

Low-Energy e-He(2¹L) Scattering Calculations

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Cross sections for e-He(2¹L) scattering have been calculated in the energy range $1 \leq E \leq 4$ eV. For $l > 0$ partial cross sections a simple analytical method, proposed by the authors before, which is essentially an extension of Seaton's exact resonance method, has been applied. In the case $l = 0$, when a complex "angular momentum quantum number" in the rotated space appears, a matching procedure has been adopted, making use of a more realistic model potential.

The results for $Q(2^1S-2^1S)$, $Q_i(2^1S-2^1P)$ and $Q(2^1P-2^1P)$ cross sections are compared with other theoretical calculations and in the case of the elastic $Q(2^1S-2^1S)$ cross section with the available experimental data as well.

The applicability of the analytical method used in the electron-atom scattering calculations is discussed, in particular for those processes which play a dominant role in the Stark broadening of spectral lines from plasmas. Finally, the relevance of the present method to searching for an eventual resonant (or virtual) state near 2¹S threshold has been discussed.

I. Introduction

Electron-atom collision processes have been the subject of extensive experimental and theoretical studies, owing to their utmost importance in many physical systems, in particular in not too high temperature plasmas. However, even in the case of e-H scattering, an exact analytical treatment of the complete collision phenomenon is beyond our present mathematical capabilities, and a number of semianalytical, approximate methods have been developed (see e.g. Drukarev [1]). Employing refined numerical procedures, many of these methods are capable to provide accurate cross sections for various processes (see e.g. Burke and Seaton [2]), usually at the expense of a considerable computing time consumed. On the other hand, in some applications scattering matrix elements (or the corresponding cross sections) of moderate accuracy, but in simple analytical form are needed, as is the case with the quantum theory of Stark broadening (Baranger [3]). In particular, in the expression for the halfwidth and shift of an isolated nonhydrogenic line one encounters the quantity

$$I = S_i S_f^{-1},$$

where $S_{i(f)}$ are the scattering matrix (diagonal) elements, for the elastic scattering on the initial (final) state of the transition. Since at low impact energies (these are usually met in plasmas where

neutral species are still present) coupling with other atomic states are important (see e.g. Barnes and Peach [4]), second and higher order processes, like $i \rightarrow i' \rightarrow i$, $i \rightarrow i' \rightarrow i'' \rightarrow i$, etc., make considerable contributions to $S_{i(f)}$ [5].

One of the most powerful low-energy approximations for treating electron-atom (ion) scattering is the close coupling equations method. Within this approximation, the only analytically completely tractable case, to our knowledge, has been the dipole exact resonance model, due to Seaton [5], which applies to the hydrogen (degenerate) target. The principal shortcoming of the original Seaton treatment seemed to be (besides the neglect of the exchange) an appearance of complex "angular momentum quantum numbers" in the rotated functional space, since these seemed to prevent a proper choice of the scattering wave functions (Mott and Massey [6]). However, as has been shown, a physical significance can be attached to these complex numbers, which indicate the presence of bound states in corresponding channels. Bottcher [7], in treating $n \rightarrow n + 1$ transition cross sections for e-H scattering, has extensively used this peculiar feature of the degenerate channel scattering. In a previous work (Grujić and Koledin [8]), to be referred to as *I*, we have extended this method to the nondegenerate case, both for real and complex values of the "rotated space" angular momentum quantum numbers λ . This procedure has been applied to the study of e-He(2¹L) low-energy scattering, in order to examine the accuracy of the approximation proposed.

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In the next section we quote some of the relevant formulae from *I* and give an outline of the additional features of the procedure employed. In the third section results for the cross sections $Q(2^1\text{S}-2^1\text{S})$, $Q(2^1\text{P}-2^1\text{P})$ and $Q_l(2^1\text{S}-2^1\text{P})$ are presented and then compared with other data and discussed in the final, fourth section.

II. Analytical Method

II.1. Coupled Equations

We start from the set of integro-differential equations for the radial part of the scattering wave functions, in matrix form (Percival and Seaton [9]) (atomic units are used, except when otherwise stated):

$$\left[\frac{d^2}{dr^2} - \frac{l_2(l_2 + 1)}{r^2} + \frac{4}{r} + \hat{K}^2 \right] \hat{F}(r) = [2\hat{V}(r) + 2\hat{W}(r)] \hat{F}(r), \quad (1)$$

where all operators on the left-hand side are in the form of diagonal matrices, $\hat{F}(r)$ is a vector column, whose components represent solutions in a particular scattering channel and \hat{V} and \hat{W} are direct and exchange potential matrices, respectively. The impact energy matrix \hat{K}^2 is given by

$$\hat{K}^2 = \|k_i^2 \delta_{ij}\|, \quad \frac{1}{2} k_i^2 + \varepsilon_i = E, \quad (2)$$

where ε_i is the energy of the target in the state ψ_i , E is the total energy of the electron-atom system, and the channel index i stands for $n l_1 s_1 l_2$. Equation (1) is, of course, impossible to solve in its complete form and one is forced to simplify the real collision model. Besides dealing only with the most important channels (close coupling approximation), the usual procedure is to expand the potentials \hat{V} and \hat{W} into multipole series and then retain only the most important, tractable terms. Further, since we shall neglect the exchange of electrons, it is a reasonable approximation to confine oneself to singlet states of the target.

II.2. The Interaction Potential

Multipole components of the direct interaction potential for e-He are given by (see Burke *et al.* [10])

$$V_{ij} = \sum_{\mu=0}^2 \{ y_0(P_{1s}^- P_{1s}^-; r) \Delta(P_{n l_1} P_{n' l_1'}) \cdot \delta_{l_1 l_1'} \delta_{l_2 l_2'} \delta_{\mu 0} + f_\mu(l_1 l_2 l_1' l_2'; L) \cdot \Delta(P_{1s}^- P_{1s}^-) y_\mu(P_{n l_1} P_{n' l_1'}; r) \}, \quad (3)$$

where f_μ , y_μ and Δ are defined in [9]. Further, we divide the space around the target into two parts.

(a) **External region.** This part of r -space is defined by the asymptotic form of $\hat{V}(\mu=1)$

$$V_{ij}(r) = \|v_{ij}(1 - \delta_{ij})r^{-2}\|, \quad r > r_0, \quad (4)$$

where r_0 is determined both by (4) and by the requirements that both $\hat{V}(\mu \neq 1)$ and \hat{W} terms may be neglected in (1) (Grujić and Koledin [11]).

(b) **Internal region.** Here, we approximate actual potential matrix elements from (3), for all possible μ -values, by

$$V_{ij}(r) = a_{ij} r^{b_{ij}} \exp(-c_{ij} r), \quad i \neq j \quad (5)$$

and introduce diagonal elements of the form

$$V_{ii}(r) = p_i r^{-2}, \quad (6)$$

which represent well the actual direct potential in this region of r . These last elements are negligible compared with centrifugal term when $l_2(l_2 + 1) \geq 2$.

II.3. Solving Eq. (1)

In the absence of a general method for solving (1) we adopt several procedures, each suited for a particular region of r and l_2 variables.

(i) **Internal region.** Here, we have $p_i \gg r^2 V_{ij}$ in case of $l_2=0$, and $l_2(l_2 + 1) \gg r^2 V_{ij}$ in case of $l_2 > 0$, where V_{ij} is given by (5). If we define an operator $\hat{Q}(K, l_2)$ by the left-hand side of (1), we obtain the zero-order solution $\hat{F}^{(0)}$ from

$$\hat{Q}(K, l_2) \hat{F}^{(0)}(r) = 0 \quad (7)$$

and, in a distorted-wave approximation manner, obtain the first order correction $\hat{F}^{(1)}$ by solving

$$\hat{Q}(K, l_2) \hat{F}^{(1)}(r) = \hat{V} \hat{F}^{(0)}(r). \quad (8)$$

This is accomplished by Lagrange's method of variation of constants (see Appendix). (The same procedure would give satisfactory results in the asymptotic region, too, provided that

$$l_2(l_2 + 1) \gg |v_{ij}|, \quad i \neq j,$$

where v_{ij} are defined in (4).)

(ii) **External region.** We employ the asymptotic form of the potential, as given by (4). If a unitary matrix [5] satisfies

$$\hat{U}^\dagger \{l_2(l_2 + 1) - v_{ij}\} \hat{U} = \lambda(\lambda + 1) \quad (9)$$

then the \hat{S} matrix can be evaluated, as shown in I, by

$$\hat{S} = \hat{K}^{1/2} \exp(i\pi l_2) \hat{U} \exp(-i\pi \lambda) \hat{U}^+ \hat{K}^{-1/2} \quad (10)$$

for those $l_2 > l_2^0$, for which λ_j in the diagonal matrix λ are real numbers. For $l_2 \leq l_2^0$, λ_j are complex numbers and one can calculate the S matrix elements (Eq. (14) in I), but they depend on the energy of the lowest lying bound state in the corresponding dipole potential V_{ij} (see e.g. Chen [12]), which in our case is not known. Besides, since for small l_2 values the internal region is important, and there V_{ij} deviate considerably from their asymptotic form, we calculate the corresponding \hat{S} matrix elements by a matching procedure, without making use of (14) from I.

The energy range of the applicability of (10) is defined by the following requirements (see Ref. I):

$$|k^2 + \Delta'_{ii}| \gg \Delta'_{ij}, \quad i \neq j, \quad (11)$$

where the elements of the energy matrices Δ' and Δ'' are defined as

$$U^+ K^2 U = \bar{k}_i^2 + \Delta' + \Delta'', \quad (12)$$

(Δ' — diagonal, Δ'' — off-diagonal).

As we shall see in the next section, condition (11) together with the adopted approximation $kr \ll 1$ (see Appendix) confines the energy range of the applicability of (10) to a rather narrow interval above the $n=2$ energy sublevels of the singlet metastable state of He.

III. Calculations and Results

The helium states considered here generate four scattering channels (see Table 1), but the channel labeled 4 does not contribute to the calculated cross sections, within the approximation adopted. Namely, as can be seen from (3), the leading term in the odd parity subspace, in the outer region, is the quadrupole potential

$$V_{44}(r) \sim f_2(1L1L; L) \Delta(P_{1s}^- P_{1s}^-) \frac{1}{r^3} \cdot \int_0^\infty P_{2p}^2(r) r^2 dr, \quad f_2 \equiv -\frac{1}{5}. \quad (4')$$

Of course, one could easily solve the corresponding differential equation from (1), with $V_{44}(r)$, numerically (single-channel case), but it would not be in the spirit of our essentially analytical approach, which pertains strictly to the dipole approximation.

Table 1. The scattering channels for the e-He(2¹L) system (l -total angular momentum quantum number).

Channel	Atomic State	Impact Electron	Parity π
1	(1s2s) ¹ S	l	$(-1)^l$
2	(1s2p) ¹ P	$l-1$	$(-1)^l$
3	(1s2p) ¹ P	$l+1$	$(-1)^l$
4	(1s2p) ¹ P	l	$(-1)^{l+1}$

In calculating the asymptotic potential matrix \hat{V} , according to (3), atomic functions due to Burke and Robb [13], based on the Hartree-Fock approximation, have been used. Numerical results for the diagonal matrix $\hat{a} \equiv \lambda(\lambda+1)$ are shown in Table 2, for the first six values of l . As can be seen in Table 2, all matrix elements, except for $l=0$, are greater than -0.25 , and consequently, only for $l=0$ a complex λ appears. This seems to be in accordance with findings in [10], where calculations of the ²S phase shift indicated a narrow resonant (or virtual) state just below the 2¹S threshold. However, since the a_3 value -0.275 differs very little from the border value -0.25 , the present method would not be convenient for determining the position of the resonance, even if a position of a negative ion He⁻(²S) level, with 2¹S parent state, were known (see e.g. Taylor [14]). This can be seen from the formula which gives the ratio of successive bound state level separations from the threshold (see e.g. Gailitis and Damburg [15])

$$E_n/E_{n+1} = \exp(2\pi/\text{Im } \lambda), \quad \lambda = -1/2 + \sqrt{a+1/4} \quad (13)$$

and which in our case yields: $E_n/E_{n+1} = 5.7 \cdot 10^{15}$. Hence, if a series of resonances above the 2¹S threshold does occur, no more than a single member could be detected (at E_0), the next one (E_1) being practically at the very threshold.

The appearance of the unique complex λ in the present calculations is to be compared with the e-H case, where complex values of λ appear for $l=0, 1, 2$. This is the direct consequence of the weaker cou-

l	a_1	a_2	a_3
0	2.275	0	-0.275
1	6.103	2	-0.103
2	12.062	6	1.938
3	20.044	12	5.955
4	30.035	20	11.965
5	42.028	30	19.972

Table 2. Elements of the diagonal matrix $\hat{a} = \lambda(\lambda+1)$ for the e-He(2¹L) system.

pling between well separated 2¹S and 2¹P helium sublevels ($\Delta\epsilon \cong 0.6$ eV). It is of interest at this point to present ratios of relevant \hat{V} matrix elements on one hand, and corresponding energy matrix elements on the other hand, for the sake of comparison, as is done in Table 3. As can be seen by comparing the second and third columns of Table 3, method (i) from Section II is not applicable for $l=0, 1$, whereas approach (ii) for the same values makes sense, but is very crude. On the other hand, method (i) should yield better results for $l>3$, than approach (ii).

Now, in calculating partial-wave cross sections we must distinguish two cases: $l=0$ and $l>0$. The reason for singling out $l=0$ partial-wave is twofold. First, since there appears in this case a complex λ , an application of the quasi exact resonance procedure, as described in I, would require knowledge of the energy of He[−](2²S) with 2¹S parent state. Second, for $l_2=0$, and this comprises half of the $l=0$ channels, the inner region is important, and an extrapolation of the asymptotic form of dipole potential to this part of the r -variable would be an oversimplification. We adopt, therefore, the matching procedure, as described in II.3 (i) (see, also, Appendix). Hence, for $l=0$ (inner region) we fit the parameters a, b, c and p in (5) and (6) to the numerical points (see Figure 1). The resulting potential matrix is given in Table 4. As can be seen from Fig. 1, the analytical values of V_{13} deviate from the actual ones considerably only for $r \leq 0.06a_0$, as indicated in more detail in the insert, but this divergency in the near-zero behaviour, being limited to the small part around the nucleus, should not

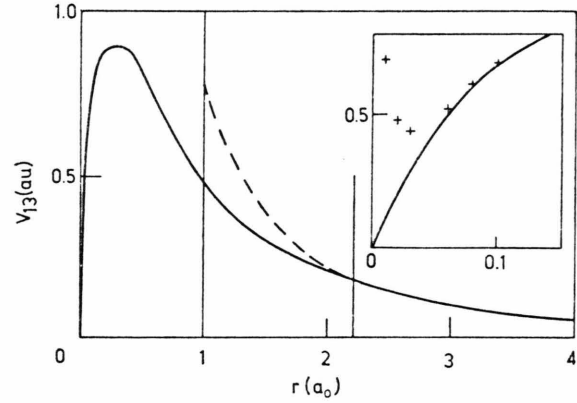


Fig. 1. Potential matrix element $V_{13}(l=0)$. Crosses (insert) are actual numerical values near the origin (see the text).

affect final results. As for the choice of r_0 , a proper value would be $\cong 2a_0$. However, the necessity for an analytical solution in the inner region dictated the adoption $r_0=a_0$. Since for $r < a_0$, $|V_{ii}| \gg |V_{ij}|$ ($i \neq j$), the system of equations decouples and an analytical solution is found (see Appendix). On the other hand, this choice results in an overestimation of the actual potential in the intermediate region (where in fact $V_{ii} \cong V_{ij}$, $i \neq j$) by the extrapolated asymptotic dipole term (dashed curve in Figure 1). Nevertheless, we believe that this deviation is partly compensated by the presence of the accurate potential for $r < a_0$, where either $V_{ij} \sim r^{-2}$ or $V_{ij} = \text{const}$, as is usually assumed, would be surely an oversimplification.

In the case $l>0$, the inner region is of minor importance, except for the channel: $l=1$, $l_2=l-1$ (i.e. $l_2=0$), when the general assumption $l_2(l_2+1) \gg V_{ij}r^2$, $r < a_0$, is not satisfied. However, since this case represents only one third of all $l=1$ channels, and since the very inner region is assumed small enough, we believe that the treatment of this particular channel by the quasi exact resonance method should negligibly affect final results. Concerning higher- l partial waves, a simple argument based on the classical trajectory model shows that, though $l_2 = 1, 2, 3$ electrons enter the atomic region ($r_A \approx 5a_0$), within the impact energy region considered, one has for $l_2>0$: $l_2(l_2+1) \gg V_{ij}r^2$, and the actual form of the true potential is of no importance here.

We have adopted the following values for the $n=2$ sublevels [10]: $\epsilon(2^1S) = -2.1445$ au and $\epsilon(2^1P) = -2.1225$ au, with the sublevels separa-

Table 3. Ratios of diagonal to off-diagonal elements for \hat{V} and Δ matrices, respectively.

l	$ V_{ii} _{\min}/ V_{ij} _{\max}$	$ \Delta_{ii} _{\min}/ \Delta_{ij} _{\max}$
0	0	1.23
1	0	2.02
2	3.28	4.00
3	10.00	5.39
4	20.34	7.14
5	34.38	10.00

Table 4. Symmetrical matrix $r^2 V_{ij}$ for $l=0$.

− 0.59	0	$3.43 r^{2.63} \exp(-2r)$
	− 0.19	0
		− 2

tion: $\Delta\varepsilon = 0.022$ au. When all channels are open, one has $k_1^2 = q\Delta\varepsilon$, $k_2^2 = k_3^2 = (q-1)\Delta\varepsilon$, where q is always taken to be greater than unity.

The diagonal matrix Δ' is energy-dependent, as different from (off-diagonal) elements of Δ'' . Therefore, as q increases, the ratio $|\Delta'_{ii}|/|\Delta''_{ij}|$ increases, too, and so does the accuracy of the procedure employed. Numerical results indicate good accuracy already for $q=2$ and for large l -values even for $q < 2$.

The partial cross sections are calculated by the standard formula [16]

$$Q_l(i \rightarrow j) = \frac{2l+1}{(2l_1+1)k_1^2} |\delta_{ij} - S_{ij}|^2 \quad (14)$$

and summing up to $l=50$, the total cross sections $Q(i \rightarrow j)$ are finally computed within the impact energy region $1 < E < 4$ eV. The lower energy limit is determined by (11), whereas the upper limit is dictated by the requirement: $kr \ll 1$ (see Appendix). The calculated S matrix does not appear completely symmetric in our calculations. Generally, those elements connecting degenerate channels possess the required symmetry, but the other ones turned out to be asymmetric. The asymmetry decreases as one moves from the threshold. As for the unitarity condition, it is fulfilled within 99%, as a test for $l=1$ has shown. It should be noted that the asymmetry does not show up in the computed cross sections. Besides, since it is diagonal elements that contribute to the half-width and shift of a spectral line, the Stark broadening is also insensitive to this break of S -matrix symmetry.

III.1. $Q(2^1S \rightarrow 2^1S)$ Cross Section

In Fig. 2 our results for the elastic scattering on the singlet metastable helium are presented, together with other theoretical and experimental data. The partial sum turned out to converge rapidly, with an asymptotic behaviour of Q_l from (14) $Q_l \sim l^{-3}$ (as in case of complete degeneracy [15]), with an analytically calculated residual term for $l > 50$ being negligible. As seen from Fig. 2, with the exception of the close coupling results [10], there is a general agreement in shape with the other theoretical results and the experimental data. It should be noted that both the distorted-wave results [18] and experimental points are likely to have overestimated actual values, the first in the lower region (neglect of the exchange) and the second in

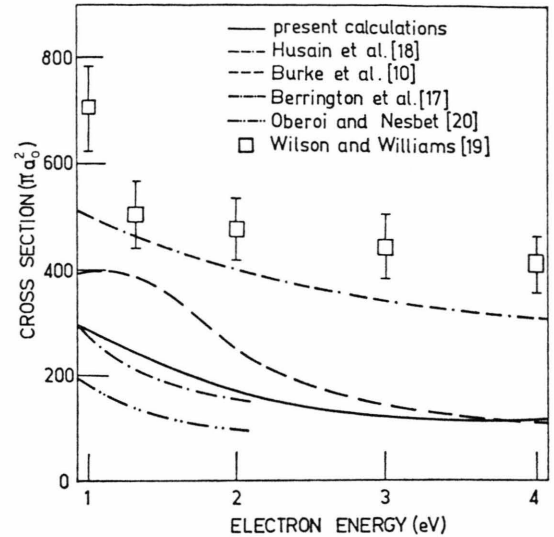


Fig. 2. Elastic cross section $Q(2^1S \rightarrow 2^1S)$. \square : Experimental points — total cross section.

the higher region, where inelastic processes have surely contributed to the values measured [19]. Note also the good agreement with the close-coupling results in the higher energy region. The broad maximum at $E \cong 1.25$ eV of the close-coupling curve is due to D-wave resonance, which appears also on both matrix-variational [20] and R -matrix [17] results below 1 eV. Since this feature is due to a combined effect of the centrifugal barrier and polarization potential of 2^1S state, our method cannot reproduce this shape resonance.

III.2. $Q(2^1P \rightarrow 2^1P)$ Cross Section

The partial sum converges more slowly than in case of $Q(2^1S \rightarrow 2^1S)$, with $Q_l(2^1P \rightarrow 2^1P) \sim l^{-2}$, $l \rightarrow \infty$, again as it was the case with the exact resonance theory. The results are shown in Figure 3. As can be seen in the figure, the matrix-variational calculations provide the smallest values, probably due to the restricted number of partial waves included. Again, the close-coupling results are close to ours in the higher energy region, whereas in the 1 eV vicinity our values are considerably higher. No experimental measurements of this cross section are reported up to now, to our knowledge.

III.3. $2^1S \rightarrow 2^1P$ Transition Partial Cross Sections

In case of this inelastic transition the partial cross sections behave as $Q_l(2^1S \rightarrow 2^1P) \sim 1/l$, $l \rightarrow \infty$, al-

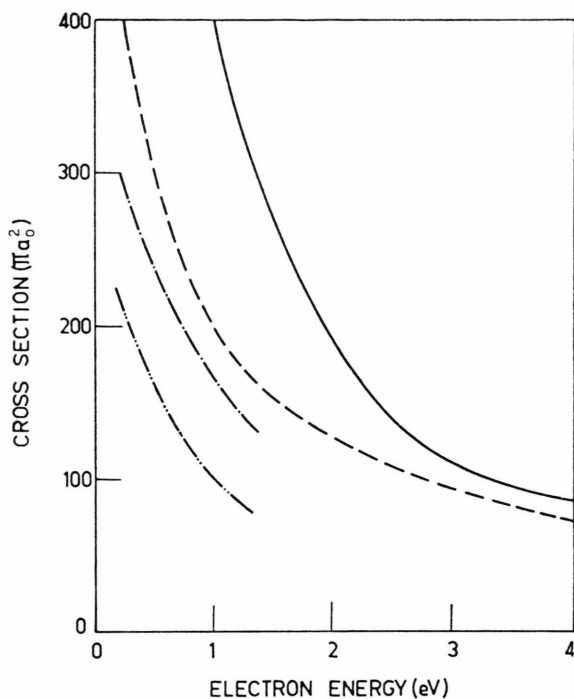


Fig. 3. Elastic cross section $Q(2^1P-2^1P)$. Curves as in Figure 2.

though the degeneracy has been removed in the present case. Partial cross sections at $E = 3$ eV are shown in Fig. 4, together with values computed by making use of the Born approximation according to Seaton's formula [21]. As can be seen from Fig. 4, although the values of the partial cross section drop

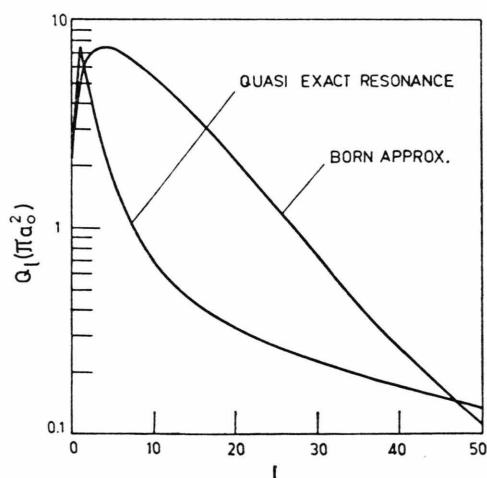


Fig. 4. Inelastic $Q_l(2^1S-2^1P)$ partial cross sections.

quickly in the interval 1–10, it goes down progressively more slowly afterwards, assuming the power law al^{-1} for $l \approx 50$ *. Born approximation cross sections have been computed for other impact energies, too, but we are not presenting them here. First, the theoretical results disagree greatly in this case (see Ref. [17]), and the Born approximation, on the other hand, surely is not competitive in this energy region. Second, as far as we know, no experimental data have been published for this transition, although measurements should be feasible with the present experimental technique.

It is to be noted that the lack of convergence is not critical as far as the Stark broadening quantum theory is concerned, since one cuts off the summation at some $l = l_{\max}$ corresponding to the Debye radius of the plasma (see, e.g., [22]). Nevertheless, the reappearance of this drawback of the exact resonance method must be regarded as a serious defect within present approximation and is to be overcome.

IV. Discussion

The principal aim of the presented calculations has been to test the accuracy of the analytical method of the quasi resonant case, for an electron-excited atom scattering, as proposed in Reference [1]. The choice of e-He(2^1L) scattering has turned out to be both advantageous and disadvantageous for that matter. As mentioned before, there is no reliable evidence for the existence of the $\text{He}^-(2^2S)$ bound state, so that we have not been able to make use of the relevant formula from I for complex λ , which appeared for $l=0$. On the other hand, the existence of elaborate calculations *via* the close coupling approximation [10], made a comparison with these numerical calculations possible. Since in the present calculations we have closely followed the setup of the scattering problem from [10], it is in order to discuss in somewhat more detail similarities and differences in our formal approaches. In [10], two separate sets of equations were solved, one comprising $n = 1, 2$, the other $n = 2$ helium states. Our calculations correspond to a part of the second set, since we have neglected completely the $n = 2$ triplet states. However, as the results from [10] show, the coupling with $n = 1$ and 2^3LS states is very weak, so

* We are indebted to the referee for drawing our attention to the convergence problem.

that our restricted model may be expected to provide reasonable results, as the present calculations show. Further, we have used somewhat more refined wave functions for He states [13], than those employed in [10], but with the same energy levels, what might have caused a major part of the disagreements.

The appearance of the complex λ seems to indicate the existence of a resonant (or virtual) state in the close vicinity of the 2¹S threshold. The eigenphase analysis in [10] (and in [17], too) points also in that direction, but no definite statement about the actual nature of an eventual singularity can be made at present. Since we have obtained a small value for the imaginary part of λ ($=0.173$), which is rather sensitive to the choice of the atomic wave functions, it would be pretentious to make use of the calculated value in predicting the ratio of the relative positions of eventual maxima (minima) of the cross sections. Moreover, because of the condition $|E_e - E_{th}| \gg \Delta\epsilon_{13}$ ($\cong 0.6$ eV), not more than a single maximum (minimum) in the cross sections is to be expected, if the calculated value of $\text{Im}(\lambda)$ is of the correct order of magnitude. It should be noted here that the appearance of the complex λ concerns all scattering channels comprised (with $l=0$), since its imaginary part is redistributed *via* (10) to all S -matrix elements.

In conclusion, we think the present calculations show that the previously proposed quasi exact resonance method may be used, in the relevant energy region, as reasonable approximate analytical procedure for calculating the \hat{S} matrix for the electron-excited atom scattering.

Acknowledgements

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Appendix

Matching Procedure for $l=0$ Partial Wave

A particular solution of Eq. (9) can be written in terms of Bessel functions $J_a(\rho)$ and Lagrange constants $C_j(r)$:

$$F_i^{(0)} = C_1^i(r) \sqrt{r} J_{q_i+1/2}(k_i r) + C_2^i(r) \sqrt{r} J_{-q_i-1/2}(k_i r), \quad (\text{A1})$$

where i denotes a scattering channel. In our case the indices of Bessel functions assume the values

$$q_i + 1/2 = \begin{cases} p_i + 1/4, & l_2 = 0, \\ l_2 + 1/2, & l_2 > 0, \end{cases} \quad (\text{A2})$$

where p_i is defined by the model potential $V_{ii} = p_i r^{-2}$ in the inner region. In a standard manner the problem of evaluating $C_j^i(r)$ reduces to evaluating an integral of the type

$$I = \int_0^{r_0} dr r^\alpha \exp(-\beta r) J_s(k_i r) J_t(k_i r). \quad (\text{A3})$$

With our choice: $r_0 = a_0$, one has $k_i r \ll 1$ within the integration interval, so that Bessel functions may be approximated by their first terms of power series and the integral is reduced to the analytically tractable form

$$I = \left\{ \frac{k_i}{2} \right\}^{s+t} \frac{1}{\Gamma(s+1) \Gamma(t+1)} \cdot \int_0^{r_0} dr r^{\alpha+s+t} \exp(-\beta r). \quad (\text{A4})$$

In the external region the solution is formally the same, with the r -dependent C_j^i coefficients replaced by the constants D_j^i . Then, from the continuity and boundary conditions at the origin (regularity) and in the asymptotic region, the unknown coefficients D_j^i , and from them the scattering matrix elements are deduced.

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