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Photon and electron ionisation of helium to the $n = 2$ state of He^+

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Abstract. Partial photoionisation cross sections, the ratios of partial cross sections and anisotropy parameters in the angular distributions of photoelectrons are calculated in the region between the second and third ionisation thresholds of helium with the inclusion of all configuration interactions for a limited number of states of the subspaces of open and closed channels. The generalised partial oscillator strengths for transitions to the continuum of helium are calculated in the same approximation. The results are compared with experiment and calculations of different authors.

1. Introduction

In the last 20 years much effort has been devoted to obtaining complete information about the photoionisation of helium-like systems by photons and electrons in the region of quasistationary states converging to the second ionisation threshold.

Modern experimental techniques together with more powerful theoretical methods enable the autoionised states of helum-like systems between the second and third thresholds to be studied. Whereas in the region below the second threshold, resonances decay exclusively via one open channel, at energies above the excitation threshold of the residual ions there exist resonances converging to the third threshold whose profiles can be studied through both the total ionisation cross sections and the partial cross sections for population of the ground and $n = 2$ excited state of the residual ion. High-resolution experiments by Woodruff and Samson (1982) provided the cross sections for resonance photoionisation of helium to the $n = 2$ state of the He^+ ion. The earliest experiments (Dhez and Ederer 1973) on the total photoabsorption cross sections for helium in the region of 3s3p, the lowest resonance, have since been repeated and improved by Lindle *et al* (1985), who also obtained partial cross sections. The first theoretical results were reported by Senashenko and Wague (1979), Burkov and Strakhova (1984a), Salomonson *et al* (1985) and Burkov *et al* (1986). In the present paper we analyse the resonance photoionisation of helium over the energy range 65.4-72.9 eV, taking into account the recent results of Lindle *et al* 1985.

Of great interest are the profiles of the resonances decaying into excited states of ions as a function of momentum transfer. Experimental data are not yet available. We have calculated the generalised partial oscillator strengths (GOS) for the ionisation of helium by fast electrons between the second and third thresholds over a wide range of momentum transfer.

The key point in the problem of ionisation of an atomic system by fast electrons and photons is a description of the continuum final state. The cross section calculations

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for the direct photoionisation of helium (Burkov and Strakhova 1984b, Berrington *et al* 1982) and the calculations for the electron scattering on He^+ ions (Haysak *et al* 1982) indicated strong coupling of open channels in helium between the second and third thresholds. In the calculations made by Senashenko and Wague (1979) such coupling was neglected.

Consistent calculations of the resonance ionisation cross sections have been carried out in the framework of the close coupling of open and closed channels (Berrington *et al* 1982). This approach is not convenient for interpreting and comparing theory with experiment because the resonance characteristics are not parameters of the theory but are derived from the calculations made, as a rule, in the approximation of non-interacting resonances. The structures observed in the cross sections are often due to several overlapping resonances (Salomonson *et al* 1985, Burkov *et al* 1986). Attractive from this viewpoint is Fano's configuration interaction method (Fano 1961, Fano and Cooper 1965) which reproduces the cross section curves to the same high precision as does the close-coupling method (Altick and Moore 1966, Burke and McVicar 1965) and, at the same time, permits estimates to be made of the spectroscopic characteristics of the resonances contributing to the shape of cross sections. However, Fano's method has been substantiated only for the cases where at least one of the subspaces (subspace of open or closed channels) is filled by no more than a single state. An attempt was later made (Starace 1972) to extend Fano's approach to the case of several resonances decaying via several open channels in the same real number representation. However, the expressions obtained for the photoabsorption cross sections (Starace 1972) were applied only to the problem with a single resonance; this was perhaps because of the presence of singularities in the energy dependence when solving the problem in cases other than those treated by Fano. A similar problem was treated by Combet-Farnoux (1982) and Davis and Feldkamp (1977, 1981).

In the present paper the general solutions of Fano's equations are given in the complex energy representation. The subspaces of open and closed channels used have been previously diagonalised. In this approach all configuration interactions are taken into account and the expressions for cross sections contain no singularities in the energy dependence.

The complex energy representation was first introduced by Siegert (1939) in the theory of nuclear resonance reactions. The concept of a complex energy is widely used to describe the nuclear disintegration in approximate versions of the unified theory of nuclear reactions (Mahaux and Weidenmüller 1969, Rotter *et al* 1975). At present there are theories based on the Siegert method (Schneider 1981, McCurdy and Rescigno 1979, Bardsley and Junker 1972) that approximately describe atomic resonances.

2. Formalism and calculation procedure

Following Fano (1961) the atomic wavefunction of helium in the region of quasi-stationary states at an excitation energy E we write

$$\Psi_\lambda^E(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_m a_{\lambda m}^E |m\rangle + \sum_{\lambda'} \int_0^\infty b_{\lambda\lambda'}^E(E')|\lambda' E'\rangle \, \mathrm{d}E'. \tag{1}$$

Here λ indicates the channel of the reaction or scattering, characterised by some definite asymptotic behaviour of the functions and by a set of quantum numbers of

ion and electron, $|m\rangle$ and $|\lambda' E'\rangle$ are the basis wavefunctions of the subspaces of open and closed channels satisfying the conditions

$$\begin{aligned} &\langle m|\hat{H}|n\rangle = \mathscr{E}_n \delta_{mn} \qquad &&\langle \lambda E|\hat{H}|\lambda' E'\rangle = E\delta_{\lambda\lambda'}\delta(E-E') \\ &\langle \lambda E|\hat{H}|n\rangle = V_{n\lambda}(E) \qquad &&[V_{n\lambda}]^* = V_{\lambda n} \end{aligned} \tag{2}$$

where $\hat{H}$ is the total Hamiltonian of the atomic system. The expansion coefficients $a^E_{\lambda n}$ and $b^E_{\lambda\lambda'}(E')$ satisfy the equations

$$\begin{cases} (\mathscr{E}_n - E)a^E_{\lambda n} + \sum\limits_{\lambda'} \int_0^\infty b^E_{\lambda\lambda'}(E') \cdot V_{n\lambda'}(E')\,\mathrm{d}E' = 0 \\ \sum\limits_m a^E_{\lambda m} \cdot V_{m\lambda'}(E') + (E'-E)b^E_{\lambda\lambda'}(E') = 0. \end{cases} \tag{3}$$

In the papers by Starace (1972) and Mies (1968) developing the Fano formalism, equation (3) are formally solved in the real number representation of eigenchannels in the scattering K matrix. The resonances in the system manifest themselves as K-matrix singularities and hence involve computational difficulties (for example when inverting the K matrix). As a result the final expressions for the cross sections explicitly contain uncompensated singularities in the numerator and denominator. The particular cases examined by Fano (1961) and Fano and Cooper (1965), with at least one subspace containing no more than one state, do not present such difficulties.

Unlike the authors mentioned above we present the formal solution of the set (3) in order to provide physical boundary conditions in the T-matrix representation:

$$b^E_{\lambda\lambda'}(E') = P\frac{\sum_m a^E_{\lambda m} V_{m\lambda'}(E')}{E-E'} + \left(A_{\lambda\lambda'} \pm \mathrm{i}\pi \sum_m a^E_{\lambda m} V_{m\lambda'}(E)\right) \cdot \delta(E-E'). \tag{4}$$

Here i is a complex unit, the complex constants $A_{\lambda\lambda'}$ are related to the normalisation of the function (1) and P is the principal value in (1) when (4) is inserted. The sign ($\pm$) corresponds to alternate phase choices of the function (1): $\Psi_\lambda^{E(\pm)}(\boldsymbol{r}_1, \boldsymbol{r}_2)$. In our further calculations the basis wavefunction $|\lambda E\rangle$ asymptotically takes the form of a standing wave and is normalised as an energy δ function, with energies in atomic units. Unlike Mahaux and Weidenmüller (1969) we expand the expression (4) as functions (2) which were previously diagonalised. Substitution of (4) in set (3) gives

$$(\mathscr{E}_n - E)a^E_{\lambda n} + \sum_m \left(\frac{1}{\pi}\fint_0^\infty \frac{\gamma_{nm}(E')}{E-E'}\,\mathrm{d}E' - \mathrm{i}\gamma_{nm}(E)\right)a^E_{\lambda m} = -\sum_{\lambda'} A_{\lambda\lambda'} V_{\lambda' n}(E) \tag{5}$$

where $\fint$ is the principal value and

$$\gamma_{nm}(E) = \sum_\lambda V_{n\lambda}(E) \cdot V_{\lambda m}(E).$$

We shall write the solution of (5) in terms of the eigenvectors and eigenvalues of the symmetric complex matrix

$$Z_{nm}(E) = \mathscr{E}_n \delta_{nm} + \frac{1}{\pi}\fint_0^\infty \frac{\gamma_{nm}(E')}{E-E'}\,\mathrm{d}E' - \mathrm{i}\gamma_{nm}(E). \tag{6}$$

Let $E_n(E) - \frac{1}{2}\mathrm{i}\Gamma_n(E)$ be eigenvalues and $B_{nm}(E)$ the corresponding complex eigenvectors of this matrix. Exploiting the orthogonality of the eigenvectors we can express $a^E_{\lambda m}$ as

$$a^E_{\lambda m} = \sum_{m'} \frac{M_{\lambda m'}(E)}{E - E_{m'}(E) + \frac{1}{2}\mathrm{i}\Gamma_{m'}/E)} B_{m'm}(E) \tag{7}$$

where

$$M_{n\lambda}(E)=\sum_{k\lambda'} B_{nk}(E)V_{k\lambda'}(E)A_{\lambda'\lambda}$$

$$[M_{n\lambda}(E)]^*=M_{\lambda n}(E).$$

It is now convenient to change to a new basis of wavefunctions:

$$\begin{aligned}\varphi_\lambda^E(\boldsymbol{r}_1,\boldsymbol{r}_2)&=\sum_{\lambda'} A_{\lambda\lambda'}|\lambda' E\rangle\\ \tilde{\varphi}_m^E(\boldsymbol{r}_1,\boldsymbol{r}_2)&=\sum_n B_{mn}(E)\cdot|n\rangle\end{aligned}\tag{8}$$

and to substitute (7) into the expressions (4) and (1) for the wavefunction $\Psi_\lambda^{E(-)}(\boldsymbol{r}_1,\boldsymbol{r}_2)$. As a result we obtain the following expression:

$$\Psi_\lambda^{E(-)}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\varphi_\lambda^E(\boldsymbol{r},\boldsymbol{r}_2)+\sum_m \frac{M_{\lambda m}(E)}{E-E_m(E)+\frac{1}{2}\mathrm{i}\Gamma_m(E)}\Bigg[\varphi_m^E(\boldsymbol{r}_1,\boldsymbol{r}_2)$$
$$+\sum_{\lambda'}\left(\int_0^\infty \frac{M_{\lambda' m}(E')}{E-E'}\varphi_{\lambda'}^{E'}(\boldsymbol{r}_1,\boldsymbol{r}_2)\,\mathrm{d}E'-\mathrm{i}\pi M_{\lambda' m}(E)\varphi_{\lambda'}^E(\boldsymbol{r}_1,\boldsymbol{r}_2)\right)\Bigg].\tag{9}$$

In first-order perturbation theory the amplitude of the transition from the initial state Ψ_0 of helium to its final state as given by the wavefunction (9) is proportional to the matrix element

$$T_\lambda(E)\sim\langle\Psi_\lambda^{E(-)}(\boldsymbol{r}_1,\boldsymbol{r}_2)|\hat{t}|\Psi_0(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle\tag{10}$$

where $\hat{t}$ is the transition operator. Substituting (9) into (10) and taking account of kinematic factors we obtain the following expression for the partial-resonance ionisation amplitudes:

$$T_\lambda(E)=t_\lambda^{\mathrm{dir}}(E)+\sum_n H_{\lambda n}(E)/(\varepsilon_n(E)+\mathrm{i})\tag{11}$$

where

$$t_\lambda^{\mathrm{dir}}(E)=\langle\varphi_\lambda^E(\boldsymbol{r}_1,\boldsymbol{r}_2)|\hat{t}|\Psi_0(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle-$$

is the matrix element of the direct transition to the continuum,

$$\varepsilon_n(E)=2(E-E_n(E))/\Gamma_n(E)$$

$$H_{n\lambda}(E)=M_{n\lambda}(E)(t_n(E)-\mathrm{i}\pi\tau_n(E))\cdot 2/\Gamma_n(E)$$

$$\tau_n(E)=\sum_\lambda M_{n\lambda}(E)\cdot t_\lambda^{\mathrm{dir}}(E)$$

$$t_m(E)=\langle\tilde{\varphi}_m^E(\boldsymbol{r}_1,\boldsymbol{r}_2)|\hat{t}|\Psi_0(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle+\int_0^\infty\frac{\tau_m(E')}{E-E'}\,\mathrm{d}E'.$$

Using the identity

$$\frac{1}{\varepsilon_m+\mathrm{i}}\frac{1}{\varepsilon_n-\mathrm{i}}=\frac{1}{E_m-E_n-\frac{1}{2}\mathrm{i}(\Gamma_m+\Gamma_n)}\left(\frac{\Gamma_n}{\varepsilon_m+\mathrm{i}}-\frac{\Gamma_m}{\varepsilon_n-\mathrm{i}}\right)\frac{1}{2}$$

we reduce the partial ionisation cross sections to the form

$$\sigma_\lambda(E)=\sigma_\lambda^{\mathrm{dir}}(E)+\sum_n\frac{P_{n\lambda}(E)\varepsilon_n(E)+R_{n\lambda}(E)}{1+\varepsilon_n^2(E)}\tag{12}$$

where $P_{n\lambda}(E)/2$ and $R_{n\lambda}(E)/2$ are the real and imaginary parts of the complex function $N_{n\lambda}(E)$ determined by the following relation:

$$N_{n\lambda}(E) = H_{n\lambda}(E)\left(\frac{1}{2}\sum_k \frac{H^*_{k\lambda}(E)\cdot\Gamma_k(E)}{E_k(E)-E_n(E)+\frac{1}{2}\mathrm{i}(\Gamma_k(E)+\Gamma_n(E))}+[t_\lambda^{\mathrm{dir}}(E)]^*\right)$$

where

$$\sigma_\lambda^{\mathrm{dir}}(E)\sim|t_\lambda^{\mathrm{dir}}(E)|^2. \tag{13}$$

One can parametrise (12) when the so-called 'resonance approximation' is valid, i.e. if the functions $E_m(E)$, $\Gamma_m(E)$ and others vary smoothly with energy and may be replaced in Fano's formalism by their values at the resonance point; the behaviour of these functions with energy should be verified in every particular case. The partial ionisation cross sections may also be expressed in terms of the Fano-type parameters:

$$\sigma_\lambda(E) = \sigma_\lambda^{\mathrm{dir}}(E)\left[1+\sum_n\left(\rho_{n\lambda}^2\frac{(q_{n\lambda}+\varepsilon_n)^2}{1+\varepsilon_n^2}-\rho_{n\lambda}^2\right)\right]. \tag{14}$$

The parameters in (14) are determined by the relations

$$\rho_{n\lambda}^2 = (|N_{n\lambda}|/\sigma_\lambda^{\mathrm{dir}})\cos^2(\tfrac{1}{2}\arg N_{n\lambda})$$
$$q_{n\lambda} = \tan(\tfrac{1}{2}\arg N_{n\lambda}). \tag{15}$$

Using (12) and (14) it is easy to verify the relation for the parameters $\{q_{n\lambda}, \rho_{n\lambda}^2\}$ and $\{P_{n\lambda}, R_{n\lambda}\}$. Since the partial parameters $\{P_{n\lambda}, R_{n\lambda}\}$ enter linearly into the expression for cross sections, the total ionisation cross section will take a form similar to (12), where the functions $\{P_m, R_m\}$ are determined as the real and imaginary parts of the complex expression:

$$\chi_m(E) = \sum_\lambda N_{m\lambda}(E).$$

The complex matrices $Z_{nm}(E)$ were diagonalised numerically and the above formulae were used to calculate the photoionisation cross section of helium. In the calculations the operator $\hat{t}$ was replaced by the dipole transition operator and the amplitude (11) was determined from the matrix elelments (10) taking into account kinematic factors.

In the Born approximation the differential GOS for ionisation are determined by the corresponding cross sections of the electron impact ionisation of atoms (Bell *et al* 1973). Specifically, the differential GOS for ionisation of helium leaving He^+ in an excited $n=2$ state will be determined from the partial cross section of the helium ionisation to the $n=2$ state of the ion. The latter can be obtained from the above formulae. In this case the operator $\hat{t}$ must be replaced by the known Born operator, which depends on momentum transfer, and the expressions (10)-(11) should include the necessary kinematic factors. The formulae for the transition GOS are given, for example, by Robb *et al* (1975) and Jacobs (1975, 1976).

The anisotropy parameter β in the angular distribution of photoelectrons is determined from the photoionisation amplitude. To calculate the anisotropy parameter $\beta_{n=2}$ in the angular distribution of photoelectrons in the helium ionisation to the $n=2$ state of the He^+ ion we used well known formulae; see, for example, Kabachnik and Sazina (1976) or Jacobs and Burke (1972). The expression (9) was used in this case as a continuum wavefunction.

3. Diagonalisation of subspaces

The diagonalisation of closed channels $|m\rangle$ involves only diagonalisation of a real matrix. This does not present any problems and was used, for example, by Altick and Moore (1965), Balashov *et al* (1970) and Haysak *et al* (1982). For the subspace of open channels we used the method suggested by Fano and Prats (1963). We have solved numerically the following set of integral equations for the K matrix of electron scattering from the He^+ ion:

$$K(\lambda, \lambda', E) + \sum_{\mu} \int_0^{\infty} \frac{\langle \psi^0_{\lambda' E} | \hat{V} | \psi^0_{\mu \varepsilon'} \rangle}{\varepsilon' - \varepsilon_{\mu}} K(\lambda, \mu, \varepsilon')\, d\varepsilon' = -\langle \psi^0_{\lambda' E} | \hat{V} | \psi^0_{\lambda \varepsilon_{\lambda}} \rangle. \tag{16}$$

Here $\varepsilon_{\lambda} = E - E_{\lambda}$, E is is the excitation energy of He, E_{λ} is the channel ionisation threshold of channel λ, $\hat{V} = \hat{H} - \hat{H}_0$, $\hat{H}$ and $\hat{H}_0$ are the exact and model Hamiltonians of He and the functions $|\psi^0_{\lambda E}\rangle$ are basis functions to channel λ at energy E which are eigenfunctions of the Hamiltonian $\hat{H}_0$.

In the present calculation the basis wavefunctions are solutions of the equation

$$\left(\hat{T} + \hat{V} + \left\langle nl(\lambda) \left| \frac{1}{r_{12}} \right| nl(\lambda) \right\rangle - \varepsilon \right) |\psi^0_{\lambda \varepsilon}\rangle = 0. \tag{17}$$

Here $\hat{T}$ and $\hat{V}$ are the kinetic and potential energy of the electron in the He^+ nuclear field, $1/r_{12}$ is the electronic interaction in helium and $|nl(\lambda)\rangle$ is the Coulomb bound-state electronic wavefunction of the He^+ ion corresponding to the channel λ of the He atom.

The expression for the diagonalised continuum wavefunction used to calculate the resonance ionisation amplitude (10) includes the K matrix in the following manner (Fano and Prats 1963, Bloch 1966, Strakhova and Zajac 1984, Strakhova and Shakirov 1982):

$$|\lambda E\rangle = \sum_{\mu} A_{\lambda \mu} \left(|\psi^0_{\mu \varepsilon_{\mu}}\rangle + \sum_{\lambda'} \int_0^{\infty} \frac{K(\mu, \lambda', \varepsilon)}{\varepsilon - \varepsilon_{\lambda'}} |\psi^0_{\lambda' \varepsilon}\rangle\, d\varepsilon \right). \tag{18}$$

In our further calculations the wavefunction $\Psi_{\lambda}^{E(-)}$ is normalised as an energy δ function and $A_{\lambda \mu} = (1 - iK(\lambda, \mu, E))^{-1}$. The set (16) was solved numerically by two methods: with iterations and without. In the latter case the set of four (three for the total momentum $L = 0$) integral equations was reduced, as by Bloch (1966) and Strakhova and Shakirov (1982), to a set of algebraic equations. Excitation energies up to 20 au = 40 Ryd were taken into account in the second term of (18). Comparison between the two methods shows that in order to obtain good accuracy the iteraction scheme should involve not less than six to eight iterations.

4. Approximate variants of the approach

There are variants of this approach, for example the diagonalisation method (Balashov *et al* 1970, Haysak *et al* 1982). In this method the interaction of the previously diagonalised subspaces of open and closed channels is considered in perturbation theory. This corresponds to the formalism in which the matrix (6) retains only the first term, i.e. the interaction of diagonalised states of the closed channels with the continuous spectrum is neglected.

The next two terms in the matrix (6) describe the configuration interaction of diagonalised closed channels through open channels at the off- and on-shell points, respectively. When removing any term in (6) it is necessary to take the corresponding physical approximations in (9) in order to avoid mismatch.

5. The structure model

In our calculations the subspace of closed channels $|m\rangle$ contained 20 configurations corresponding to two-electron excitations between the second and third thresholds. Coulomb functions for charge $Z=2$ were used as basis functions to describe these states. The subspace of open channels contained four (three for the zero total momentum) configurations corresponding to the electron above the ground and first $n=2$ excited state of the residual ion. In the GOS calculations the sum over the total momentum of the system included the contribution of the first four terms. As follows from the non-resonance GOS calculations, the contribution of other terms can be neglected. The calculations were made using the Tweed (1972) 41-term wavefunction to describe the ground state.

6. Results

The positions and total widths were determined as the real and imaginary parts of eigenvalues of the complex matrix (6) taking into account all configuration interactions. In the diagonalisation approach the resonance energies were determined, as by Balashov *et al* (1970), through the eigenvalues of the real matrix, taking into account the interactions within the subspace of closed channels, and the widths were calculated following the perturbation approach.

The calculations yielded the positions and widths of the singlet S, P, D and F resonances in helium converging to the threshold $n=3$. Energies and widths of the lowest resonances of this series were calculated in a variety of papers (see, for example, Senashenko and Wague 1979, Burkov and Strakhova 1984a, Salomonson *et al* 1985, Ho and Callaway 1985, Oberoi 1972, Chung 1972, Herrick and Sinanoğlu 1975, Burke and Taylor 1969, Wakid and Callaway 1980 and the references therein). Our data on positions and widths agree with the results obtained in similar physical approximations. In the present paper we do not analyse positions and widths because these data have been intensely discussed in the literature.

6.1. The cross sections of the direct photoionisation of helium

The close-coupling calculations of the partial and total cross sections of the direct photoionisation of helium were carried out by Chang (1980) and twice by Burke and collaborators (Jacobs and Burke 1972, Berrington *et al* 1982). It is interesting to compare the calculation of Chang (1980) with the calculation of Burke and Jacobs (1972). In these two calculations the continuum wavefunction far away from the threshold is calculated in the same manner, i.e. the coupling between the four open channels is taken into account. A slight difference between the results is probably due to the fact that Jacobs and Burke employ the Hylleraas (1929) He ground-state wavefunction with 56 parameters and Chang (1980) uses his own method of accounting for the ground-state correlation. The difference near the threshold can result from the

inclusion of pseudostates, in addition to four open channels, into the Jacobs and Burke calculations of the He continuum wavefunctions. These two calculations lead to opposite conclusions. Chang predicts the near-threshold photoionisation of helium to the 2s state of the He^+ ion and Jacobs and Burke predict if to the 2p state (figure 1). The total cross section of helium photoionisation to the $(n=2)$ state of the He^+ ion is almost the same in both cases (figure 2). The experimental research by the techniques of fluorescence yield (Woodruff and Samson 1982) and photoelectron spectroscopy (Bizau *et al* 1982) failed to resolve this discrepancy definitely. More accurate and powerful calculations of Berrington *et al* (1982) made in the *R*-matrix representation of the close-coupling of 1s-2s-2p states and 3s-3p-3d pseudostates of the He^+ ion to determine the He ground- and final-state wavefunctions and also the special experiments conducted by Schmidt *et al* (1982) and Lindle *et al* (1985) with the use of photoelectron spectroscopy, have substantiated the main physical conclusions made by Jacobs and Burke (1972).

It is to be noted, however, that the experimental data of different authors are in poor agreement. A detailed description of the behaviour of the direct photoionisation cross section between the second and third threshold is lacking. What is required is a more frequent scanning in this interval of the excitation spectrum because here the energy dependence of the direct transitions strongly affects the resonance profiles.

Our calculations (figure 1) agree with the data of Jacobs and Burke (1972) and Berrington *et al* (1982) over a wide energy region.

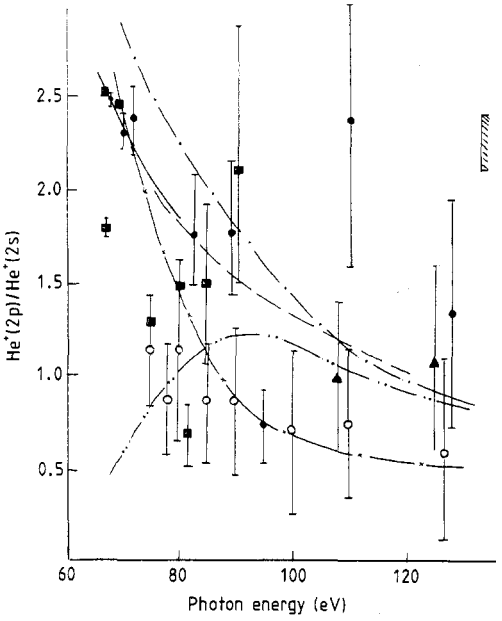

Figure 1. Ratio of the cross sections of the direct photoionisation of helium to the 2p and 2s states of the He^+ ion. The present calculations with the inclusion of the close coupling of four open channels are shown by the full curve; for comparison are the celebrations of: Jacobs and Burke (1972), —·—·—; Chang (1980), —··—··—; Berrington *et al* (1982), —×—×—; Salomonson *et al* (1985), - - .24- -. Experimental data is also shown: ■, Lindle *et al* (1985); ○, Bizau *et al* (1982); ●, Schmidt *et al* (1982); ▲, Krause and Wuilleumier (1972). Only the *L* form of calculations is presented.

Differences between our results and those by Burke *et al* (1982) are observed in a narrow energy interval between the second and third thresholds. Here the simplifying assumptions of different approaches play a significant role; among others the inclusion of pseudostates, the ground-state correlations and subthreshold states. We have obtained a different energy dependence of the background of direct transitions: the resonances are on the high-energy side of the partial cross sections. The calculations of Jacobs and Burke (1972) and Berrington *et al* (1982) locate resonances on the low-energy side. This will lead to rather different estimates of the spectroscopic characteristics of the resonances converging to the ($n = 3$) threshold and can be verified by comparing the calculated characteristics with the available experimental data.

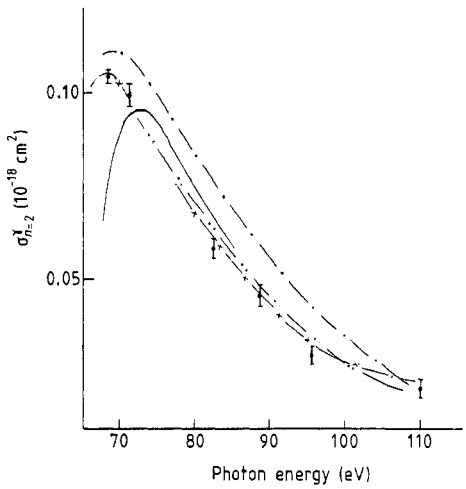

Figure 2. Cross sections of the direct photoionisation of helium to the $n = 2$ state of the He^+ ion. The notation is the same as in figure 1. The experimental data are from Woodruff and Samson (1982).

6.2. Resonance photoionisation

In figure 3 the cross section of the resonance ionisation of helium to the $n = 2$ state of the He^+ ion is shown, and in figure 4 the ratio of the partial cross sections of the helium photoionisation to the $n = 2$ and $n = 1$ state of the He^+ ion between the second and third thresholds. Our calculations reproduce the experimental data. Of particular interest is the region of the minimum at 70 eV. The experimental partial $n = 2$ cross sections (Woodruff and Samson 1982) drop to zero in this region while the measurements by Lindle *et al* (1985) do not reproduce this effect (figure 3, 4). It will be noted (table 1) that the error bars in the data by Woodruff and Samson (1982) are higher compared with those of Lindle *et al* (1985), and at the same time the experimental resolution of Woodruff and Samson (1982) is better. The theoretical *R*-matrix calculation by Salomonson *et al* (1985) also yields non-zero cross sections. We find it desirable to improve both the theoretical and experimental data in this region.

Figure 5 gives the values of the anisotropy parameter in the angular distributions of photoelectrons in the helium ionisation to the $n = 2$ states of the He^+ ion (the comparison between the calculated and experimental curves). The structure in the

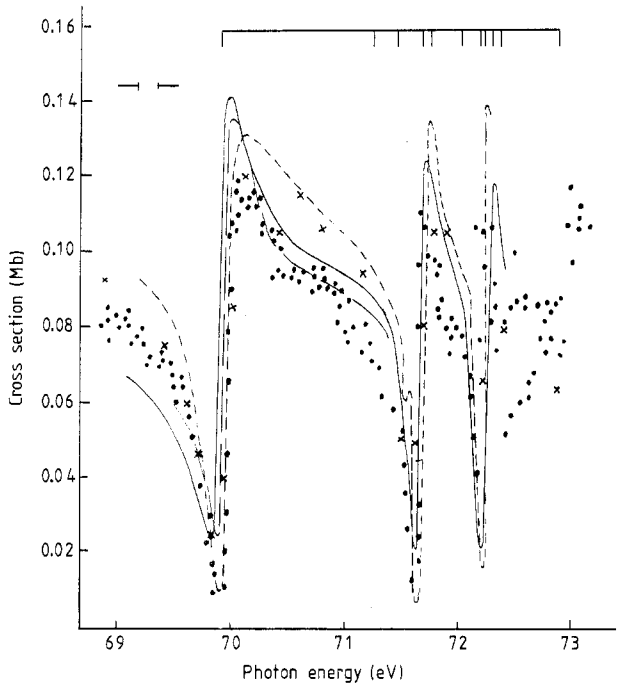

Figure 3. Cross sections of the resonance photoionisation of helium to the $n=2$ state of the He^+ ion between the second and third thresholds. Present calculations: ——, the method of configuration interaction in the complex number representation; — — —, the diagonalisation approximation with the inclusion of the close coupling of open channels; - - - -, the calculation of Salomonson *et al* (1985) in K-matrix theory. Experimental data: ●, Woodruff and Samson (1982); ×, Lindle *et al* (1985).

anisotropy parameter, also in the partial photoionisation cross sections, is due to contribution from several resonances. Only the first peak corresponds to the lowest resonance ($3s3p^1p$).

6.3. Fast electron ionisation

In figure 6 the partial GOS in the helium ionisation to the $n=2$ state of the He^+ ion are shown. As in the photoionisation cross section, the structures in the GOS are due to contributions from several resonances, and therefore the treatment of these structures in the single-resonance approximation is not optimal. Table 1 lists the momentum transfer dependence of the profile parameter q of the lowest resonances in the partial GOS. The dependence of the profile parameter of the lowest ^1S resonance contains a singularity in the region of momentum transfer $Q=3$–4 au. Such singularities (see expression (15)) were also observed in the dependences of the profile resonance parameter below the second threshold of helium ionisation (Lipovetsky and Senashenko 1974). The ionisation cross section does not exhibit any singularities in this case, as follows from the above formalism. Dependences of the type given in table 2 help one to a better understanding of how the GOS curves from figure 5 will change at different values of momentum transfer.

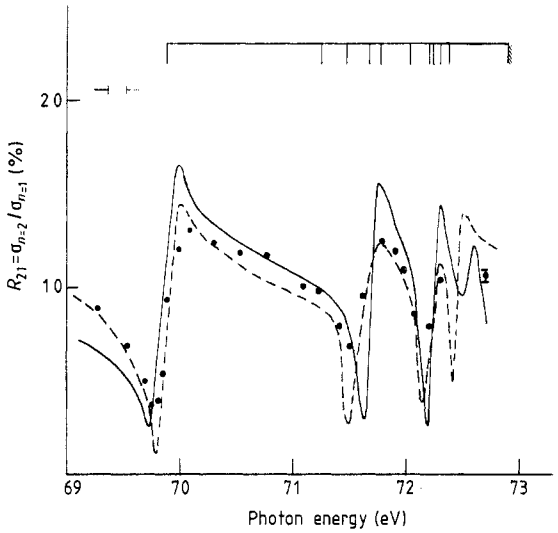

Figure 4. Ratio of partial cross sections of the photoionisation of helium to the $n = 2$ and $n = 1$ states of He^+. The full curve is the present calculation by the method of interaction configurations in the complex number representation. The dots are the experimental data of Lindle *et al* (1985). The broken curve is the fitting of the experimental data by Lindle *et al* (1985) with the monochromator broadening removed. The calculated position of the ^1P resonances and the monochromator resolution in the experiments of Lindle *et al* (1985) are given at the top of the figure.

Table 1. Parameters of the lowest ^1P resonance in He from the series of resonances converging to the threshold $n = 3$ in the total and partial photoionisation cross sections. The notation is as in Woodruff and Samson (1982). Errors are given in parentheses.

Parameter		This work	Experimental data		Calculation of Senashenko and Wague (1979)
$\sigma_{n=2}$	A (Mb)	0.120	0.120 (2)[a]	0.081 (14)[b]	0.072
	B (Mb)	−0.005	−0.044 (2)[a]	−0.065 (8)[b]	−0.004
	q	0.960	0.7[a,d]	0.48 (9)[b]	0.95
	ρ^2	0.670	0.88[a,d]	$0.98^{(+2)[b]}_{(-26)}$	0.39
	C (Mb)	0.061	0.097 (1)[a]	0.086 (7)[b]	
	A (Mb)	0.068	0.18 (8)[a]	0.032 (6)[c]	0.046
	B (Mb)	−0.042	−0.032 (56)[a]	0.010 (5)[c]	0.015
σ_{total}	q	0.553	0.84 (30)[a]	1.36 (20)[c]	1.37
	ρ^2	0.067	0.11 (3)[a]	0.012 (3)[c]	0.018
	C (Mb)	1.050	0.989 (20)[a]	0.957 (30)[c]	

[a] Lindle *et al* (1985).
[b] Woodruff and Samson (1982).
[c] Dhez and Ederer (1973).
[d] The Fano parameters obtained by recalculating the Shore (1968) parameters by the formulae given, for example, by Lindle *et al* (1985).

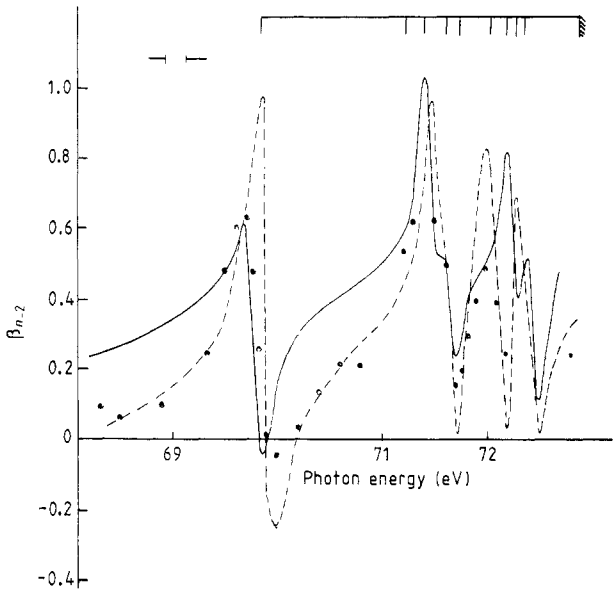

Figure 5. Anisotropy parameter in the angular distribution of photoelectrons in the helium ionisation to the $n = 2$ states of the He^+ ion. The notation is the same as in figure 4.

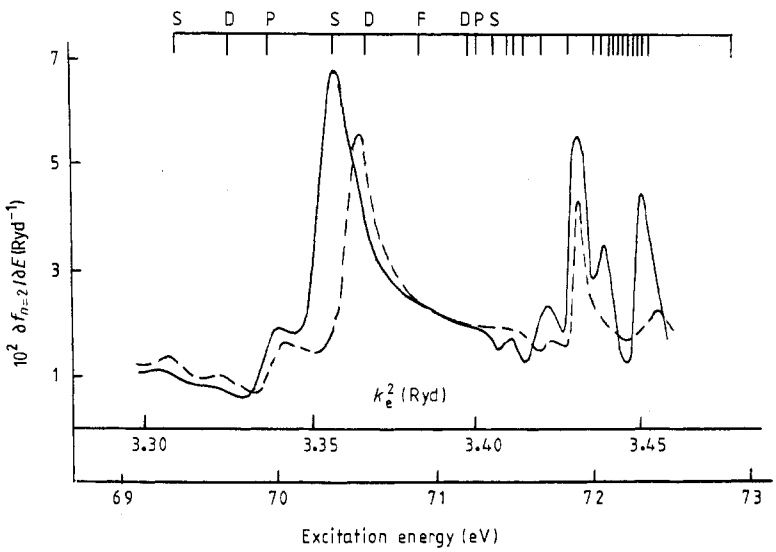

Figure 6. Generalised partial oscillator strengths in the helium ionisation to the $n = 2$ state of the He^+ ion at the momentum transfer $Q = 1$ au. Present calculations: ——, the method of configuration interaction in the complex number representation; - - - -, the diagonalisation approximation.

Table 2. Profile of the lowest singlet resonances of the series converging to the $n = 3$ threshold in He^+ as a function of momentum transfer in the helium ionisation by fast electrons to the $n = 2$ state of the He^+ ion. The present configuration interaction calculation is in the complex number representation

Momentum transfer (au)	Profile of resonances with the total momentum L			
	$L = 0$	$L = 1$	$L = 2$	$L = 3$
0.1	6.18	0.98	2.70	1.20
0.3	4.76	1.07	9.80	1.15
0.5	3.55	1.08	10.0	1.38
1.0	−0.54	1.06	3.86	1.81
1.5	−1.37	1.03	1.84	2.10
3.0	−5.19	1.02	0.64	2.12
3.5	300	1.00	0.55	1.50
4.0	4.75	1.00	0.50	0.81
5.0	2.67	1.14	0.44	−1.10

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