Convergent *R* matrix with pseudostates calculation for e^--He collisions

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The *R* matrix with pseudostates method has been used to study e^--He collisions at low and intermediate energies up to 80 eV. Since target correlation effects and target continuum states are both accurately represented by this method, the associated program package can now be used to obtain reliable results at intermediate energies for more complex atomic and ionic targets, which are urgently required in many applications. [S1050-2947(96)50907-8]

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Electron collisions with atoms and ions has attracted considerable attention since the earliest days of quantum mechanics, because these processes provide an ideal means of investigating the quantum dynamics of many-particle systems at a fundamental level [1]. In addition, a detailed understanding of these processes is of crucial importance in many other fields, particularly in the interpretation of observations in astronomy, planetary atmospheric studies, plasma physics, and laser physics.

Until recently, most detailed theoretical investigations concentrated either on the ''low-energy region,'' where the electron-impact energy is insufficient to ionize the target, or on the ''high-energy region,'' which is usually taken to be above about four times the ionization threshold energy. At low energies, close-coupling or *R*-matrix calculations, including in recent years an increasing number of *physical* target states in the expansion, have usually given satisfactory results (see, for example, Burke and Berrington [2]). On the other hand, at high energies perturbative methods such as the first-order distorted-wave Born approximation (DWBA) [3] or the first-order many-body theory (FOMBT) [4] can be used. However, while many calculations based on these low-energy or high-energy methods have been reported for energies lying between the ionization threshold and about four times this threshold, their reliability is often questionable in view of their underlying assumptions. The fundamental difficulty at these ''intermediate energies'' is that the theoretical method adopted must be able to accurately allow for loss of flux into the infinity of continuum states of the target atom or ion that become open and are, in addition, strongly coupled in this energy region.

One method of treating the intermediate-energy region that has been considered for many years is based on augmenting the physical target state basis included in the close-coupling expansion by a set of square-integrable ''pseudostates.'' These pseudostates are not eigenstates of the target Hamiltonian, but are chosen to represent in an average way the higher-lying Rydberg and continuum states of the target. Intermediate-energy e^--H collisions were first considered using this approach by Burke and Webb [5]. More recently, Callaway and Oza [6], using a Slater-orbital basis to represent the pseudostates, obtained accurate e^--H $1s\rightarrow 2s$ and $1s\rightarrow 2p$ excitation cross sections at intermediate energies. These cross sections were also successfully studied by Scott *et al.* [7] using an intermediate-energy *R*-matrix (IERM) basis for the pseudostates, and by Bray and Stelbovics [8,9] using a Laguerre basis. The method adopted by Bray and Stelbovics, referred to as the ''convergent close-coupling'' (CCC) method, has also recently been successfully extended to e^--He scattering at intermediate energies by Fursa and Bray [10]. They treated the helium target in a one-electron frozen-core approximation to yield impressive agreement with nearly all the available experimental data, including electron-impact ionization. Furthermore, Konovalov and McCarthy [11], using a ''convergent *J*-matrix calculation,'' which also represented the continuum by a square-integrable basis, obtained accurate results for resonances in e^--He collisions in the vicinity of the $n=2$ and $n=3$ thresholds.

In this Rapid Communication we present an application of a general method and program to e^--He collisions. This method, described in detail by Bartschat *et al.* [12] and called the ''*R*-matrix with pseudostates method'' (RMPS), extends the *R*-matrix program package RMATRX II [13], which has been developed to enable accurate electron-impact excitation cross sections for arbitrary complex atoms and ions to be calculated at low energies, by including a large square-integrable set of pseudostates. The results reported here represent an example of calculations for a multielectron target, where *both* important target correlation effects and target continuum states are accurately represented.

Turning now to a detailed description of our calculation for e^--He collisions, we obtained an accurate representation of the target states and pseudostates using the following set of physical orbitals and pseudoorbitals. (i) The analytically known 1*s* orbital of He^+ was included, since it is a very good approximation of the inner orbital in all excited states of neutral helium. (ii) Next, two pseudoorbitals $2\overline{s}$ and $2\overline{p}$ were included, which have the same exponential behavior (e^{-2r}) as the 1*s* orbital; in addition, the $2\overline{p}$ orbital was chosen to represent the full dipole polarizability of the He^+ ground state. (iii) Two more pseudoorbitals, $3\overline{s}$ and $3\overline{p}$, were constructed by using the configuration-interaction code CIV3 [14] to optimize the energy of the $(1s^2)^1S$ ground state of

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TABLE I. Absolute energies of the He targets states (in atomic units). The accurate nonrelativistic results are taken from Pekeris [15] for the $1\,^1S$ ground state and from Accad, Pekeris, and Schiff [16] for the excited states.

State	Ref. [18]	Ref. [10]	This work	Nonrel.	Moore [17]
$1\,^1S$	−2.85687	−2.87227	−2.89966	−2.90372	−2.90317
$2\,^3S$	−2.17420	−2.17419	−2.17517	−2.17523	−2.17484
$2\,^1S$	−2.14333	−2.14336	−2.14569	−2.14597	−2.14558
$2\,^3P^o$	−2.13132	−2.13130	−2.13306	−2.13316	−2.13278
$2\,^1P^o$	−2.12229	−2.12245	−2.12365	−2.12384	−2.12345

TABLE II. Oscillator strengths for $n=1,2$ transitions in He. The two rows in the theory columns represent the length (top) and velocity (bottom) forms, respectively.

Transition	Ref. [18]	This work	Ref. [19]
$1\,^1S\rightarrow 2\,^1P^o$	0.255	0.2755	0.2762
	0.273	0.2766	
$2\,^1S\rightarrow 2\,^1P^o$	0.363	0.3754	0.3764
	0.290	0.3760	
$2\,^3S\rightarrow 2\,^3P^o$	0.554	0.5398	0.5391
	0.519	0.5389	

neutral helium, where all possible configurations were included in the CI expansion that could be formed from the five $1s$, $2\overline{s}$, $2\overline{p}$, $3\overline{s}$, and $3\overline{p}$ orbitals. (iv) The next three pseudoorbitals, $4\overline{s}$, $4\overline{p}$, and $3\overline{d}$, were also constructed with CIV3 to optimize the energies of the $n=2$ states of neutral helium. (v) Further pseudoorbitals $n\overline{\ell}$ were constructed to represent the target continuum by taking the minimum linear combination of Sturmian-type orbitals $r^i e^{-\alpha r}$ orthogonal to the above-mentioned orbitals. Although the range parameter α is, in principle, arbitrary, the convergence of the results for specific transitions will depend on its choice. In the present calculation, we chose $\alpha=1.2$ and included $\overline{s}$ orbitals up to $n=10$, $\overline{p}$ orbitals up to $n=9$, and $\overline{d}$ orbitals up to $n=6$. It was not necessary to choose an angular-momentum-dependent parameter $\alpha(\overline{\ell})$. (vi) Finally, the target states and pseudostates were constructed as multiconfiguration expansions through diagonalization of the target Hamiltonian. To make the subsequent scattering calculation both tractable and consistent with the structure part, we included only configurations where at least one electron occupied one of the five orbitals that were used in the optimization of the $(1s^2)^1S$ ground state.

The main reason for the inclusion of the Sturmian-type orbitals described in (v) above is to represent the target continuum states in the close-coupling expansion. Nevertheless, these orbitals also further improve the five physical target states. Indeed, an important advantage of our present approach is that N-electron target correlation effects and $(N+1)$-electron continuum effects are treated in a consistent way. An improvement in the treatment of one thus automatically yields an improvement in the treatment of the other.

Our results for the physical target energies are shown in Table I, in comparison with experiment and other theoretical work. Note the very good energy positions compared to the other collision calculations, particularly the absolute energies of the two ^1S states. Since more than 90% of the electron correlation energy of the ground state is included in the present model, we also expect to obtain very reliable low-energy phase shifts. Due to relativistic effects omitted in our model, our absolute energies for the excited states even lie slightly below the experimental values [17].

We also note the very good agreement between the experimental values and the length and velocity forms of the oscillator strengths for the transitions between the physical target states included in our calculation. Our results are summarized in Table II, where we compare them with those used by Berrington and Kingston [18] in a 19-state R-matrix calculation and with the highly accurate results given by Wiese, Smith, and Glennon [19].

With the above orbitals and target states, we performed an R-matrix calculation, including a total of 41 states (ten ^1S, nine ^3S, eight ^1P, eight ^3P, three ^1D, and three ^3D). Our choice of the α parameter and the R-matrix radius of $27a_0$ ensured that all pseudostates as well as the five physical states $1\,^1S$, $2\,^{3,1}S$, and $2\,^{3,1}P^o$ fit into the R-matrix box. Tests with an increased box size of $40a_0$ and a decrease in the α parameter to ensure a proper representation of the tail of the wave functions showed that we can obtain similarly good representations of the $n=3$ (and, in principle, higher n) target states using the same *general* method.

We obtained excellent agreement with low-energy phase-shift results [20,21] for incident energies below the first excitation threshold, indicating the quality of both our target description and the collision model [22]. At higher energies in the elastic region, the present calculation yields the position of the well known ^2S resonance at 0.453 eV below the $2\,^3S$ excitation threshold, with a width of 10.7 meV. On the experimental energy scale, this position corresponds to 19.366 eV above the ground-state energy. This result is in nearly perfect agreement with the experimental findings of Cvejanovic, Comer, and Read [23] who give a position of 19.367 ± 0.009 eV with a width of 9 meV. Consequently, we believe that the present calculation yields the most accurate results available to date for the resonance region near the $n=2$ excitation thresholds.

Figures 1 and 2 show total cross-section results for excitation of the $1\,^1S\rightarrow 2\,^{3,1}S$ and $2\,^3S\rightarrow 2\,^1S$ transitions for incident electron energies in the vicinity of the $n=2$ thresholds and for higher energies between 30 and 80 eV. In the latter energy region, some small oscillations (due to pseudothresholds) with amplitudes of less than 10% of the absolute values were smoothed out. Convergence checks, including more D and F states in the close-coupling expansion, indicate that the results presented here are converged to better than 2% with respect to the effect of such states.

In the resonance region near the $n=2$ thresholds, the agreement with the 29-state R-matrix calculation of Fon, Lim, and Sawey [24] and the J-matrix results of Konovalov and McCarthy [11] is satisfactory. Like Konovalov and McCarthy (see their Fig. 1), we observe a small reduction in the total cross section compared to the 29-state calculation, due to the effect of continuum channels that were omitted in that work. We support the view of Konovalov and McCarthy that the remaining differences between the theories are likely to

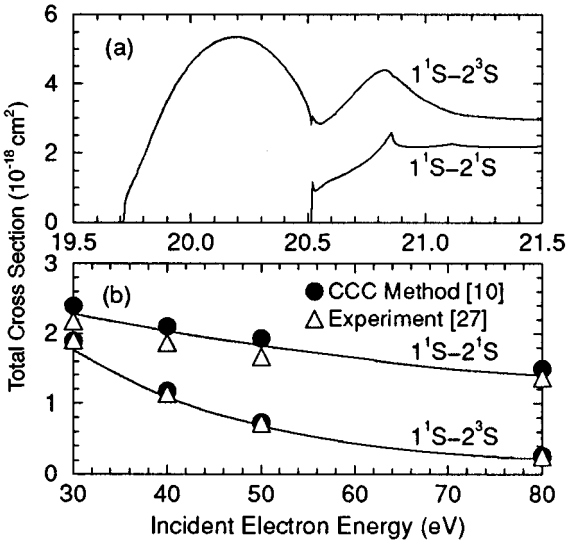

FIG. 1. Total cross sections (in 10^{-18} cm^2) for electron-impact excitation of the $1\,^1S \rightarrow 2\,^{3,1}S$ transitions in helium near the $n=2$ thresholds (a) and between 30 and 80 eV incident electron energy (b).

be due to differences in the target description. As discussed above, we believe that effects due to the target structure are accounted for very accurately in the present calculation.

Our results at incident energies of 30, 40, 50, and 80 eV are compared in Table III with experiment and with the 75-state CCC results of Fursa and Bray [10]. In light of the experimental uncertainties discussed by de Heer *et al.* [26], which are about 5% for the elastic cross section, 30% for the $1\,^1S \rightarrow 2\,^3S$ cross section, and 10% for the $1\,^1S \rightarrow 2\,^1S$ cross section, the agreement between the predictions from the two models and experiment is very satisfactory, indicating once more the reliability of the theoretical methods [27,28].

For comparison, we also present results obtained in a standard physical five-state frozen-core calculation, including the $1s$ orbital of He^+, a $2\overline{s}$ pseudoorbital optimized on the ground-state energy, and $3\overline{s}$ and $2p$ orbitals optimized on

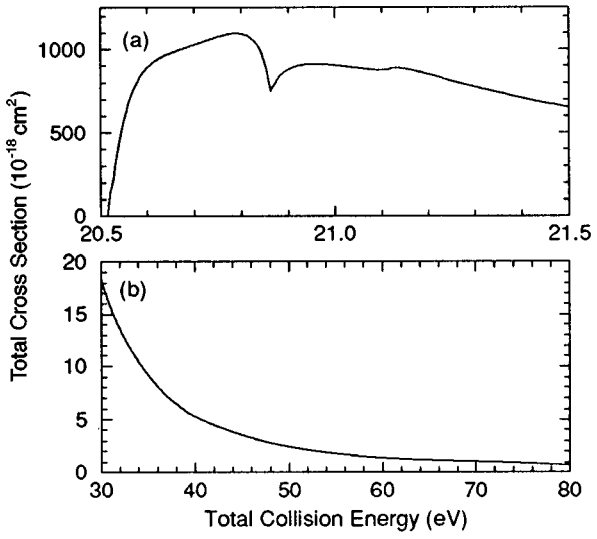

FIG. 2. Same as Fig. 1 for the transition $2\,^3S \rightarrow 2\,^1S$.

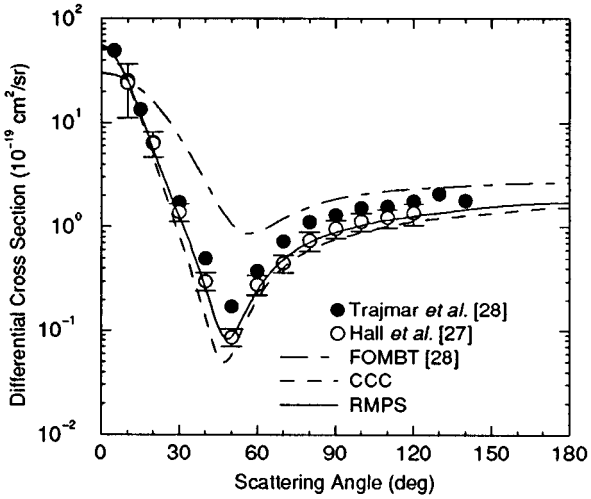

FIG. 3. Differential cross section for electron-impact excitation of the $1\,^1S \rightarrow 2\,^1S$ transition in helium at an incident electron energy of 50 eV.

the sums of the $2\,^{3,1}S$ and $2\,^{3,1}P^o$ eigenvalues, respectively. As one would expect, the results for the elastic cross section are nearly unchanged, with the CCC and RMPS values being slightly larger due to the inclusion of the full dipole polarizability in these models. On the other hand, the CCC and RMPS results for the $1\,^1S \rightarrow 2\,^{3,1}S$ transitions at the lower energies quoted are less than 50% of their values in the five-state model. This dramatic reduction is due to the effect of the target continuum states and is similar to that found by Burke and Webb [5] for electron-impact excitation of atomic hydrogen. It is therefore likely that this effect is of similar importance for other more complex atomic targets, and *must be* included to obtain accurate results in collision calculations for the intermediate-energy region.

On a more detailed level, Fig. 3 shows differential cross

TABLE III. Total cross sections (in 10^{-18} cm^2) for electron-impact excitation of helium. CCC refers to the 75-state calculation of Fursa and Bray [10] and five-state to a frozen-core model with physical states alone (see text). The experimental data for the elastic cross section are taken from Register *et al.* [25] and for excitation from de Heer *et al.* [26].

Transition	Energy (eV)	Five-state	CCC	This work	Experiment
$1\,^1S \rightarrow 1\,^1S$	30	201	225	219	211
	40	154	169	166	158
	50	124	134	133	126
	80	73.2	75.9	78.4	71.2
$1\,^1S \rightarrow 2\,^3S$	30	4.95	1.91	1.76	1.90
	40	1.63	1.14	1.10	1.18
	50	0.709	0.732	0.694	0.740
	80	0.151	0.256	0.225	0.260
$1\,^1S \rightarrow 2\,^1S$	30	5.84	2.19	2.29	2.40
	40	3.97	1.87	2.02	2.11
	50	3.12	1.67	1.84	1.94
	80	1.66	1.37	1.40	1.50

section results for excitation of the $2\,^1S$ state at an incident electron energy of 50 eV. Excellent agreement exists between RMPS, CCC, and the experimental data, while the perturbative FOMBT calculation is inadequate.

In conclusion, we have shown that the RMPS method yields accurate elastic and inelastic $1\,^1S \rightarrow 2\,^{3,1}S$ cross sections for e^--He collisions at low and intermediate energies. We are now extending this calculation to obtain accurate results for transitions involving the $2\,^{3,1}P^o$ states as well as higher Rydberg states with $n=3$ and 4. For these transitions, physical and pseudo *D* and *F* states will need to be included in the expansion. Also, since the RMPS method and the associated program package include target correlation effects and target continuum states in a completely general and consistent way, reliable cross sections for arbitrary targets at low and intermediate energies can now be readily obtained. We are therefore planning to extend our work to more complex targets such as carbon and oxygen where reliable cross sections are urgently required in many applications.

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