

## Electron-impact ionization of $\text{Ne}^{6+}$

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**Abstract.** We have calculated total and single differential cross sections for electron impact ionization of  $\text{Ne}^{6+}(1s^2 2s^2 \ ^1S)$  using a method that combines the distorted-wave Born approximation for the incident/scattered electron with an  $R$ -matrix treatment of the  $\text{Ne}^{6+}$  system. Our calculation included eight states of the final  $\text{Ne}^{7+}$  ion, namely  $1s^2 2s \ ^2S$ ,  $1s^2 2p \ ^2P^o$  and six states with the configuration  $1s2\ell 2\ell'$ , and up to the  $2^4$ -pole component of the interaction between the ionizing electron and the target. The single differential cross sections exhibit considerable structure due to autoionizing resonances, including a large resonance due to the quasi-bound state  $\text{Ne}^{6+}(1s2s^2 2p \ ^1P^o)$ . In the calculation of the total cross section, a modification to the usual half-range approximation is proposed, which ensures that the contributions from autoionizing resonances have the correct thresholds. Our theoretical results for the total cross section are in good agreement with the experimental results.

### 1. Introduction

In the calculation of the cross section for the electron-impact ionization of complex positive ions it is insufficient to consider only direct ionization, whereby one of the target electrons is removed while the others remain in the same orbitals throughout. (Cross sections for direct ionization may be calculated adequately by the configuration-average distorted-wave method of Younger (1980)). Rather, it is necessary to include the indirect processes which are mediated by doubly excited, quasi-bound states (cf the review by Moores and Reed 1994).

The computational method we have used in the present work is the distorted-wave Born approximation (DWBA)  $R$ -matrix method of Bartschat and Burke (1987). This method incorporates the indirect process of excitation autoionization (EA) by treating the final continuum states (comprised of the final ion plus the ejected electron) by an accurate  $R$ -matrix formulation. The initial bound state of the target ion is treated in a similar way, and this consistency between the initial bound state and the final continuum states is a major strength of the method. However, a weakness of the method is that the incident electron and the scattered electron (i.e. the faster of the two free electrons in the final state) are treated only in a distorted-wave Coulomb–Born approximation. (The formulation by Bartschat and Burke is similar to that by Jakubowicz and Moores (1981), except that in the former an inner region is treated by expansions in a basis that is independent of the impact energy, whereas in the latter coupled integro-differential equations are solved throughout for each impact energy.) A major feature

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of the present paper is that we introduce a correction to a threshold anomaly in the calculation of the total cross section.

Another approach to ionization, using the  $R$ -matrix formulation of the one-continuum-electron problem, which we mention only to distinguish it from the DWBA  $R$ -matrix method, is to apply the  $R$ -matrix formulation to the entire system comprised of the incident electron and the target ion. The doubly excited states of the target are included in the set of target states as if they were genuinely bound states, and their excitation gives the excitation-autoionization mechanism. This full  $R$ -matrix treatment incorporates resonant capture of the incident electron and hence can account for indirect processes such as resonant-excitation double autoionization (cf the review by Henry and Kingston (1988) and more recent work such as that of Gorczyca *et al* (1994) or Tayal (1994)). Electron exchange is fully taken into account, which is not the case in the DWBA  $R$ -matrix method. On the other hand, the full  $R$ -matrix method is limited in practice to the calculation of total cross sections, whereas the DWBA  $R$ -matrix method can be used not only for single differential and total cross sections but also for double differential (Schwienhorst *et al* 1995) and triple differential (Reid *et al* 1998) cross sections.

In the present paper we calculate the single differential and total cross sections for the ionization of  $\text{Ne}^{6+}$ . Because there have been several previous calculations using the DWBA  $R$ -matrix method (Bartschat and Burke 1988, Reid *et al* 1992, Raeker *et al* 1994, Laghdas *et al* 1995), we shall recall the necessary features of the method in the context of this particular case, rather than repeating the generalities. The computational details of the method have been described by Bartschat (1993).

## 2. Wavefunctions and energies

We have considered ionization of the Be-like  $\text{Ne}^{6+}$  ion in its ground state:

$$e_0^-(E_0) + \text{Ne}^{6+}(1s^2 2s^2 {}^1S) \longrightarrow e_0^-(E_1) + \{\text{Ne}^{7+}(f) + e^-(E_2)\} \quad (1)$$

where  $E_0$ ,  $E_1$  and  $E_2$  denote the energies of the free electrons (with corresponding wavenumbers  $k_i = \sqrt{2E_i}$ ), and  $f$  denotes the state of the final ion. The energy of the final continuum state of the  $\text{Ne}^{6+}$  system is conveniently characterized by the energy loss  $\Delta E$ :

$$\Delta E \equiv E_0 - E_1 = E_2 + I_f \quad (2)$$

where  $I_f$  is the energy of the final ion state  $f$  relative to the initial bound state. Clearly, for a given  $E_0$ , only one of  $\Delta E$ ,  $E_1$  or  $E_2$  is independent. We have denoted the incident/scattered electron by  $e_0^-$  to emphasize that it is regarded as distinguishable from the electrons of the  $\text{Ne}^{6+}$  system. Thus, in the absence of spin dependence in the interaction between  $e_0^-$  and the  $\text{Ne}^{6+}$  system, only doublet states of  $\text{Ne}^{7+}$  can be produced. We have included the eight states with configurations  $1s^2 2\ell$  or  $1s 2\ell 2\ell'$ :

$$f \in \left\{ \begin{array}{lll} 1s^2 2s {}^2S & 1s^2 2p {}^2P^o & \\ 1s 2s {}^2S & 1s 2s ({}^1S) 2p {}^2P^o & 1s 2s ({}^3S) 2p {}^2P^o \\ 1s 2p {}^2D & 1s 2p {}^2P & 1s 2p {}^2S \end{array} \right\}. \quad (3)$$

Within the framework of the DWBA  $R$ -matrix method, the wavefunctions and eigenenergies of the final ion states are input data which have a major effect on the accuracy of the calculation. We have used simple,  $LS$ -coupled, configuration-interaction wavefunctions for the eight  $\text{Ne}^{7+}$  states, based on three radial orbitals  $g_{1s}$ ,  $g_{2s}$  and  $g_{2p}$ , each of which is a sum of Slater-type orbitals (cf Clementi and Roetti 1974)

$$g(r) = \sum_k c_k R(n_k, \zeta_k | r) \quad \text{where} \quad R(n, \zeta | r) \equiv \sqrt{(2\zeta)^{2n+1} / (2n)!} r^{n-1} e^{-\zeta r}. \quad (4)$$

**Table 1.** Coefficients  $\{c_k, n_k, \zeta_k\}$  for each of the three radial orbitals  $g_{1s}(r)$ ,  $g_{2s}(r)$  and  $g_{2p}(r)$  (cf equation (4)).

1s			2s			2p		
$c$	$n$	$\zeta$	$c$	$n$	$\zeta$	$c$	$n$	$\zeta$
0.9594	1	9.5139	-0.3525	1	8.9078	0.9940	2	4.1364
0.0413	1	15.5969	-0.0103	1	15.0357	0.0113	2	11.6934
0.0117	2	4.5217	1.2574	2	4.2690			
-0.0054	2	4.7067	-0.2302	2	7.4140			

**Table 2.** Wavefunctions  $\phi$  for  $Ne^{7+}$  in terms of single-configuration wavefunctions  $\varphi$ , and the wavefunction  $\psi_0$  for  $Ne^{6+}(1s^2 2s^2 {}^1S)$  in terms of correlation functions  $\Theta$  and product functions  $\phi_f \otimes u_{n\ell}$ . The *ab initio* calculated energies are expressed relative to  $-102.6163$  au, the absolute *ab initio* energy of the ground state of  $Ne^{7+}$ . Observed energies (Bashkin and Stoner 1981) are shown below in parentheses. The energies used in our ionization calculation,  $I_f$ , are relative to the ground state of  $Ne^{6+}$ .

Adopted wavefunction	Expansion in known functions	Energy (au)	
		<i>ab initio</i>	$I_f$
$\phi(1s2p^2 {}^2S)$	$= 0.00473 \varphi(1s^2 2s) - 0.32571 \varphi(1s2s^2) - 0.94546 \varphi(1s2p^2)$	34.2864	41.9040
$\phi(1s2p^2 {}^2P)$	$= \varphi(1s2p^2)$	33.9113	41.5288
$\phi(1s2p^2 {}^2D)$	$= \varphi(1s2p^2)$	33.8592	41.4768
		(33.8262)	
$\phi(1s2s2p[b] {}^2P^o)$	$= 0.00121 \varphi(1s^2 2p) + 0.69134 \varphi(1s2s[{}^1S]2p) - 0.72253 \varphi(1s2s[{}^3S]2p)$	33.6401	41.2577
$\phi(1s2s2p[a] {}^2P^o)$	$= -0.00420 \varphi(1s^2 2p) + 0.72252 \varphi(1s2s[{}^1S]2p) + 0.69133 \varphi(1s2s[{}^3S]2p)$	33.3592	40.9767
		(33.3715)	
$\phi(1s2s^2 {}^2S)$	$= 0.00210 \varphi(1s^2 2s) + 0.94547 \varphi(1s2s^2) - 0.32571 \varphi(1s2p^2)$	32.7361	40.3537
$\phi(1s^2 2p^2 {}^2P^o)$	$= 0.99999 \varphi(1s^2 2p) + 0.00219 \varphi(1s2s[{}^1S]2p) + 0.00378 \varphi(1s2s[{}^3S]2p)$	0.5736	8.1911
		(0.5889)	
$\phi(1s^2 2s^2 {}^2S)$	$= 0.99999 \varphi(1s^2 2s) - 0.00045 \varphi(1s2s^2) + 0.00515 \varphi(1s2p^2)$	0.0000	7.6175
$\psi_0(1s^2 2s^2 {}^1S)$	$= -0.96199 \Theta(1s^2 2s^2) + 0.25072 \Theta(1s^2 2p^2)$	-7.6215	0.0000
	$-0.07598 \phi(1s^2 2s^2 S) \otimes u_{1s} - 0.04143 \phi(1s^2 2s^2 S) \otimes u_{3s}$	(-7.6175)	
	$-0.03977 \phi(1s^2 2s^2 S) \otimes u_{2s} + \dots$		

The single-configuration wavefunction  $\varphi_f$  for each  $Ne^{7+}(f)$  state is constructed uniquely from these orbitals, and the required wavefunctions  $\phi_f$  are then obtained in the form  $\phi_f = \sum_{f'} C_{f'f} \varphi_{f'}$  by allowing for configuration interaction. The values of the parameters  $\{c, \zeta\}$  in the radial orbitals and the configuration mixing coefficients  $\{C\}$  were determined by the code CIV3 (Hibbert 1975), by starting with orbitals taken from Clementi and Roetti (1974) and adjusting  $\{c, \zeta\}$  to minimize the sum of the eigenenergies of the  $1s^2 2s^2 {}^2S$ ,  $1s^2 2p^2 {}^2P^o$ ,  $1s2s^2 {}^2S$  and  $1s2p^2 {}^2S$  states. The resulting values are shown in tables 1 and 2.

Our calculated energy of the ground state of  $Ne^{7+}$  is  $-102.6163$  au, which is slightly higher than the value of  $-102.6311$  au given by Clementi and Roetti (1974). Clearly, our  $1s$  and  $2s$  orbitals have become compromised by having to also represent the higher states. In table 2 we give our calculated  $Ne^{7+}$  energies relative to this ground state, and compare them with the available measured data (Bashkin and Stoner 1981). Again, the discrepancies are of the order of 0.02 au.

All the wavefunctions for the  $Ne^{6+}$  system, including the wavefunction  $\psi_0$  for the initial  $1s^2 2s^2 {}^1S$  state and the wavefunctions for the final continuum states, are constructed by the *R*-matrix method. Because the initial symmetry is  ${}^1S^e$  and because the coupling to that symmetry

is by electric  $2^\lambda$ -pole operators, the only symmetries of the  $\text{Ne}^{6+}$  system that are required are  $^1L^\pi$ , with parity  $\pi = (-1)^L$ . In practice, we considered only the interaction components with  $\lambda \leq 4$ , so that only the symmetries  $L = 0, \dots, 4$  are required. We took an  $R$ -matrix radius of  $3.76 a_0$  and constructed radial continuum orbitals  $u_{n\ell}(r)$  ( $n = 1, \dots, 17$ ) for each angular momentum  $\ell = 0, \dots, 6$ . For each symmetry  $L$ , the  $R$ -matrix basis functions that are used to represent the  $\text{Ne}^{6+}$  system in the inner region are built from two types of function: first, the functions obtained from the  $\text{Ne}^{7+}$  functions  $\phi_f$  by adding a further electron in a continuum orbital, which we denote loosely by  $\phi_f \otimes u_{n\ell}$  and, secondly, the ‘correlation functions’  $\Theta$ , which are  $\text{Ne}^{6+}$  wavefunctions constructed from the input bound orbitals  $\{g_{n\ell}\}$ .

The wavefunction  $\psi_0$  and the eigenenergy of the bound  $1s^2 2s^2 ^1S$  state are determined by requiring an exponentially decreasing solution in the outer region. Our calculated energy is  $-110.2378$  au, which compares favourably with the value  $-110.1110$  au given by Clementi and Roetti (1974). Our calculated ionization potential for  $\text{Ne}^{6+}(1s^2 2s^2 ^1S)$  is thus  $7.6215$  au, compared with the observed value of  $7.6175$  au (Bashkin and Stoner 1981). Table 2 lists the first few terms of the wavefunction  $\psi_0$  in order of decreasing coefficients, showing that  $\psi_0$  is dominated by all-bound configurations.

The wavefunctions  $\psi_{f\ell_2 k_2 L}^{(-)}$  for the final continuum states of the  $\text{Ne}^{6+}$  system are also calculated by the  $R$ -matrix method. We recall that  $\psi_{f\ell_2 k_2 L}^{(-)}$  is the scattering state with symmetry  $^1L^\pi$  ( $\pi = (-1)^L$ ) in which the  $\ell_2$ th partial wave of an electron with energy  $E_2 = k_2^2/2$  is incident on  $\text{Ne}^{7+}(f)$  with incoming scattered waves. By virtue of the accurate determination of  $\psi_{f\ell_2 k_2 L}^{(-)}$  by the  $R$ -matrix method, the functions  $\psi_{f\ell_2 k_2 L}^{(-)}$  contain coherent admixtures of quasi-bound states of the  $\text{Ne}^{6+}$  system, and it is in this way that the EA mechanism is included in the formulation. In the calculation of  $\psi_{f\ell_2 k_2 L}^{(-)}$ , we have adopted the observed value for the ionization potential, but otherwise we have used our calculated  $\text{Ne}^{7+}$  energies. The resulting energies, relative to the  $\text{Ne}^{6+}$  ground state (i.e. the quantities  $I_f$ ) are shown in the rightmost column of table 2.

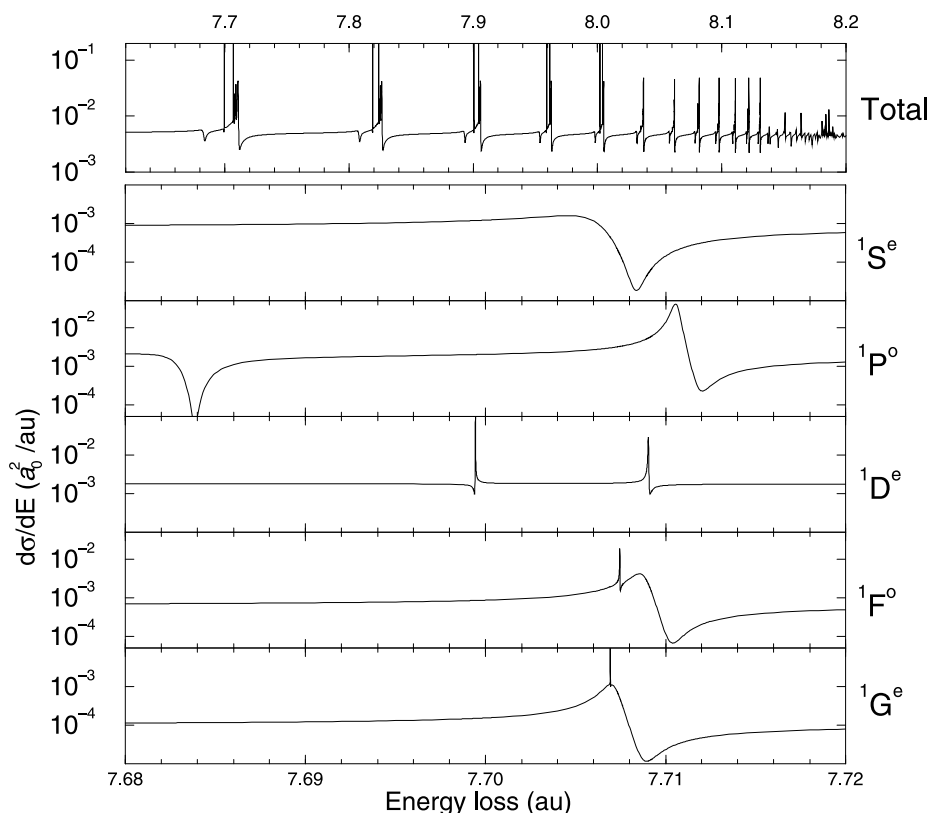
### 3. Single differential cross sections

The single differential cross section for ionizing the  $1s^2 2s^2 ^1S$  state of  $\text{Ne}^{6+}$  and leaving the resulting  $\text{Ne}^{7+}$  ion in state  $f$  is resolved into a contribution from each symmetry  $L$  of the final continuum state of the  $\text{Ne}^{6+}$  system:

$$\frac{d\sigma_f^L}{dE}(E_2, E_0) = \frac{16}{E_0} \sum_{\ell_0 \ell_1 \ell_2} |\langle \psi_{f\ell_2 k_2 L}^{(-)} \| V^{(L)}(\ell_1 k_1 \ell_0 k_0) \| \psi_0 \rangle|^2. \quad (5)$$

Here we have shown the cross section as a function of  $E_2$ , but it can as readily be regarded as a function of  $\Delta E$ . Also we have written  $d/dE$  for  $d/dE_2$  or  $d/d\Delta E$ . The continuum radial orbitals in (5) are normalized so that asymptotically their incident parts are  $1/k_2$  times a sine function.

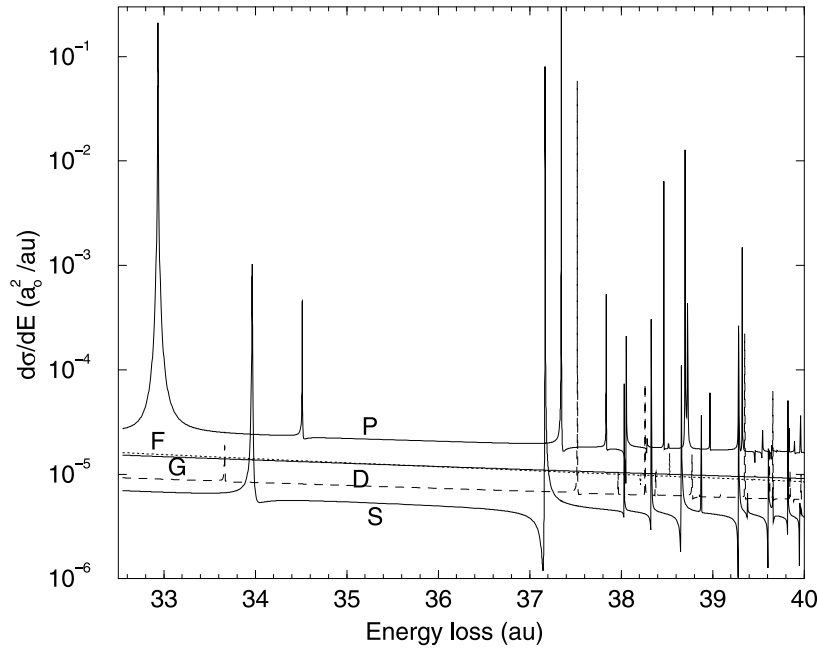
In equation (5), the operator  $V_\mu^{(\lambda)}(\ell_1 k_1 \ell_0 k_0)$  is proportional to the  $2^\lambda$ -pole component of the interaction between  $e_0^-$  and the  $\text{Ne}^{6+}$  system overlapped between the  $\ell_0$ th and  $\ell_1$ th partial waves of  $e_0^-$  at energies of  $E_0 = k_0^2/2$  and  $k_1^2/2$ , respectively (cf Jakubowicz and Moores 1981, Bartschat and Burke 1987). These partial waves were calculated using the static potential of  $\text{Ne}^{6+}(1s^2 2s^2 ^1S)$  obtained from the wavefunction given by Clementi and Roetti (1974). The maximum value of  $\ell_0$  and  $\ell_1$  that was used,  $\bar{\ell}$ , was sufficient to ensure convergence of the single differential cross section, and ranged from  $\bar{\ell} = 11$  for  $E_0 = 8$  au to  $\bar{\ell} = 43$  for  $E_0 = 100$  au. For our adopted range of  $\lambda$ , namely  $0 \leq \lambda \leq 4$ , the number of  $(\lambda, \ell_0, \ell_1)$  combinations is  $15\bar{\ell} - 18$ , and so there can be up to 627 operators for each  $(k_0, k_1)$  pairing. For a given value of



**Figure 1.** Single differential cross section for electron-impact ionization of  $\text{Ne}^{6+}(1s^2 2s^2 ^1S)$  for impact energy  $E_0 = 35$  au and energy loss  $\Delta E$  between the thresholds for producing  $\text{Ne}^{7+}(1s^2 2s^2 ^2S)$  and  $\text{Ne}^{7+}(1s^2 2p^2 ^2P^o)$ . The top graph shows the cross section summed over the continuum symmetries of  $\text{Ne}^{6+}$ . The resolution is not uniform: only the first five groups of resonances are fully resolved. The lower graphs show the contributions from each symmetry (see labels in the right-hand margin) for the resonances with  $\Delta E \approx 7.7$  au.

$k_0$ , these operators should be evaluated for each  $k_1$  ( $\Delta E$ ), and, because  $\psi_{f\ell_2 k_2 L}^{(-)}$  is generally a rapidly varying function of  $k_2$  ( $\Delta E$ ), several thousand values of  $k_1$  ( $\Delta E$ ) are required to obtain  $d\sigma_f^L/dE$  as a function of  $\Delta E$ . Thus, in principle, very many distinct operators are required. In practice, since the operators are slowly varying functions of  $k_1$ , they are evaluated only at a few representative values  $\bar{k}_1$ . With  $k_1$  held fixed at  $\bar{k}_1$ , equation (5) is used to determine the quantity  $d\sigma_f^L/dE(E_2, E_0, \bar{k}_1)$  for the complete range of  $E_2$  values. Then, for each  $E_2$ , the required quantity at the physically correct value of  $k_1$  is found by interpolating with respect to  $\bar{k}_1$ .

In figures 1 and 2 we present some single differential cross sections, resolved into the contribution from each final  $\text{Ne}^{6+}$  symmetry  $L$ . Figure 1 shows the cross sections for  $E_0 = 35$  au and for  $\Delta E$  between the  $\text{Ne}^{7+}(1s^2 2s^2 ^2S)$  and  $\text{Ne}^{7+}(1s^2 2p^2 ^2P^o)$  thresholds. The top graph shows the cross section summed over symmetry and demonstrates the regular Rydberg series of resonances. The lower graphs show the contributions from each symmetry  $L$  for the group of resonances with  $\Delta E \approx 7.7$  au. The resonances here are all due to quasi-bound states of  $\text{Ne}^{6+}$  with a  $\text{Ne}^{7+}(1s^2 2p^2 ^2P^o)$  core. Details of some of these resonances are listed in table 3. The effective principal quantum numbers  $n^*$  are high, starting at 6.84. Indeed,



**Figure 2.** Single differential cross section for electron-impact ionization of  $\text{Ne}^{6+}(1s^2 2s^2 \ ^1S)$  for impact energy  $E_0 = 73.5$  au and energy loss  $\Delta E$  below the threshold for producing  $\text{Ne}^{7+}(1s 2\ell' 2\ell'')$ . The cross section is summed over the final states of  $\text{Ne}^{7+}$ , but is resolved into the contributions from the various continuum symmetries of  $\text{Ne}^{6+}$ . Each curve is labelled by the  $L$ -value of its symmetry. The resonances are due to quasi-bound states  $\text{Ne}^{6+}(1s 2\ell' 2\ell'' n\ell)$ , with the lowest, at  $\Delta E = 32.9$  au, due to  $\text{Ne}^{6+}(1s 2s^2 2p \ ^1P^o)$ .

with this core, the  $\text{Ne}^{6+}$  states with  $n^* < 6.45$  lie below the  $\text{Ne}^{7+}(1s^2 2s^2 \ ^1S)$  level, and so are genuinely bound. The regularity between the  $n = 7$  and the  $n = 8$  resonances is clear from table 3. For example, corresponding states have very close quantum defects  $n - n^*$ , and their widths  $\Gamma_r$  exhibit the expected  $(n^*)^{-3}$  proportionality. Finally, the quantum defects seen in the  $n^*$ -values in table 3 are consistent with the values for the bound states listed by Bashkin and Stoner (1981), for example,  $1s^2 2p 3p \ ^1S$ ,  $n^* = 2.974$ ;  $1s^2 2p 3p \ ^1D$ ,  $n^* = 2.954$ ;  $1s^2 2p 4s \ ^1P^o$ ,  $n^* = 3.864$ ;  $1s^2 2p 4d \ ^1P^o$ ,  $n^* = 4.050$ ;  $1s^2 2p 4d \ ^1F^o$ ,  $n^* = 4.026$ .

Figure 2 shows the cross sections for  $E_0 = 73.5$  au and for  $\Delta E$  between 32.5 and 40.0 au. These cross sections have been summed over the two final ion states. The resonances are due to quasi-bound states of  $\text{Ne}^{6+}$  with a  $\text{Ne}^{7+}(1s 2\ell' 2\ell'')$  core. The lowest of them, the strong resonance at  $\Delta E = 32.9$  au, is due to the quasi-bound state  $\text{Ne}^{6+}(1s 2s^2 2p \ ^1P^o)$ . The lowest four resonances, between 32.9 and 34.5 au, are from the  $1s 2s^{3-k} 2p^k$  configurations, and for them the assignment of an  $n^*$ -value is inappropriate. Nevertheless, if they were assigned an  $n^*$ -value relative to one of the  $\text{Ne}^{7+}$  cores, the  $2s$  orbital would have  $n^* \approx 1.77$  and the  $2p$  orbital would have  $n^*$  between 1.82 and 1.88. We take this to show that quantum defects for  $n \geq 3$  are less than about 0.25, which is a useful first step in identifying the resonances. Thus we can say that the ranges of binding energies are: 3.24–2.72 au for  $n = 3$ ; 1.74–1.53 au for  $n = 3$ ; etc. We conclude that the lowest  $n = 4$  states, namely,  $\text{Ne}^{6+}(1s 2s^2 4\ell)$ , lie in the range 38.61–38.82 au, and that, apart from these, all the resonances up to 39.18 au have  $n = 3$ , since the  $\text{Ne}^{6+}(1s 2s 2p[a] 4\ell)$  states start at 39.23 au. Table 3 shows the designation and properties of several of the  $n = 3$  resonances. We note that, for each  $\ell$ , the  $n_{3\ell}^*$  values calculated with the various cores are reasonably consistent.

**Table 3.** Details of some singlet autoionizing states of  $Ne^{6+}$ . The energies are relative to the ground state,  $Ne^{6+}(1s^2 2s^2 \ ^1S)$ . The thresholds for production of the various states of  $Ne^{7+}$  are given as  $I_f$  in table 2. These values have been used to calculate the effective principal quantum number  $n^*$ .

Energy $\mathcal{E}_r$ (au)	Width $\Gamma_r$ ( $10^{-3}$ au)	$Ne^{6+}$ term	$n^*$
7.683 42	2.39	$1s^2 2p[{}^2P^o]$	$7s \ ^1P^o$ 6.844
7.699 428	0.0054	...	$7p \ ^1D^e$ 6.9511
7.706 43	3.81	...	$7p \ ^1S^e$ 7.000
7.706 923	0.0005	...	$7h \ ^1G^e$ 7.0031
7.707 11	1.09	...	$7f \ ^1G^e$ 7.004
7.707 45	0.014	...	$7g \ ^1F^o$ 7.0068
7.708 80	1.30	...	$7d \ ^1F^o$ 7.016
7.709 038	0.033	...	$7f \ ^1D^e$ 7.0180
7.710 60	0.55	...	$7d \ ^1P^o$ 7.029
7.808 28	1.56	$1s^2 2p[{}^2P^o]$	$8s \ ^1P^o$ 7.844
7.818 915	0.0034	...	$8p \ ^1D^e$ 7.9508
7.823 54	2.53	...	$8p \ ^1S^e$ 7.999
7.823 972	0.0003	...	$8h \ ^1G^e$ 8.0032
7.824 10	0.71	...	$8f \ ^1G^e$ 8.004
7.824 321	0.010	...	$8g \ ^1F^o$ 8.0068
7.825 17	0.86	...	$8d \ ^1F^o$ 8.016
7.825 382	0.023	...	$8f \ ^1D^e$ 8.0180
7.826 36	0.36	...	$8d \ ^1P^o$ 8.028
32.935 50	2.81	$1s 2s^2 2p$	$^1P^o$
33.665 56	5.65	$1s 2s 2p^2$	$^1D^e$
33.965 50	4.27	$1s 2s 2p^2$	$^1S^e$
34.513 51	2.38	$1s 2p^3$	$^1P^o$
37.169 22	0.31	$1s 2s^2[{}^2S^e]$	$3s \ ^1S^e$ 2.774
37.345 10	0.044	$1s 2s^2[{}^2S^e]$	$3p \ ^1P^o$ 2.854
37.521 21	0.088	$1s 2s^2[{}^2S^e]$	$3d \ ^1D^e$ 2.941
37.836 77	0.98	$1s 2s 2p[a \ ^2P^o]$	$3s \ ^1P^o$ 2.788

#### 4. Total cross sections

The total cross section for ionization that leaves the final ion in state  $f$  is

$$\sigma_f(E_0) = \int_0^{\bar{E}/2} \frac{d\sigma_f}{dE}(E_2, E_0) dE_2 \quad (6)$$

where

$$\frac{d\sigma_f}{dE}(E_2, E_0) = \sum_L \frac{d\sigma_f^L}{dE}(E_2, E_0) \quad (7)$$

and where

$$\bar{E} \equiv E_0 - I_f. \quad (8)$$

In equation (6), the upper limit of ejected-electron energy  $E_2$  is taken to be half of the maximum possible value  $\bar{E}$ , because the case in which  $E_2 = x$  and  $E_1 = \bar{E} - x$  is physically identical to the case in which  $E_2 = \bar{E} - x$  and  $E_1 = x$ . However, this requires that electron exchange between the two unbound electrons in the final state be taken into account in the single differential cross section. If exchange has been ignored, as is the case in the present calculation, then

equation (6) is only approximate (the *half-range approximation*) and a threshold error occurs in (6) for the following reason. A quasi-bound state of  $\text{Ne}^{6+}$  which has energy  $\mathcal{E}_r$  relative to the initial bound state will cause a resonance in the single differential cross section for  $\Delta E \approx \mathcal{E}_r$ , that is, for  $E_2 \approx \mathcal{E}_r - I_f$ . Hence, since the integration in (6) is over the interval  $0 \leq E_2 \leq (E_0 - I_f)/2$ , the quasi-bound state contributes to the total cross section evaluated by (6) only when  $\mathcal{E}_r - I_f \leq (E_0 - I_f)/2$ , that is, only when  $E_0 \geq 2\mathcal{E}_r - I_f$ . This is clearly incorrect, since the quasi-bound state should contribute for  $E_0 \geq \mathcal{E}_r$ —with increasing  $E_0$ , the resonance first appears at  $\Delta E \approx E_0$ , that is, at  $E_1 \approx 0$  and  $E_2 \approx E_0 - I_f$ . Thus the total cross section  $\sigma_f(E_0)$  will be seriously in error for  $\mathcal{E}_r \leq E_0 \leq 2\mathcal{E}_r - I_f$ .

If the exchange between the two unbound electrons in the final state is taken into account, the single differential cross section, as a function of  $E_2$ , is symmetric about  $\bar{E}/2$ . The resonance due to a quasi-bound state with energy  $\mathcal{E}_r$  occurs at  $E_2 \approx E_0 - \mathcal{E}_r$  through the exchange amplitude. Thus, with increasing  $E_0$ , the resonance first appears at  $E_2 = 0$ , which lies in the integration range in (6), so that the threshold is dealt with correctly.

The present calculation provides an illustration of this threshold error, because a major contribution to ionization comes from the quasi-bound state  $\text{Ne}^{6+}(1s2s^22p^1P^o)$  which has an excitation energy  $\mathcal{E}_r = 32.9$  au. Figures 3(a) and (b) show our calculated single differential cross sections for producing  $\text{Ne}^{7+}(1s^22s^2S)$  and  $\text{Ne}^{7+}(1s^22p^2P^o)$  at an impact energy of  $E_0 = 35.0$  au. The values of  $I_f$  for these final states are 7.6 and 8.2 au, respectively. The figures show the large resonant contribution due to  $\text{Ne}^{6+}(1s2s^22p^1P^o)$  at  $\Delta E = 32.9$  au. In both cases, the resonance lies above the half-range point, and so makes no contribution to the total cross section evaluated by (6). This is physically inappropriate, since  $E_0$  exceeds the energy of the resonance.

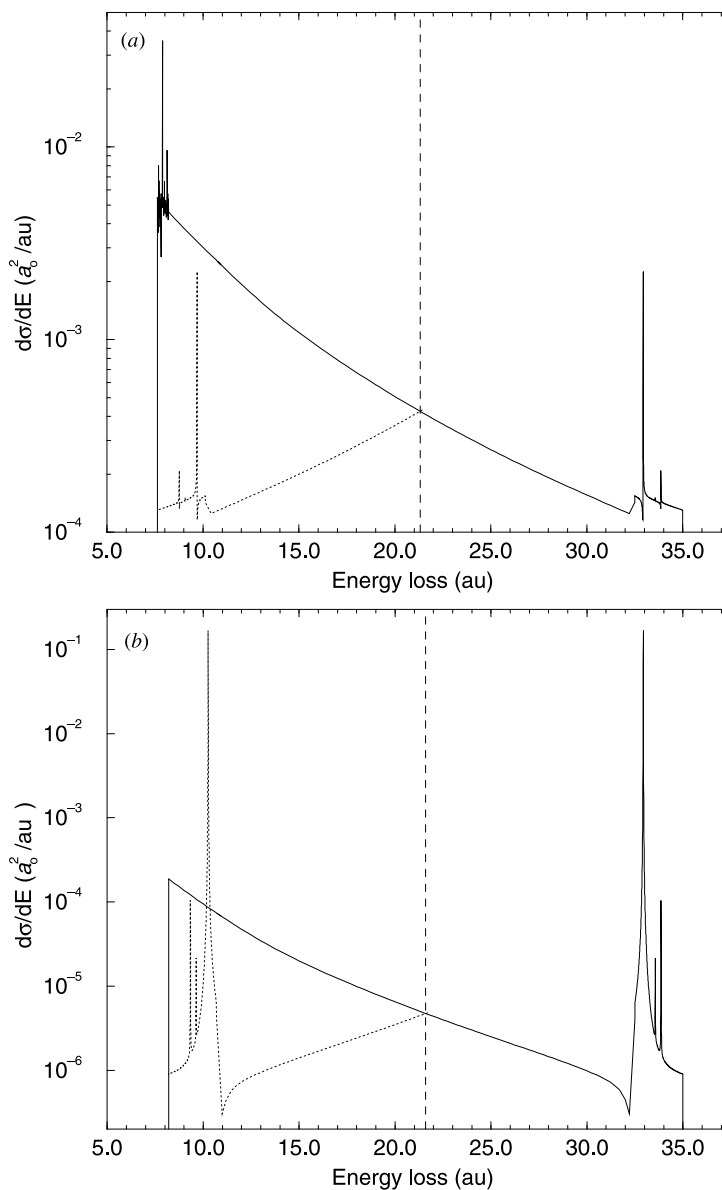
We now propose an *ad hoc* correction to this threshold error that is consistent with the level of approximation which led to (6).

Firstly, we recall the usual justification for the approximation of using (6) when there has been no allowance for exchange. If  $d\sigma_f/dE$  is calculated with proper allowance for the exchange between the two final-state continuum electrons, then it is comprised of three terms: a *direct-only* term  $[d\sigma_f/dE]^D$  arising from the absolute square of the direct scattering amplitude; an *exchange-only* term  $[d\sigma_f/dE]^X$  arising from the absolute square of the exchange amplitude; and an *interference* term  $[d\sigma_f/dE]^I$  arising from a product of the direct and exchange amplitudes (cf Rudge 1968). The justification for taking  $d\sigma_f/dE \approx [d\sigma_f/dE]^D$  is that the interference term and the exchange-only term cancel each other completely. (A less radical assumption, which is widely adopted (cf Younger 1980), is that the interference is maximum. The consequences of the various approximations in handling the exchange and interference terms have been studied by Jakubowicz and Moores (1981)).

Secondly, let us consider a case in which the exchange-only term is larger than the direct-only term. Then we would argue that it is unreasonable to assume that the exchange-only and the interference terms cancel. Rather, in the spirit of the original justification, we should assume that it is the direct-only term and the interference term which cancel each other, leaving  $d\sigma_f/dE \approx [d\sigma_f/dE]^X$ . Hence, generally, we should use the larger of  $[d\sigma_f/dE]^D$  and  $[d\sigma_f/dE]^X$  as the integrand in (6).

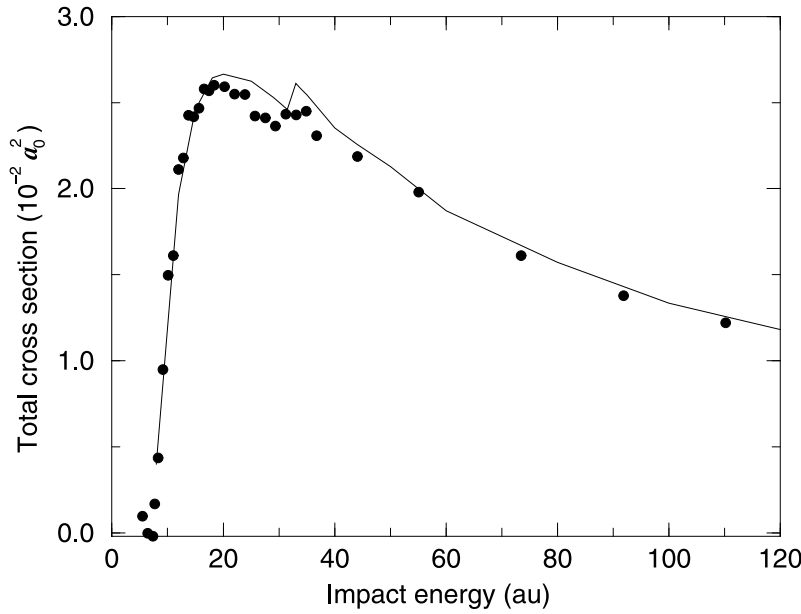
Finally, we recall the result due to Peterkop (1961) that  $[d\sigma_f/dE]^X(E_2) = [d\sigma_f/dE]^D(\bar{E} - E_2)$ . This result requires that the two final-state continuum electrons be treated similarly, for example, both treated exactly in an accurate final-state wavefunction, or both treated by similar distorted waves (cf Younger 1980). In our formulation this is certainly not true, since the ejected electron and the ionizing electron  $e_0^-$  are treated completely differently. Nevertheless, we shall assume that our calculated  $[d\sigma_f/dE]^D(\bar{E} - E_2)$  is a





**Figure 3.** Single differential cross sections (full curves) for ionization of  $\text{Ne}^{6+}(1s^2 2s^2 {}^1S)$  by electrons with energy  $E_0 = 35$  au in which the final ion  $\text{Ne}^{7+}$  is left in state (a)  $1s^2 2s^2 S$  or (b)  $1s^2 2p^2 P^o$ . (The continuum symmetries of  $\text{Ne}^{6+}$  have been summed over.) The full range  $I_f \leq \Delta E \leq E_0$  is shown. The vertical broken line indicates the half-range point. For the lower half-range, the dotted curves show the single differential cross sections as functions of  $(I_f + E_0 - \Delta E)$ .

reasonable approximation to  $[d\sigma_f/dE]^X(E_2)$ .



**Figure 4.** Total cross sections for electron impact ionization of  $\text{Ne}^{6+}$ , summed over the final states  $\text{Ne}^{7+}(1s^2 2s^2 S)$  and  $\text{Ne}^{7+}(1s^2 2p^2 P^o)$ . The full curve shows the result of the present calculation. The full circles are the experimental results of Duponchelle *et al* (1997).

Combining these three points, we arrive at our proposed modification to the usual half-range approximation (6):

$$\sigma_f(E_0) = \int_0^{\bar{E}/2} \max \left[ \frac{d\sigma_f}{dE}(E_2, E_0), \frac{d\sigma_f}{dE}(\bar{E} - E_2, E_0) \right] dE_2. \quad (9)$$

We note that there is a correction to (6) only from an  $E_2$  region in which the exchange term exceeds the direct one. Also, we note that (9) is identical to (6) when  $d\sigma_f/dE$  is exact.

Figures 3(a) and (b) show our calculated values of  $d\sigma_f/dE(\bar{E} - E_2)$  as dotted curves. In the case when the  $\text{Ne}^{7+}$  is left in its ground state, figure 3(a), the total cross section is not altered by using (9) rather than (6). On the other hand, figure 3(b) shows that the total cross section for ionization with production of  $\text{Ne}^{7+}(1s^2 2p^2 P^o)$  is enhanced by using (9), the increase being the area above the full curve and below the dotted curve. A feature of (9) is that the contribution from the resonance increases with  $E_0$ , because more of the dotted curve lies above the full curve as the peak in the dotted curve at  $E_2 = \bar{E} - \varepsilon_r$  moves to higher  $E_2$  with increasing  $E_0$ .

Figure 4 shows the total cross section for ionization of  $\text{Ne}^{6+}(1s^2 2s^2 {}^1S)$  calculated using approximation (9). The plotted quantity is the sum over the  $1s^2 2s$  and  $1s^2 2p$  final states. The theory agrees well with the experimental results by Duponchelle *et al* (1997). In particular, the location and size of the EA contribution from the  $\text{Ne}^{6+}(1s^2 2s^2 2p {}^1P^o)$  resonance is accounted for satisfactorily. Our calculated total cross sections are also presented in table 4. Again, we have presented only the results for the production of the two  $1s^2 2\ell$  states of  $\text{Ne}^{7+}$  and not the results for the six  $1s^2 2\ell 2\ell'$  states, even though the latter were included in the calculation. The  $1s^2 2\ell 2\ell'$  states would give a contribution of less than 9% to the summed total cross section for impact energies above their thresholds at about 41 au, but in any case we believe that they should be regarded as contributing to double, rather than single, ionization. We address this

issue separately (Laghdas *et al* 1999).

**Table 4.** Total cross sections for electron-impact ionization of  $\text{Ne}^{6+}(1s^2 2s^2 \ ^1S)$  with production of  $\text{Ne}^{7+}(1s^2 2s \ ^2S)$  or  $\text{Ne}^{7+}(1s^2 2p \ ^2P^o)$ . Column ‘ $\Sigma$ ’ is the cross section summed over the  $1s^2 2s$  and  $1s^2 2p$  states.

Cross section ( $10^{-2} a_0^2$ )				Cross section ( $10^{-2} a_0^2$ )			
Impact energy (au)	$\Sigma$	$1s^2 2s$	$1s^2 2p$	Impact energy (au)	$\Sigma$	$1s^2 2s$	$1s^2 2p$
8.0	0.40	0.40		34.0	2.58	2.37	0.207
12.0	1.97	1.92	0.050	35.0	2.54	2.34	0.200
15.0	2.46	2.39	0.063	40.0	2.35	2.16	0.191
18.0	2.64	2.58	0.066	44.0	2.26	2.09	0.162
20.0	2.66	2.60	0.066	50.0	2.13	1.97	0.156
25.0	2.62	2.56	0.062	60.0	1.87	1.73	0.146
29.0	2.53	2.47	0.059	80.0	1.57	1.44	0.130
31.5	2.46	2.40	0.056	100.0	1.33	1.22	0.118
33.0	2.61	2.40	0.214	140.0	1.03	0.93	0.099

A different approach to the potential threshold error due to resonances in the single differential cross section has been taken by Moores and Reed (1989) in their study of ionization of  $\text{Se}^{24+}$  using the DWBA close-coupled formulation of Jakubowicz and Moores (1981). For each prominent resonance in the single differential cross section, they separated the resonant contribution from the non-resonant background. The non-resonant cross section was integrated by formula (6), while the resonant parts were integrated separately to give independent-process-type additions to the total cross section. They were thus able to allow for radiative decay of the autoionizing states by the usual device of multiplying each resonant contribution by a branching ratio. They found that, for this highly charged Ne-like ion, the radiative damping reduced their cross section by a factor of about two.

## 5. Summary

Our calculation has demonstrated the capacity of the Bartschat–Burke formulation of electron-impact ionization to include the EA mechanism by automatically generating the quasi-bound states of the target and including them coherently in the single differential cross section. We have analysed the properties of several of these autoionizing resonances, although the main feature is the  $\text{Ne}^{6+}(1s2s^2 2p \ ^1P^o)$  resonance. The position and width of this quasi-bound state may be sensitive to our adopted set of radial orbitals  $\{g_{nl}\}$ , and we are conscious that this is an area of our calculation that might bear improvement, judging from the accuracy of our calculated energies for  $\text{Ne}^{7+}$ .

The significant contribution to ionization made by the  $\text{Ne}^{6+}(1s2s^2 2p \ ^1P^o)$  autoionizing state has served to demonstrate a threshold error in the half-range approximation for the total cross section. We have proposed a modification to that approximation, and the resulting total cross section agrees well with the experimental results of Duponchelle *et al* (1997).

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## References

- Bartschat K 1993 *Comput. Phys. Commun.* **17** 219  
Bartschat K and Burke P G 1987 *J. Phys. B: At. Mol. Phys.* **20** 3191  
——1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2969  
Bashkin S and Stoner J O 1981 *Atomic Energy-Levels and Grotian Diagrams* vol 2 (Amsterdam: North-Holland) pp 250–3  
Clementi E and Roetti C 1974 *At. Data Nucl. Data Tables* **14** 177  
Duponchelle M, Khoulid M, Oualim E M, Zhang H and Defrance P 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 729  
Gorczyca T W, Pindzola M S, Griffin D C and Badnell N R 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** 2399  
Henry R J W and Kingston A E 1988 *Adv. At. Mol. Phys.* **25** 267  
Hibbert A 1975 *Comput. Phys. Commun.* **9** 141  
Jakubowicz H and Moores D L 1981 *J. Phys. B: At. Mol. Phys.* **14** 3733  
Laghdas K, Reid R H G, Joachain C J and Burke P G 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 4811  
——1999 in preparation  
Moores D L and Reed K J 1989 *Phys. Rev. A* **39** 1747  
——1994 *Adv. At. Mol. Phys.* **34** 301  
Peterkop R K 1961 *Proc. Phys. Soc.* **77** 1220  
Raeker A, Bartschat K and Reid R H G 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** 3129  
Reid R H G, Bartschat K and Burke P G 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 3175  
Reid R H G, Bartschat K and Raeker A 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 563  
Rudge M R H 1968 *Rev. Mod. Phys.* **40** 564  
Schwienhorst, Raeker A, Reid R H G and Bartschat K 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 4651  
Tayal S S 1994 *Phys. Rev. A* **49** 2561  
Younger S M 1980 *Phys. Rev. A* **22** 111