCC	0.0014	0.0055	0.0127	0.0239	0.0389	0.0582	0.0839
	IERM		0.005	0.013	0.024	0.039	0.058	
	CC	0.0010	0.0041	0.0089	0.0147	0.0207	0.0260	0.0303
3	CCC	0.0004	0.0018	0.0040	0.0075	0.0121	0.0191	0.0287
	IERM		0.0018	0.0040	0.0073	0.0124	0.0200	
	CC	0.0004	0.0014	0.0032	0.0056	0.0086	0.0122	0.0163