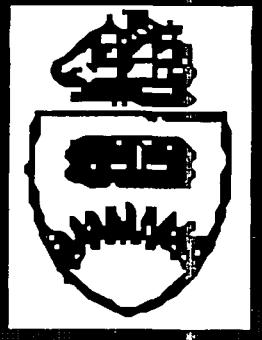

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ELECTRONIC STRUCTURE OF MATERIALS CENTRE

Convergent J-Matrix Calculation of Electron-Helium Resonances

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Abstract

Resonance structures in n=2 and n=3 electron-helium excitation cross sections are calculated using the J-matrix method. The number of close-coupled helium bound and continuum states is taken to convergence, e.g. about 100 channels are coupled for each total spin and angular momentum. It is found that the present J-matrix results are in good shape agreement with recent 29-state R-matrix calculations. However the J-matrix absolute cross sections are slightly lower due to the influence of continuum channels included in the present method. Experiment and theory agree on the positions of n=2 and n=3 resonances.

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Recently, a number of electron-atom scattering problems have been solved exactly using various forms of close-coupling methods. The problems are solved exactly in the sense that the calculations converge for physical observables when the number of coupled channels, including a discrete representation of the target continuum, is increased.

This trend is most clearly represented by Convergent-Close-Coupling (CCC) calculations for electron scattering on hydrogen (Bray and Stelbovics 1992*a*), sodium (Bray 1994), helium (Bray *et al* 1994) and references therein. Such a benchmark problem as the simplified model of electron-hydrogen scattering (only zero angular momentum is allowed), or Poet-Temkin model, has been also solved by the CCC method (Bray and Stelbovics 1992*b*, Bray and Stelbovics 1994).

One of the other close-coupling methods which can provide a solution of the scattering problem is the J-matrix method, see Broad and Reinhardt (1976) and references therein. Konovalov and McCarthy (1994*a*) have shown that the method could be used to solve the Poet-Temkin model of electron-hydrogen scattering to any required accuracy. The method uses an expansion of the target and projectile states in complete sets of square-integrable (L^2) Laguerre functions. The authors called the method convergent, in a fashion similar to the CCC method, to emphasise that if convergence by the number of L^2 states is achieved the result does not depend on the parameters of the L^2 basis used.

The J-matrix method is attractive to use for study of resonances as a number of incident electron energies can be calculated at once. Also, the method is very computer undemanding, for example, in comparison to the R-matrix method. All calculations are performed on a SUN SS10/512 workstation.

Konovalov and McCarthy (1994*b*) used the method to describe resonances in electron-hydrogen scattering. It was shown that, as for the Poet-Temkin problem, such physical observables as cross sections can be calculated to any required accuracy.

In this work we continue the study of resonances in electron-atom scattering. We present calculations of electron-helium scattering in the energy region of the n=2 and n=3 resonances using the J-matrix method.

In the case of electron-hydrogen resonances there is a pseudostate close-coupling calculation of Callaway (1982) which is in complete agreement with absolute measurements of Williams (1988). The J-matrix calculation of Konovalov and McCarthy (1994*b*) is in complete agreement with both. The R-matrix calculation of Fon *et al* (1994), which coupled only exact bound states of hydrogen, obtained absolute cross sections about 10% higher.

The situation with electron-helium resonances is more complex. Firstly, relative experiments of Brunt *et al* (1977) and Buckman *et al* (1983) predict different yields of metastable (2^3S and 2^1S) helium atoms resulting from electron impact on helium, as a function of the incident electron energy. Secondly, multiconfiguration wave-functions are required for the ground and excited states of helium (Froese-Fischer 1977) to be able to reproduce their energies to sufficient accuracy.

The aim of this work is to calculate the absolute values of n=2 and n=3 excitation cross sections of helium. The full problem is solved to an accuracy of better than 3% for n=2 and 5% for n=3 excitation cross sections. The number of coupled bound and continuum

target states is increased until convergence in the cross sections is achieved, e.g. about 100 channels were coupled for each LS. The resonances can be considered as decaying states of the He^- system. In the present calculation about 1000 He^- states were generated for each LS. We therefore present the the resulting cross sections rather than giving a table of a vast number of resonance energies and widths, e.g. there are about 20 He^- S-states only in the energy region up to 20 eV.

Quite a complete formulation of the J-matrix method was given by Broad and Reinhardt (1976) and references therein. Here we present details of a calculation specific to electron-helium scattering.

A complete set of orthogonal Laguerre functions

$$\phi_{nl}(r) = \phi_{k+l,l}(r) = (\lambda_l r)^{l+1} e^{-\lambda_l r/2} L_k^{2l+2}(\lambda_l r), \quad k = n - l = 0, 1, ..., \bar{N}_l - 1, \tag{1}$$

is used to create the basis functions by diagonalizing the one electron Hamiltonian,

$$\langle \psi_{nl} | -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{Z}{r} | \psi_{n'l} \rangle = \epsilon_{nl}\delta_{nn'} \quad Z = 2, \text{ if } l = 0; \quad Z = 1, \text{ if } l \neq 0, \tag{2}$$

where nl denotes the principal quantum number and angular momentum of a one-electron state. The coordinate space of the same size is covered for each l if the following set of λ_l is used

$$\lambda_l = \lambda_0 \frac{\bar{N}_l + l + 1}{\bar{N}_0 + 1}. \tag{3}$$

The ϕ_{nl} functions (1) are directly related to the non-orthogonal Laguerre functions used in the J-matrix method via

$$L_k^{\alpha+1}(x) = \sum_{k'=0}^{k} L_{k'}^{\alpha}(x). \tag{4}$$

Helium states are created by diagonalising its nonrelativistic Hamiltonian in the following set of correctly-antisymmetrised configurations with a total target spin S_t and orbital angular momentum L_t. One electron has always $l = 0$ and can be in $1s, 2s, ..., n_0 s$-states. The second electron can be in any nl state with $n - l \leq \bar{N}_l$. We use the set of $\bar{N}_l = 12, 8, 6, 5$ with $\lambda_0 = 1.2$ and $n_0 = 4$. The resulting eigenvalues are presented in table 1. All excited-state energies are described to an accuracy of better than 0.1%. Our description of the ground state does not include such configurations as $(2p)^2, (3p)^2$ and $(3d)^2$ which are needed to get the same accuracy as for the excited states (Froese-Fischer 1977). Excitation thresholds

are calculated using the MCHF ground state energy (E_0=-2.90303 a.u.) instead of the first eigenvalue (E_1=-2.87247). We have made this energy shift (0.8316 eV) in comparing our cross sections with experiment. Comparison with the experimental values of Moore (1971) shows that all considered excitation thresholds are reproduced to an accuracy of about 0.1% or better except for 2^1S (0.3%).

The J-matrix method requires wave functions of the whole system, target plus the scattering electron. He^- states are created by adding one more electron to the target configurations with the electron being in one-electron states with $n - l \leq N_l$. The total Hamiltonian of He^- is diagonalised for each total spin S and orbital angular momentum L. More than 1000 configurations were used for some LS. We used the convenient formulas of Fano (1965) to calculate the He^- matrix elements. The eigenvalues of He^- are invariant under any linear transformation of the initial basis ψ_{nl} (2), e.g. if the basis is made directly from Laguerre functions (1) (diagonalisation step (2) is omitted). This property is satisfied when all possible He^- configurations are included in the diagonalisation for each L and S. However the usage of ψ_{nl} defined by Eq.2 speeds up convergence for the cross sections by $\bar{N}_l$ and n_0.

It has been found that all physical observables converge faster by $\bar{N}_l$ than by N_l which is used in the J-matrix formalism to solve the scattering equations. To shorten the notation for an individual basis set we used the following notation

$$\{\lambda_0, n_0; (\bar{N}_0, N_0), (\bar{N}_1, N_1), ...\} = \{1.2, 4; (12, 17), (8, 15), (6, 12), (5, 10)\}. \quad (5)$$

The parameters were obtained by increasing $\bar{N}_l$, N_l, and n_0 for a particular λ_0 until further increase led to a difference in the cross section within the required accuracy. Small variations of λ_0 further confirmed that convergent results are achieved.

In figure 1*a*, *c* and figure 2 we present our results and compare them with the 29-state R-matrix results of Fon *et al* (1993). As in the case of electron-hydrogen resonances (Konovalov and McCarthy 1994*b*) the R-matrix results are slightly higher in the energy region above the n=2 thresholds ($2^3S, 2^1S, 2^3P$ and 2^1P). This is due to the influence of the continuum channels, which are not included in the R-matrix calculations (Fon *et al* 1993, Fon *et al* 1994). Some discrepancy in the 20 to 21 eV region is most likely due to different ways of describing the ground state of helium. We assumed that the results of Fon *et al* (1993) had a misprint in their presentation of 2S-cross sections. That is the scales in their figures are meant to be 10 times smaller, as in their earlier 19-state R-matrix calculations (Fon *et al*

1989).

In figure 1*b*, *d* we compare our results with curves describing the relative experiments of Brunt *et al* (1977) and Buckman *et al* (1983), which are normalised at the 20-21eV energy range to the present calculation. The plotted experimental values have some additional small errors, as we had to extract the experimental data by hand from figures in the papers. We agree with the position of n=2 and n=3 resonances described by the experiments. However we do not support the overall behavior of the metastable yield measured by Buckman *et al* (1983). If the experiment is normalised in the 20-21 eV range, than the value is too high at the higher energies. This is further supported by the comparison with the R-matrix results and variational calculations of Nesbet (1979) in figure 1*c*.

Some additional excitation cross sections are presented in figure 3 for future reference.

In conclusion, inclusion of helium continuum states has only a small effect in comparison with the R-matrix calculations, which coupled only bound states. Some remaining differences between theories is likely due to some differences in the description of the helium ground and excited states.

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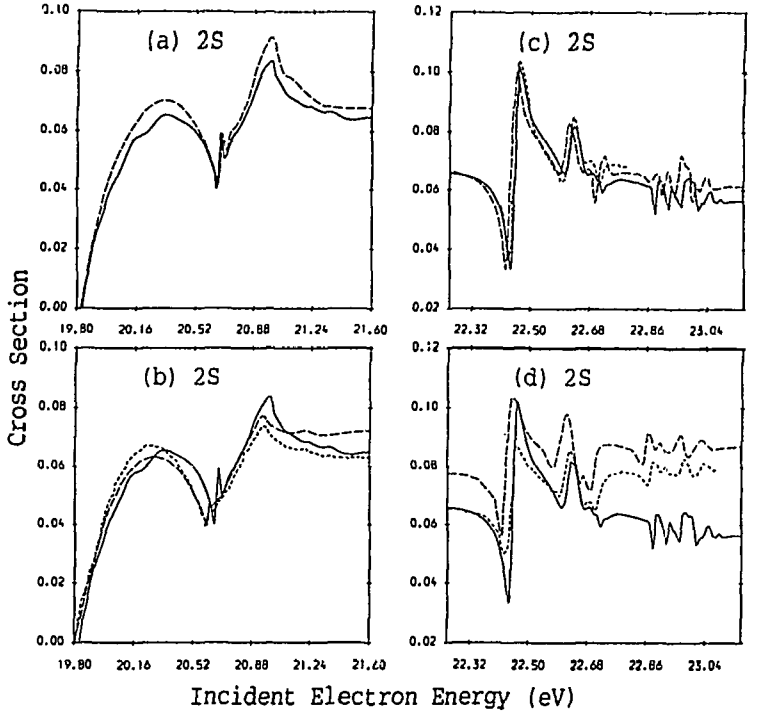

Fig.1

Figure 1.

Cross sections (πa_0^2) for the excitation of metastable ($2^1S + 2^3S$) states of helium. The solid line is the present convergent J-matrix calculation {1.2,4;(12,17)(8,15)(6,12)(5,10)}. Dashed line in *a* and *c* is the 29-state R-matrix calculation of Fon *et al* (1993). Short-dashed line in c is the variational calculation of Nesbet (1979). Arbitrarily normalised relative experimental results of Brunt *et al* (1977) and Buckman *et al* (1983) (b, d) are denoted by the short-dashed and long-dashed lines, respectively.

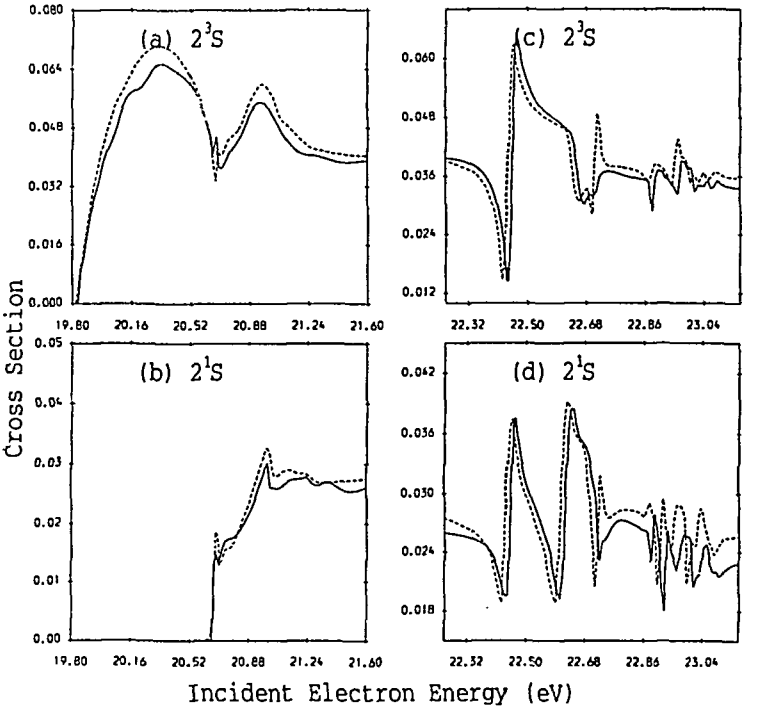

Fig. 2

Figure 2.

Cross sections (πa_0^2) for the excitation of 2S-triplet (a, c) and singlet (b, d) states of helium. The solid line is the present convergent J-matrix calculation. Dashed line is the R-matrix calculation of Fon *et al* (1993). Note the displaced zero on the cross section scale in figures c and d.

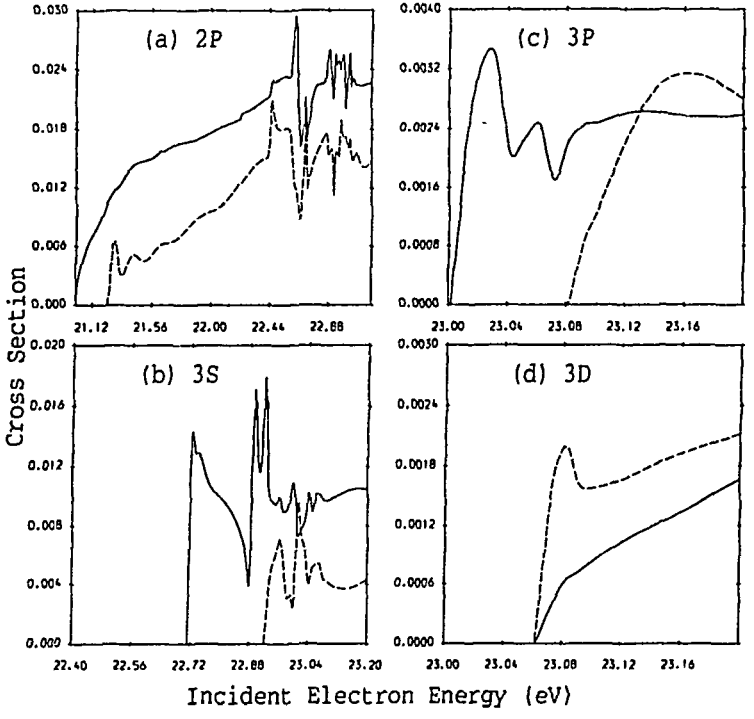

Fig 3

Figure 3.

Cross sections (πa_0^2) for the excitation of 2P (a), 3S (b), 3P (c), and 3D (d) states of helium. The solid line denotes triplet and dashed line denotes singlet.

Table 1.

The ground and n=2,3 states eigenvalues of the non-relativistic Hamiltonian of the helium atom ($-E$ in a.u.) together with corresponding excitation thresholds (eV) used in the calculations. Highly accurate non-relativistic energy levels of helium are by Pekeris (1958) for 1^1S and by Accad *et al* (1971) for the excited states. MCHF denotes the multiconfiguration Hartree-Fock calculations of Froese-Fischer (1977). HF and denotes the ground state Roothaan-Hartree-Fock calculation of Clementi and Roetti (1974). Excitation thresholds are calculated using the MCHF ground state energy (E_0=-2.90303). Experimental values derived from the analysis of optical spectra are by (Moore 1971).

Level	**Pekeris (1958) Accad *et al* (1971)	Present	MCHF	HF	Excitation thresholds (eV) Present	Moore (1971)
1^1S	2.90372**	2.87247	2.90303	2.86168	0.0	0.0
2^3S	2.17523	2.1742			19.834	19.8135
2^1S	2.14597	2.1434	2.14587		20.670	20.6095
2^3P	2.13316	2.1312			21.004	20.9577
2^1P	2.12384	2.1223			21.244	21.2115
3^3S	2.06869	2.0684			22.712	22.7116
3^1S	2.06127	2.0605			22.927	22.9134
3^3P	2.05808	2.0575			23.009	23.0001
3^3D		2.05547			23.0638	23.0667
3^1D		2.05544			23.0645	23.0671
3^1P	2.05515	2.0546			23.087	23.0800