Calculation of electron-helium scattering at 40 eV

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We apply the convergent close-coupling (CCC) method to calculation of 40-eV electrons scattering on the ground state of helium. We present the differential cross sections up to the $n \leq 3$ levels, as well as the electron-impact coherence parameters for the $3\,^1D$ state. We find our results to be in excellent agreement with the measurements. It is shown that at this energy treating the target continuum has a large effect on the presented results, and for this reason the CCC theory is the only one that is able to obtain agreement with experiment. Integrated, total ionization, and total cross sections are also presented, and are found to be in excellent agreement with experiment.

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We wish to develop a general reliable method for the calculation of electron-atom and electron-ion scattering phenomena. To this end we choose the close-coupling (CC) formalism because, having expanded the total wave function in a set of target states, it attempts to solve the resulting scattering equations without approximation. Thus the major issue in the CC calculations is whether a sufficiently complete set of target states has been taken in the expansion. The convergent close-coupling (CCC) method provides a systematic approach to increasing the multichannel expansion due to the use of an orthogonal Laguerre basis for the generation of target states. As the basis sizes are increased we can be confident that the expansions approach completeness, and that if convergence to a required accuracy is observed, then any larger expansions are unlikely to significantly alter the result.

The formal theory of the CCC method for the e-H scattering problem has been given by Bray and Stelbovics [1], and then extended to hydrogenlike targets by Bray [2]. The numerous applications of the CCC method have shown it to be equally reliable across the entire energy range where the Born approximation is invalid. It is able to obtain accurate results for elastic, inelastic, ionization, and total cross sections simultaneously for a particular energy. Having thoroughly tested the CCC method for the three-body Coulomb problem of electron scattering on hydrogenlike targets, we have now moved on to the four-body Coulomb problem of electron scattering on helium.

This problem has attracted a great deal of interest from many experimental and theoretical groups. The large quantity of experimental data allows the theorists to thoroughly test their scattering calculation methods. There are a number of R-matrix calculations at the low- [3–5], intermediate- [6], and high- [7] energy ranges. Most of these treat only the target discrete states. Above the one-electron ionization threshold, inclusion of some treatment of the target continuum becomes necessary, something which these calculations find difficult.

There are also theories that are based on the perturbative approach. There are many applications of the first-order many-body theory (FOMBT), see, for example, Cartwright *et al.* [8] and Trajmar *et al.* [9]. There are also distorted-wave calculations of Bartschat and Madison [10]. While some of the transitions are well described by these theories they usually have considerable difficulty when compared with available measurements.

Our first application of the CCC method to e-He scattering at 30 eV [11] showed that we were able to get very good agreement with the measurements of the differential cross sections for excitation of the helium ground state up to $n \leq 3$ levels. We found that this was only possible if the target continuum was treated in the close-coupling formalism. This may be done accurately with the CCC method using positive energy, but still square-integrable states. In this work we apply the method to the projectile energy of 40 eV not only to differential cross sections but also to the electron-impact coherence parameters (EICPs) for the $3\,^1D$ state. We expect that comparison with the measurements of the latter will prove to be a more sensitive test of our method.

In the CCC method the solution of the Schrödinger equation takes the form of a coupled set of Lippmann-Schwinger equations for the T matrix,

$$\langle \boldsymbol{k}_f\phi_f|T|\phi_i\boldsymbol{k}_i\rangle = \langle \boldsymbol{k}_f\phi_f|V|\phi_i\boldsymbol{k}_i\rangle + \sum_n \int d^3k \frac{\langle \boldsymbol{k}_f\phi_f|V|\phi_n\boldsymbol{k}\rangle\langle \boldsymbol{k}\phi_n|T|\phi_i\boldsymbol{k}_i\rangle}{E-\epsilon_n-k^2/2+i0}, \quad (1)$$

where projectile momentum and corresponding energy are denoted by $\boldsymbol{k}$ and $k^2/2$, the helium target states and corresponding energy are denoted by ϕ_n and ϵ_n, and $E = \epsilon_i + k_i^2/2 = \epsilon_f + k_f^2/2$ is the total energy. The V-matrix elements and the method for obtaining the target states are given in Ref. [11]. In both the earlier work and here we use the frozen-core approximation when generating the helium target states.

We solve (1) with an ever increasing number of target states obtained by diagonalizing the target Hamiltonian using a large Laguerre basis [11] until satisfactory con-

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vergence is obtained. The following results have been obtained using a total of 62 states which are comprised of 11 states of each of the ^1S, ^3S, ^1P, and ^3P symmetries, and nine states of each of the ^1D and ^3D symmetries. These calculations we denote by CCC. Of the 62 states 29 lie in the discrete spectrum. We use these to indicate the effect of the continuum on the presented results.

In Fig. 1 we present our calculations for the differential cross sections for electrons scattering on the ground state of helium up to the $n \leq 3$ levels. We see that it is only the CCC calculation that is able to obtain almost complete quantitative agreement with the measurements. Comparison of the CCC and the CC calculations shows the quite considerable effect of the treatment of the target continuum. Similar observations have been made earlier by Brunger *et al.* [12], who used a more approximate method of treating the continuum via the CCO model. The first-order many-body theory of Cartwright *et al.* [8] and Trajmar *et al.* [9] is very successful in describing the singlet nP excitations, but is less reliable for other transitions.

We now turn to Fig. 2, where we present our calculations of the electron-impact coherence parameters for the $3\,^1D$ excitation of helium. A major motivation for us in applying the CCC method here is due to the recent detailed investigations performed by Donnelly and Crowe [13], McLaughlin, Donnelly, and Crowe [14], McLaughlin *et al.* [15], Batelaan, van Eck, and Heideman [16], and Mikosza *et al.* [17]. The measurements are in good agreement with each other, but are in poor agreement with the then available theory. We are therefore particularly pleased to find excellent agreement between the CCC calculations and the measurements. It should be noted that the Stokes parameters P_1, P_2, P_3, and P_4 are sufficient to determine the other presented parameters. For the relevant relations see Andersen, Gallagher, and Hertel [18]. Once more, comparison of the CCC and the CC calculations shows the very large effect of the treatment of the continuum within the close-coupling formalism. The other presented theory is due to Bartschat and Madison [10]. This is a first-order distorted-wave approximation whose results have a strong dependence on the choice of the distorting potential [10]. We have presented only one of their calculations for the sake of clarity. For the same reason the FOMBT results of Cartwright and Csanak [19] are not presented.

In Table I we give various integrated cross sections, all of which are in excellent agreement with experiment. It is particularly worthwhile to note the excellent agreement for the total ionization cross section. Any calculation that uses only the discrete states, such as the CC ones above, yields identically zero for this cross section.

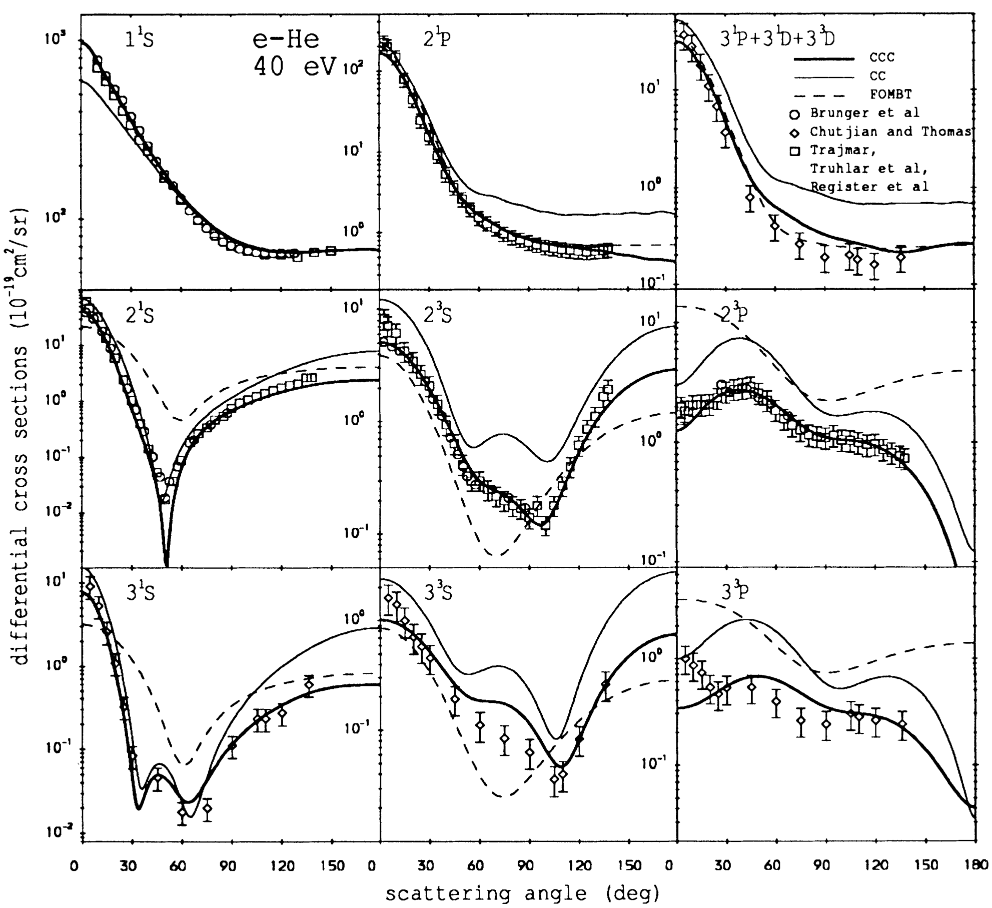

FIG. 1. Differential cross sections for e-He scattering at a projectile energy of 40 eV. The present CCC calculations are obtained by coupling a total of 62 states. The CC calculations use just the first 29 of these that have negative energies relative to the $He^+(1s)$ frozen core. The measurements are due to Brunger *et al.* [21] (elastic), Brunger *et al.* [12] (ratio measurements multiplied by our theoretical $2\,^1P$), Trajmar [22] ($2\,^1S, 2\,^3S, 2\,^3P$), Register, Trajmar, and Srivastava [26] (elastic), Truhlar *et al.* [27] ($2\,^1P$), and Chutjian and Thomas [23] ($n = 3$). Quantitative results may be obtained from the authors.

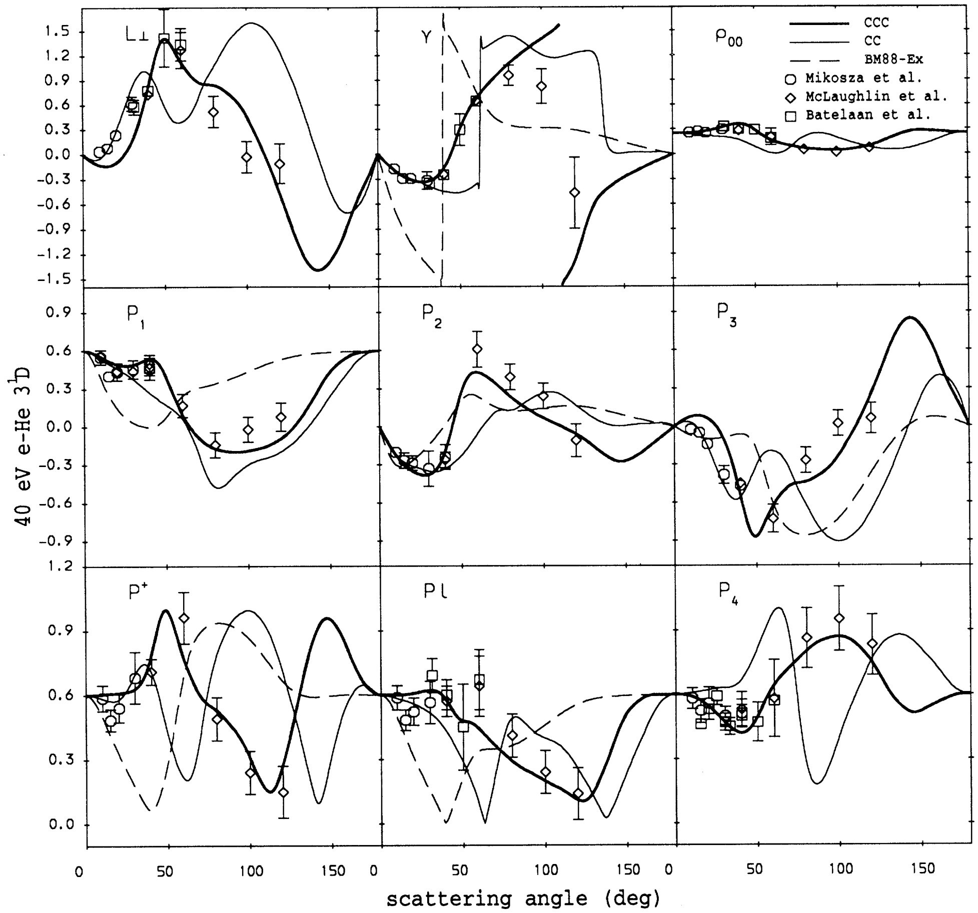

FIG. 2. The $3\,^1D$ EICPs for 40-eV e-He scattering. The CCC and CC calculations are as in Fig. 1. The calculations denoted by BM88 are due to Bartschat and Madison [10]. The measurements are due to McLaughlin, Donnelly, and Crowe [14], McLaughlin *et al.* [15], Batelaan, van Eck, and Heideman [16], and Mikosza *et al.* [17]. Quantitative results may be obtained from the authors.

It will be very interesting to apply the CCC method to calculating $(e,2e)$ differential cross sections for the e-He scattering problem. This should be as successful as the application to the atomic hydrogen target [20] so long as the frozen-core approximation is sufficiently accurate.

In conclusion, we have demonstrated that to date only the CCC method is able to reliably describe e-He scattering phenomena from the ground state up to $n \leq 3$ levels in the intermediate-energy range. The primary reason for this is that above the ionization threshold the effect of treating the target continuum may be very large. It is because such large effects require accurate treatment that many other available theories are less reliable.

It remains for us to apply the method to the wide range

TABLE I. Integrated cross sections ($10^{-18}\,\text{cm}^2$) for 40-eV electrons scattering on the ground state of helium. The ionization and total cross sections are denoted by σ_i and σ_t, respectively.

	$1\,^1S$	$2\,^1S$	$3\,^1S$	$2\,^3S$	$3\,^3S$
CCC	169.2	1.82	0.38	1.08	0.30
Expt.	167.0±8[a]	2.11±0.4[b]	0.24±0.06[c]		
	$2\,^1P$	$3\,^1P$	$2\,^3P$	$3\,^3P$	$3\,^1P+3\,^1D+3\,^3D$
CCC	6.73	1.38	1.73	0.49	1.79
Expt.	6.7±0.3[d]		1.77±0.32[b]	0.41±0.09[c]	1.59±0.38[c]
	$3\,^1D$	$3\,^3D$	σ_i	σ_t	
CCC	0.29	0.11	16.2	203.4	
Expt.			16.8±0.8[e]	194.0±6[f]	

[a] Bunger *et al.* [21].
[b] Trajmar [22].
[c] Chutjian and Thomas [23].
[d] Trajmar *et al.* [24].
[e] Montague, Harrison, and Smith [25].
[f] Register, Trajmar, and Srivastava [26].

of energies and various observables that have been measured for the e-He scattering problem. Initial indications suggest that the method is equally reliable at other energies both for the cross sections and various EICPs. Subsequently, the method will be extended to calculate $(e, 2e)$ differential cross sections for e-He ionization, and then to the treatment of heliumlike targets.

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[1] I. Bray and A. T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).
[2] I. Bray, Phys. Rev. A **49**, 1066 (1994).
[3] T. F. O'Malley, P. G. Burke, and K. A. Berrington, J. Phys. B **12**, 953 (1979).
[4] W. C. Fon and K. P. Lim, J. Phys. B **25**, 3513 (1992).
[5] W. C. Fon, K. P. Lim, K. Ratnavelu, and P. M. J. Sawey, J. Phys. B **27**, 1561 (1994).
[6] W. C. Fon, K. A. Berrington, and A. E. Kingston, J. Phys. B **21**, 2961 (1988).
[7] S. Nakazaki, K. A. Berrington, K. Sakimoto, and Y. Itikawa, J. Phys. B **24**, L27 (1991).
[8] D. C. Cartwright, G. Csanak, S. Trajmar, and D. F. Register, Phys. Rev. A **45**, 1602 (1992).
[9] S. Trajmar, D. F. Register, D. C. Cartwright, and G. Csanak, J. Phys. B **25**, 4889 (1992).
[10] K. Bartschat and D. H. Madison, J. Phys. B **21**, 153 (1988).
[11] I. Bray, D. V. Fursa, and I. E. McCarthy, J. Phys. B **27**, L421 (1994).
[12] M. J. Brunger *et al.*, J. Phys. B **23**, 1325 (1990).
[13] B. P. Donnelly and A. Crowe, J. Phys. B **21**, L637 (1988).
[14] D. T. McLaughlin, B. P. Donnelly, and A. Crowe, Z. Phys. D **29**, 259 (1994).
[15] D. T. McLaughlin *et al.*, J. Phys. B **27**, L19 (1994).
[16] H. Batelaan, J. van Eck, and H. G. Heideman, J. Phys. B **24**, L397 (1991).
[17] A. G. Mikosza, R. Hippler, J. B. Wang, and J. F. Williams, Z. Phys. D **30**, 129 (1994).
[18] N. Andersen, J. W. Gallagher, and I. V. Hertel, Phys. Rep. **165**, 1 (1988).
[19] D. C. Cartwright and G. Csanak, J. Phys. B **20**, L583 (1987).
[20] I. Bray, D. A. Konovalov, I. E. McCarthy, and A. T. Stelbovics, Phys. Rev. A **50**, 2818 (1994).
[21] M. J. Brunger *et al.*, J. Phys. B **25**, 1823 (1992).
[22] S. Trajmar, Phys. Rev. A **8**, 191 (1973).
[23] A. Chutjian and L. D. Thomas, Phys. Rev. A **11**, 1583 (1975).
[24] S. Trajmar, J. M. Ratliff, D. C. Cartwright, and G. Csanak, Z. Phys. D **22**, 457 (1992).
[25] R. G. Montague, M. F. A. Harrison, and A. C. H. Smith, J. Phys. B **17**, 3295 (1984).
[26] D. F. Register, S. Trajmar, and S. K. Srivastava, Phys. Rev. A **21**, 1134 (1980).
[27] D. G. Truhlar *et al.*, Phys. Rev. A **8**, 2475 (1973).