Overlapping resonances in dielectronic recombination of highly charged ions

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Abstract. The effects of overlapping resonances in dielectronic recombination (or in photoionization) of a highly-charged ion are investigated. The example taken in this report is the coupling between 2s3s and 2p3p resonance states of an helium-like ion. The energy separation of the 2s3s and the 2p3p resonance states is always larger than the autoionizing widths for all ions. However, the energy separation becomes smaller than the radiative decay widths for a highly-charged ion. This report discusses the case that resonances become overlapping owing to the radiative decay effect. An isolated-resonance approximation usually employed in the calculation of dielectronic recombination processes is also examined.

1. Introduction

Recently, the effects of overlapping resonances have been investigated for the resonance structure forming a high-lying Rydberg series in dielectronic recombination processes (Pradhan and Seaton 1985, LaGattuta and Hahn 1985). With increasing principal quantum number $n$ of the Rydberg resonance state, the separation ($\Delta E$) of the nearest-neighbouring two resonances becomes small ($\sim n^{-3}$). On the other hand, the radiative decay width ($\Gamma_r$) of the resonance state is nearly independent of $n$. Hence, the resonances overlap each other when $n$ is very large. The effect of the overlapping resonances is nicely described by using a quantum defect theory (Bell and Seaton 1985). We can have a similar situation for low-lying resonances if we consider a highly-charged ion. The autoionizing width ($\Gamma_a$) is nearly independent of ion charge $z$ while the radiative decay width is roughly proportional to $z^4$. Hence, it is expected that some low-lying resonances will overlap for a highly-charged ion. However, the quantum defect theory (Bell and Seaton 1985) is not applicable to treating low-lying resonances. Although there have been several formal studies on overlapping resonances (Treftz 1967, Mies 1968, Roszman 1982), none of them pays attention to the resonances which overlap due to the radiative decay effect.

The importance of the overlapping effect in plasma diagnostics is pointed out by Inal and Dubau (1989). The interference effects of overlapping resonances make a change in the polarization of dielectronic satellite lines. However, an isolated-resonance approximation is usually introduced in the calculation of dielectronic recombination processes related to low-lying resonances (Dubau and Volonté 1980, Hahn and LaGattuta 1988). Therefore, it is desired to investigate the effect of overlapping resonances further on these processes.
In the present work, we study the overlapping resonances. For this purpose, we employ a numerical method developed by Sakimoto et al. (1990). This method is based on the general theory of Davies and Seaton (1969) for bound–free transitions. If we have a dipole matrix element fitted well in an analytical function, we can easily use the formula of Davies and Seaton. Whenever $\Delta E \gg \Gamma_a$, the fitting of the dipole matrix element is always possible (Bartschat and Burke 1988). Since this method does not assume $\Delta E \gg \Gamma_e$, it allows us to treat the resonances which overlap due to the radiative decay effect.

The content of the present paper is as follows. Section 2 briefly outlines the theory. We give an explicit form for the probability for dielectronic recombination in terms of a dipole matrix element fitted in a simple function. Section 3 demonstrates some results of the application. Finally, section 4 provides the summary of the present study.

2. Theory

By solving a radiation-damping equation, Davies and Seaton (1969) provided an $S$-matrix for bound–free transitions in the form

$$S_{bf}(E) = -2\pi i[1 + L(E)]^{-1}D^\dagger(E)$$

where $E$ is the energy of the free electron, $D(E)$ is the reduced dipole matrix for bound–free transitions (Davies and Seaton 1969, Sakimoto et al 1990), and $L(E)$ is given in terms of $D(E)$ by

$$L(E) = -i\pi \int dE' \frac{D^\dagger(E')D(E')}{E' - E - i\epsilon}.$$  \hspace{1cm} (2)

From equations (1) and (2), we see that the dipole matrix element is the fundamental quantity in the calculation of the $S$-matrix.

In this study, we assume that the energy separation $\Delta E$ of autoionizing states is much larger than the autoionization width $\Gamma_a$. Furthermore, for simplicity, we assume that the non-resonant contribution is negligible and there is only a single channel for each initial continuum and final bound state. Therefore, we consider the case that the dipole matrix element is fitted in the simple form

$$D(E) = \sum_\lambda \frac{A^\lambda}{E - (Z^\lambda)^*}.$$  \hspace{1cm} (3)

As long as we discuss a narrow energy range around resonances, the dipole matrix element can be well fitted in this form (Bartschat and Burke 1986, Sakimoto et al 1990). The complex resonance energy $Z^\lambda$ is

$$Z^\lambda = E_a^\lambda - \frac{i}{2} \Gamma_a^\lambda.$$  \hspace{1cm} (4)

It should be noted that this complex resonance energy is the one obtained by neglecting the radiative decay effect. The summation in equation (3) is taken over the autoionizing states denoted by $\lambda$. When the energy positions of the autoionizing states
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$(E_a^\lambda)$ are very close to each other, the fitting parameters $A^\lambda$ can be chosen to be a real value without loss of generality (Bell and Seaton 1985). Substituting equation (3) into the integral (2) and evaluating it, we obtain (Sakimoto et al 1990)

$$L(E) = 2\pi^2 \sum_{\lambda, \lambda'} \frac{A^\lambda A^{\lambda'}}{(E - Z^\lambda)(Z^\lambda - (Z^{\lambda'})^*)}.$$  \hspace{1cm} (5)

Since the probability for dielectronic recombination (or for photoionization) is given by $P_O = |S_{fr}|^2$, we have

$$P_O(E) = 4\pi^2 \left| \frac{D(E)}{1 + L(E)} \right|^2.$$  \hspace{1cm} (6)

In obtaining equation (6), we have not introduced the assumption that the energy separation $\Delta E$ is much larger than the radiative decay width. This means that we can use equation (6) to treat the overlapping resonances. In the present study, however, we only consider the resonances which overlap due to the radiative decay effect but not due to the autoionizing effect. This is because the condition $\Delta E \gg \Gamma_a^\lambda$ must be satisfied to have equation (3) and thereby (5).

If the resonances are well isolated, we can approximate $L(E)$ at $E \sim E_a^\lambda$ by

$$L(E \sim E_a^\lambda) = 2\pi^2 \frac{(A^\lambda)^2}{(E - Z^\lambda)(Z^\lambda - (Z^\lambda)^*)}.$$  \hspace{1cm} (7)

Then, equation (6) reduces to

$$P_O(E) = 4\pi^2 \left| \sum_{\lambda} \frac{A^\lambda}{(E - E_a^\lambda) + \frac{1}{2}(\Gamma_a^\lambda + \Gamma_r^\lambda)} \right|^2.$$  \hspace{1cm} (8)

The radiative decay width $\Gamma_r^\lambda$ is defined by

$$\Gamma_r^\lambda = \frac{(2\pi A^\lambda)^2}{\Gamma_a^\lambda}.$$  \hspace{1cm} (9)

It should be noted that the quantity $\Gamma_r^\lambda$ has the meaning of a width only if the resonances are well isolated. Expression (8) was used to study the effect of overlapping resonances in dielectronic satellite lines by Inal and Dubau (1989).

In the case of a perfectly isolated resonance (Davies and Seaton 1969, Bell and Seaton 1985), the interference terms in equation (8) may be neglected. Then, we have

$$P_O(E) = \sum_{\lambda} \frac{\Gamma_a^\lambda \Gamma_r^\lambda}{(E - E_a^\lambda)^2 + \frac{1}{4}(\Gamma_a^\lambda + \Gamma_r^\lambda)^2}.$$  \hspace{1cm} (10)

This equation is usually employed in the calculation of dielectronic recombination processes.

Since we have neglected the non-resonant contribution, there is no shift of the resonance position from $E_a^\lambda$ in equations (8) and (10). (If we add the non-resonant part to the dipole matrix element (3), the resonance position will shift.) However, even if we neglect the non-resonant contribution, owing to the coupling between the resonance states, we can have a resonance shift in equation (6).
3. Calculations

We take up the following resonance process:

\[ A^{(z+1)+}[1s_{1/2}] + e = A^{z+}[2l'_j 3l'_j (J = 1)] \rightarrow A^{z+}[1s_{1/2}3p_{1/2}(J = 1)] + \gamma. \]

To have the interference effect, the autoionizing states must be coherent. Hence, we restrict ourselves to the case that the autoionizing states have the same total angular momentum. (Here, we choose \( J = 1 \).) In this process, many autoionizing states are coherent (i.e. \( 2s_{1/2}3s_{1/2}, 2p_{1/2}3p_{1/2}, 2p_{1/2}3p_{3/2}, \ldots, 2s_{1/2}3p_{1/2}, \ldots \)). Among these autoionizing states, we only focus on the \( 2s_{1/2}3s_{1/2} \) and the \( 2p_{1/2}3p_{1/2} \) states. This is because the energy separation of these two states is very small and they are well isolated from the others.

<table>
<thead>
<tr>
<th>( z )</th>
<th>Resonance</th>
<th>( E_a )</th>
<th>( \Delta E )</th>
<th>( \Gamma_a )</th>
<th>( \Gamma_f )</th>
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</thead>
<tbody>
<tr>
<td>16</td>
<td>2p3p</td>
<td>121.504</td>
<td>0.248</td>
<td>1.16(−6)</td>
<td>5.71(−3)</td>
</tr>
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<td></td>
<td>2s3s</td>
<td>121.256</td>
<td>3.00(−4)</td>
<td>1.27(−3)</td>
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</tr>
<tr>
<td>28</td>
<td>2p3p</td>
<td>340.284</td>
<td>0.335</td>
<td>1.77(−5)</td>
<td>6.22(−2)</td>
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<tr>
<td></td>
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<td>2.34(−4)</td>
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<td>3.20(−5)</td>
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<td>2.12(−4)</td>
<td>2.21(−2)</td>
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<td>40</td>
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<td>4.69(−5)</td>
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<td>52</td>
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<td>7.74(−5)</td>
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<td>1132.049</td>
<td>1.90(−4)</td>
<td>0.276</td>
<td></td>
</tr>
</tbody>
</table>

This resonance process was theoretically investigated by Nilsen (1987) under the assumption of isolated resonances. Table 1 shows the parameters for the \( 2s_{1/2}3s_{1/2} \) and the \( 2p_{1/2}3p_{1/2} \) resonances of several ions with charge \( z \) calculated by Nilsen. (Here, the ion charge \( z \) means the one for the ion in a resonance state.) We can see that the energy separation is always much larger than the decay width for autoionization. However, this is not the case for radiative emission. With an increase in the ion charge, the radiative decay width becomes large, and accordingly the radiative decay width is comparable with or larger than the energy separation for \( z > 40 \). Therefore, the overlapping effect in these resonances is very important for \( z > 40 \).

In the calculation of Nilsen (1987), the wavefunctions of the resonance (autoionizing) states are determined by using a computer code for bound states, and the radiative decay width is defined as the Einstein coefficient for spontaneous emission. As we have seen earlier, the quantity \( \Gamma_\lambda^\Delta \) given in equation (9) does not have the meaning of a width for \( z > 40 \) because of the overlapping effect. However, we should note that a bound-state code can also provide the accurate dipole matrix element (3) for \( z > 40 \). That is to say, if we know the value of \( \Gamma_\lambda^\Delta \) calculated by a bound-state code, the fitting coefficients \( A_\lambda \) in equation (3) can be deduced from equation (9) which is merely a numerical relation in the case of \( z > 40 \). In this way, we take the value of
Figure 1. Dielectronic recombination probabilities as a function of the incident electron energy for $z = 28$ ($z$ being the charge of a recombined ion). The two peaks show the resonances in the 2s3s and the 2p3p states.
Figure 2. The same as in figure 1 except for $z = 40$. 

Electron energy (in atomic units)

$P_0^-$, $P_1^-$, $P_A^-$

Probability

$z = 40$
Figure 3. The same as in figure 1 except for $z = 52$. 

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the coefficient $A^z$ from the data of Nilsen. Nevertheless, the sign of $A^z$ remains still unknown. We assume that the sign is always positive. When a bound-state code is not applicable to describe the autoionizing state, we can make a scattering calculation to obtain an accurate dipole matrix element (including a non-resonant part) as was done in the previous study (Sakimoto et al 1990). In the present case, however, a bound-state code is satisfactory since the autoionizing widths are sufficiently narrow.

We have calculated the probabilities by using equations (6), (8) and (10), respectively. In figures 1–3, we compare the three results of $P_O$, $P_I$ and $P_A$ for $z = 28$, 40 and 52. Since $\Delta E \gg \Gamma_a^z + \Gamma_r^z$, there is only a negligible difference between the three results for $z = 28$ (figure 1). When $z = 40$, we can see some difference but that is still small. Table 1 shows that the energy separation of the autoionizing states is comparable with but a little larger than $\Gamma_r^z$ of the 2p3p state for $z = 40$. Hence, as figure 2 shows, the interference between the two resonances is partly important. Consequently, the isolated-resonance approximation $P_I$ is relatively poor; on the other hand, the approximation $P_A$ reproduces better the accurate one $P_O$. When $z = 52$, the radiative decay width of Nilsen for the 2p3p state is larger than the energy separation. The interference effect is significant for $z = 52$. Figure 3 shows that both of the two approximations $P_I$ and $P_A$ are quite unsatisfactory. In the isolated-resonance approximation, the 2p3p resonance appears only as a shoulder of the 2s3s resonance. However, the accurate result $P_O$ clearly shows two peaks. Furthermore, the two approximations $P_I$ and $P_A$ fail to have a deep well between the two resonance peaks.

Comparing the accurate result with the isolated-resonance approximation, we see that the overlapping of resonances causes not only a change in the peak height but also a shift in the peak position.

4. Summary and discussion

There are plenty of calculations on the dielectronic recombination process. In the previous calculations particularly concerned with low-lying resonances, the isolated-resonance approximation is employed. Very recently, cross sections for dielectronic recombination have been measured for extremely highly-charged ions ($z \geq 80$) (see Pindzola and Badnell 1991, Badnell and Pindzola 1991 and references therein). The effects of the overlapping resonances may be very important in that case. However, the calculations for the corresponding process also assume isolated resonances (Pindzola and Badnell 1991, Badnell and Pindzola 1991). By using the present method, we can easily take the overlapping effect into account.

It is not always possible to resolve the details of a resonance profile. In that case, an important quantity is a probability averaged over energies. Consider one of the present examples: $z = 52$. Averaging the probability shown in figure 3 over the energies considered there ($E = 1131.3–1133.2$ au), we have $\bar{P}_O = 6.73 \times 10^{-4}$ and $\bar{P}_I = 7.72 \times 10^{-4}$. The difference between the two is about 15%, which is not yet so significant. This is because the radiative decay width shown in table 1 is not much larger than the resonance separation for $z = 52$. For extremely highly-charged ions (i.e. $\Delta E \ll \Gamma_r$), the isolated-resonance approximation would also become poor for an averaged probability. A further study on the overlapping resonances of highly-charged ions would be very stimulating.

In this study, we have assumed $\Delta E \gg \Gamma_a$. Since the case of $\Delta E < \Gamma_a$ is rarely found for low-lying resonances, the present method would be applicable to most of the low-lying overlapping resonances.
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