Unified dielectronic and radiative-recombination cross sections for U^{90+}

N. R. Badnell and M. S. Pindzola
Department of Physics, Auburn University, Auburn, Alabama 36849-5311
(Received 16 August 1991)

We have calculated unified photorecombination cross sections and independent-processes photorecombination cross sections for U^{90+} in the vicinity of the *KLL* resonances. For this case, where the radiative width of a level dominates the Auger width, we find relatively strong interference effects between the direct (radiative) and indirect (dielectronic) recombination processes. In particular, we find that the unified photorecombination cross section for the $1s^2+e^- \to 1s^2 2s + h\nu$ line is suppressed by a factor of 2 in the presence of the $1s2s(1)2p(\frac{3}{2})$ resonance. Overall, however, the *KLL* recombination cross section is reduced by only 2–3 %, at most.

PACS number(s): 34.80.Kw

I. INTRODUCTION

In recent years, there have been great advances in techniques for the measurement of dielectronic recombination (DR) cross sections, both with regard to the energy resolution [1–3] and to the charge-state accessibility [4,5]. So far, the results of such measurements have been well described by calculations [5–10] that make use of the independent-processes and isolated-resonance approximations, but for how long? A good deal of effort [11–23] has gone into developing a formal description of DR, including overlapping resonances, and into electron-ion recombination in general, following the recognition that the separation into dielectronic and radiative recombination is purely artificial. Most of these theoretical calculations to date have been for model problems. One notable exception is the study of interference effects on DR satellite intensities by Jacobs *et al.* [18]; however, they only included part of the interference effect (see Sec. II). Jacobs *et al.* [18] studied the case for which the autoionization rate from a given level dominates the radiative rate out of that level. It turns out that a different term dominates the interference effect when the radiative rate dominates over the autoionization rate (see Sec. II), as is the case for the *KLL* resonances formed in the photorecombination of U^{90+}. We have already studied [9] the DR of U^{90+} in the independent-processes and isolated-resonance approximations using a multiconfiguration Dirac-Fock-Breit description for the required energies and rates, and the results [9] were found to be in good agreement with low-energy-resolution experimental results [4] for U^{90+} on H_2. But, high-resolution [24] results can be expected in the not-too-distant future from heavy-ion storage rings [25] and the super-EBIT (electron-beam ion trap) [26]. So, in this paper, we investigate interference effects on the photorecombination of U^{90+}, but still within the isolated-resonance approximation. The allowance for both interference and overlapping resonances in a practical calculation requires a further nontrivial effort. We utilize the formulation of Haan and Jacobs [20] for the unified dielectronic and radiative-recombination cross section, denoted as the unified photorecombination cross section. The working formulas and analyses of them are given in Sec. II. Our results for the unified photorecombination cross sections are then presented and discussed in Sec. III. We conclude with a short summary in Sec. IV.

II. THEORY

We utilize the projection-operator formalism of Haan and Jacobs [20] for the unified electron-ion photorecombination process. We assume that the sum over degenerate magnetic sublevels can be absorbed into each individual rate or cross section, following the work of Jacobs [17]. We assume that there exists a single electron continuum with a single partial-wave expansion but that there may be multiple photon continua. Then, the unified photorecombination cross section $\sigma(i \to f)$ from an initial level i to a final level f in the presence of a single resonance level j is given by [20]

$$\sigma(i \to f) = \sigma_{\mathrm{RR}}(i \to f) \frac{\left\{ (\xi+q_f)^2 + \left[\sum_{f'} \left[1 - \frac{q_f}{q_{f'}} \right] \frac{\gamma_{f'}}{\Gamma} \right]^2 \right\}}{\psi^2[(\xi-\Delta)^2+\eta^2]} , \tag{1}$$

where the width of the modified Lorentzian $\Gamma\eta$ is given by

$$\Gamma\eta = \frac{1}{\psi} \left[\Gamma + \psi \sum_f \gamma_f - \frac{1}{\Gamma} \left[\sum_f \frac{\gamma_f}{q_f} \right]^2 \right] , \tag{2}$$

and the energy shift by $\Gamma\Delta\hbar/2$, where

$$\Delta = \frac{-2}{\Gamma\psi} \sum_f \frac{\gamma_f}{q_f} . \tag{3}$$

 ©1992 The American Physical Society

Furthermore,

$$\xi=\frac{2}{\Gamma\hbar}(\varepsilon_i+E_i-E_j)\ , \tag{4}$$

where ε_i is the continuum electron energy, E_i is the target ion energy, and E_j is the unperturbed resonance energy. The continuum-continuum coupling parameter ψ is given by

$$\psi=1+\sum_f \frac{\gamma_f}{\Gamma q_f^2} \tag{5}$$

and the Fano line-profile parameter q_f by

$$q_f=\frac{\langle j\|P\|f\rangle}{v_{\varepsilon_i}\langle i\|P\|f\rangle}=\pm\left[\frac{\gamma_f}{\Gamma\Omega\sigma_{\text{RR}}(i\to f)}\right]^{1/2}\ , \tag{6}$$

where

$$\Omega=\frac{\varepsilon_i\omega}{2I\omega_j\pi a_0^2}\ . \tag{7}$$

The remaining quantities are the unperturbed $j\to f$ radiative rate denoted by γ_f, the unperturbed $j\to i+e^-$ autoionization rate Γ, the unperturbed $i+e^-\to f+h\nu$ radiative-recombination cross section σ_{RR}, the statistical weight of the target ω_i, the statistical weight of the resonance level ω_j, the ionization potential of the hydrogen atom I, Planck's constant $\hbar$, and the Bohr radius a_0.

We can energy average Eq. (1) over a bin width $\delta\varepsilon_i$ to obtain the energy-averaged unified photorecombination cross section $\langle\sigma(i\to f)\rangle$ given by

$$\begin{aligned}\langle\sigma(i\to f)\rangle=&\frac{\sigma_{\text{RR}}(i\to f)}{\psi^2}\\&+\frac{(2\pi a_0 I)^2\omega_j\tau_0\gamma_f\Gamma}{\varepsilon_i\delta\varepsilon_i 2\omega_i\psi^2\Gamma\eta}\\&\times\left\{\left[1+\frac{\Delta}{q_f}\right]^2-\left[\frac{\eta}{q_f}\right]^2\right.\\&\left.+\left[\sum_{f'}\left[1-\frac{q_f}{q_{f'}}\right]\frac{\gamma_{f'}}{q_f\Gamma}\right]^2\right\}\end{aligned} \tag{8}$$

which reduces to the usual independent-processes result in the limit of $q_f\to\infty$. We may apply the isolated-resonance approximation in the many-level case by simply summing (1) or (8) over all resonance levels j.

It is of interest to consider Eq. (8) in some limiting cases. We first note that for all practical purposes the continuum-continuum coupling parameter ψ can be taken to be unity. To see this, just substitute for q_f from Eq. (6) into Eq. (5) and use, for example, a Bethe-Salpeter-type [27] approximation for the radiative-recombination cross section. Thus, we may write Eq. (8) as (with $\psi=1$)

$$\langle\sigma\rangle=\sigma_{\text{RR}}+\langle\tilde{\sigma}_{\text{DR}}\rangle+\langle\sigma_{\text{int}}\rangle\ , \tag{9}$$

where $\langle\tilde{\sigma}_{\text{DR}}\rangle$ is the modified DR term of Jacobs *et al.* [18,19], but in its energy-averaged form. Likewise, $\langle\sigma_{\text{int}}\rangle$ is the interference term of Jacobs, Cooper, and Haan [19], but energy averaged. For the case of a single photon continuum we have [18,19]

$$\langle\tilde{\sigma}_{\text{DR}}\rangle\approx\langle\sigma_{\text{DR}}\rangle\left[1+\frac{\gamma_f^2}{\Gamma^2 q_f^2}\right]\left[1+\frac{1}{q_f^2}\right]\ , \tag{10}$$

where $\langle\sigma_{\text{DR}}\rangle$ is the usual unperturbed energy-averaged DR cross section [see, e.g., Ref. [6], Eq. (1)].

First, we consider $\gamma_f\ll\Gamma$, then from Eq. (10) we have

$$\langle\tilde{\sigma}_{\text{DR}}\rangle\approx\langle\sigma_{\text{DR}}\rangle\left[1+\frac{1}{q_f^2}\right] \tag{11}$$

but from Eq. (8) we have

$$\langle\tilde{\sigma}_{\text{DR}}\rangle+\langle\sigma_{\text{int}}\rangle\approx\langle\sigma_{\text{DR}}\rangle\left[1-\frac{1}{q_f^2}\right]\ , \tag{12}$$

i.e.,

$$\langle\sigma_{\text{int}}\rangle\approx-\frac{2}{q_f^2}\langle\sigma_{\text{DR}}\rangle\ . \tag{13}$$

Thus, if the modified DR cross section $\langle\tilde{\sigma}_{\text{DR}}\rangle$ in Eq. (11) is considered alone [18], then the magnitude of the effect is correct but an enhancement of the unperturbed DR cross section (or rate) is predicted rather than a suppression, as found for $\langle\tilde{\sigma}_{\text{DR}}\rangle+\langle\sigma_{\text{int}}\rangle$ in Eq. (12). In fact, for $1/q^2>1$ a "window" resonance is carved out of the nonresonant background. Furthermore, the largest effects are on the weakest lines [see Eq. (6)], which turn out to be orders of magnitude weaker than the nonresonant background (σ_{RR}) and would make their detection by experiment extremely difficult; see, for example, the case of the *KLL* resonances of Ar^{16+} as discussed by Jacobs *et al.* [18]. The same results [Eqs. (11)–(13)] hold for the case of multiple-photon continua. The case of $\gamma_f\approx\Gamma$ is uninteresting since, from Eq. (6) and Bethe-Salpeter [27], we have $1/q^2\ll 1$ and so

$$\langle\sigma\rangle\approx\sigma_{\text{RR}}+\langle\sigma_{\text{DR}}\rangle\ . \tag{14}$$

Next, we consider $\Gamma\ll\gamma_f$, initially for a single-photon continuum; then, from Eq. (8) we have

$$\langle\sigma\rangle\approx\sigma_{\text{RR}}+\langle\sigma_{\text{DR}}\rangle\left[1-\frac{\gamma_f^2}{\Gamma^2 q_f^2}\right] \tag{15}$$

and, again, the incorrect effect would be deduced on retaining only $\langle\tilde{\sigma}_{\text{DR}}\rangle$ since

$$\langle\tilde{\sigma}_{\text{DR}}\rangle\approx\langle\sigma_{\text{DR}}\rangle\left[1+\frac{\gamma_f^2}{\Gamma^2 q_f^2}\right]\ . \tag{16}$$

The largest interference effects are now seen for the weakest Γ, but it turns out (see Sec. III) that the size of the effect and the strength of the line can be of the same order of magnitude as the nonresonant background (σ_{RR}). This is a much more favorable arrangement for measurement than $\gamma_f\ll\Gamma$. The expression for multiple-photon continua (and $\Gamma\ll\sum_f\gamma_f$) is less simple, viz.,

$$\langle \sigma \rangle \approx \sigma_{RR} + \langle \sigma_{DR} \rangle \times \left\{ 1 - \frac{1}{q_f^2 \Gamma^2} \left[\sum_{f'} \gamma_{f'} \right]^2 + \frac{1}{q_f^2 \Gamma^2} \left[\sum_{f'} \left[1 - \frac{q_f}{q_{f'}} \right] \gamma_{f'} \right]^2 \right\} . \quad (17)$$

Thus, if all the q_f are comparable we have a straightforward generalization of Eq. (16), but the final levels f' with $q_{f'} < q_f$ tend to reduce the size of the effect through the third term in the large braces of Eq. (17). The net result for each *KLL* resonance for U^{90+} is presented in Sec. III.

The above formalism assumes an isolated-resonance approximation, but this is not a particular drawback to the study of interference effects since they are strongest for low-lying resonances, and these tend to be well separated. An alternative approach is the close-coupling approximation for photoionization [28] (and, through detailed balance, photorecombination), which automatically takes into account overlapping resonances and interference between the direct and indirect processes. Furthermore, the *R*-matrix approach to photoionization [29] is particularly efficient at generating the resonance structure, and it has been implemented in a number of general computer codes using nonrelativistic [30], Breit-Pauli [31] and Dirac-Coulomb [32] Hamiltonians. However, it uses the first-order perturbation theory [29] expression for the photoionization cross section, which is only valid for the resonant contribution in the weak-field limit ($\gamma \ll \Gamma$), e.g., low-lying resonances in low-charge ions. For an isolated resonance and a single-electron continuum, but multiple-photon continua, it can be shown (see, e.g., Ref. [33]) that the form of the close-coupling photorecombination cross section is the same as that used here, in the weak-field limit [see, e.g., Eqs. (9)–(13)]. It is a nontrivial problem to apply the close-coupling approximation in the strong-field ($\gamma \gg \Gamma$) or intermediate-field ($\gamma \sim \Gamma$) cases. Some progress [34,35] has been made by fitting the resonances to a known functional form and then using the resulting information to evaluate the photorecombination cross section for arbitrary values of γ / Γ, but this approach can only deal with weakly overlapping resonances when $\gamma \lesssim \Gamma$. A practical difficulty also arises with the use of the close-coupling approximation, namely, that of missing resonances. In the weak-field limit, where the close-coupling approximation is valid, the resonant contribution to the photorecombination cross section is proportional to the radiative width, and it is necessary to resolve all resonances down to the radiative width since both "narrow" and "broad" resonances contribute equally (as long as they still satisfy $\gamma \ll \Gamma$). In practice [36], some of the narrow resonances are missed, and this can lead to an underestimate of the resonant contribution [36]. A more elegant solution is to solve the close-coupling equations that treat the photon continua on an equal level with the electron continua, but this approach [37] is less well developed computationally.

III. RESULTS

The unperturbed energy levels, radiative rates, and autoionization rates required by the theory outlined in the previous section were taken from our earlier work [9] on electron capture by U^{90+}. In addition, we now require radiative-recombination cross sections as well. These were calculated using the same approach as before [9], namely, a multiconfiguration Dirac-Fock-Breit approximation. In Table I we compare our unperturbed energy-averaged dielectronic recombination cross sections with our energy-averaged unified photorecombination cross sections, minus the unperturbed radiative-recombination cross section, calculated according to Sec. II [see Eq. (8)]. We see that the difference for some of the transition lines (index nos. 2, 7, and 8) is of the same order of magnitude as the background ($\sim \delta\varepsilon \times 10^{-23}$ cm^2 Ry), and they are not necessarily particularly weak lines. Thus, this case ($\Gamma \ll \gamma_f$) is quite different from that studied by Jacobs *et al.* [18] ($\gamma_f \ll \Gamma$).

The most promising candidate for an observation of the breakdown of the independent-processes approximation in the photorecombination of U^{90+} is the

TABLE I. Photorecombination cross sections for $U^{90+} + e^-$.

Index	Level	Energy (Ry)	$\delta\varepsilon \langle \sigma_{DR} \rangle$ (Mb Ry)	$\delta\varepsilon (\langle \sigma \rangle - \sigma_{RR})$ (Mb Ry)
1	$1s2s^2(1/2)$	4635	2.64[−3]	2.64[−3]
2	$1s2s(1)2\bar{p}(3/2)$	4638	1.64[−4]	7.88[−5]
3	$1s2s(1)2\bar{p}(1/2)$	4640	1.40[−3]	1.39[−3]
4	$1s2s(0)2\bar{p}(1/2)$	4659	4.51[−3]	4.49[−3]
5	$1s2\bar{p}^2(1/2)$	4663	1.29[−5]	9.02[−6]
6	$1s2s(1)2p(5/2)$	4952	0.0	0.0
7	$1s2s(1)2p(3/2)$	4960	2.35[−5]	−7.80[−5]
8	$1s2s(1)2p(1/2)$	4966	1.75[−5]	−1.46[−5]
9	$1s2\bar{p}(1)2p(5/2)$	4971	1.78[−3]	1.73[−3]
10	$1s2\bar{p}(0)2p(3/2)$	4973	6.15[−4]	5.99[−4]
11	$1s2s(0)2p(3/2)$	4976	2.18[−3]	2.14[−3]
12	$1s2\bar{p}(1)2p(1/2)$	4976	9.42[−3]	9.42[−5]
13	$1s2\bar{p}(1)2p(3/2)$	4982	8.23[−4]	7.62[−4]
14	$1s2p^2(2)(5/2)$	5290	1.04[−3]	1.02[−3]
15	$1s2p^2(2)(3/2)$	5297	1.02[−4]	9.86[−5]
16	$1s2p^2(0)(1/2)$	5300	2.03[−4]	1.97[−4]

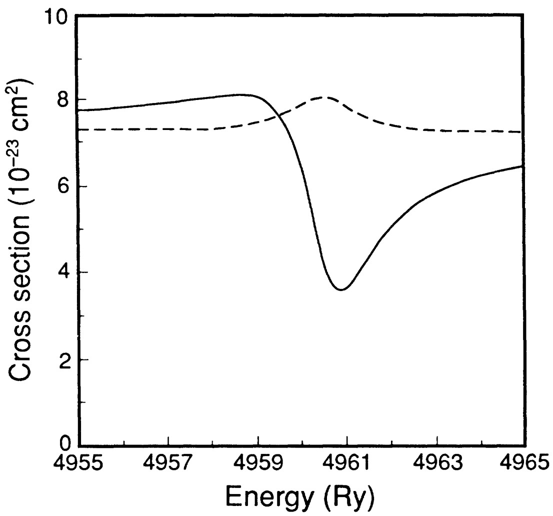

FIG. 1. Photorecombination cross sections for U^{90+} ($1s^2$) to U^{89+} ($1s^22s$) in the vicinity of the $1s2s(1)2p(3/2)$ resonance. Solid line, unified cross section; dashed line, independent-processes cross section; both this work.

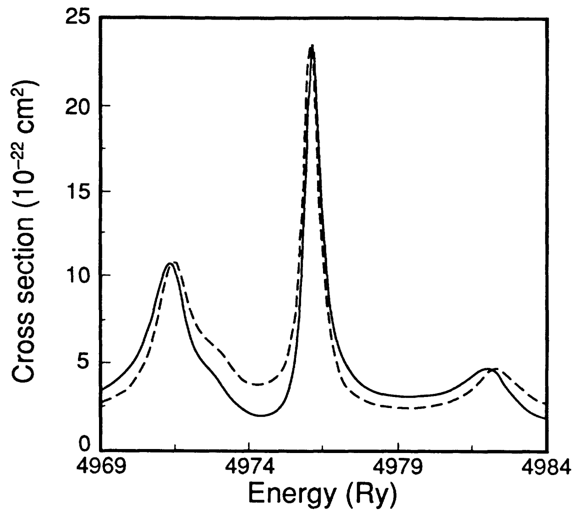

FIG. 2. Photorecombination cross sections for U^{90+} to the L-shell of U^{89+} in the vicinity of the resonances of the $1s2s2p$ and $1s2\bar{p}2p$ subconfigurations; as in Fig. 1.

$1s^2+e^- \rightarrow 1s^22s+h\nu$ line in the presence of the $1s2s(1)2p(3/2)$ resonance (index no. 7), which is well isolated from any nearby resonances with the same $J\pi$. We present our results for the unperturbed and perturbed Lorentzians [see Eq. (1)] in Fig. 1. We see that the unified photorecombination cross section is suppressed by a factor of 2, on resonance, compared to the independent-processes cross section.

As noted previously [9] (see also Table I), the KLL resonances fall into three energy-ordered groups. Our results for the unperturbed and perturbed Lorentzian spectra for the middle group of resonances (due to the $1s2s2p$ and $1s2\bar{p}2p$ subconfigurations) are shown in Fig. 2, the asymmetry due to the finite q value is quite noticeable. There is less difference for the low- and high-energy groups. We note that, in general, the strong resonances are well isolated from each other. The worst case is for the levels with index nos. 10 and 13, which have a separation of 9.5 Ry and widths of about 1.8 Ry, each. If we convolute our KLL unified photorecombination cross sections with the Compton profile for the hydrogen molecule, we find that the middle peak is only 5.5% smaller than our independent-processes results; while the lower- and higher-energy peaks are only reduced by about 2%. This size of effect is too small to have been seen in the Bevalac experiment [4]. However, the results that we have presented here (e.g., Fig. 1) should be a stimulus to experimentalists involved with heavy-ion storage rings [25], the super-EBIT [26], and high-resolution x-ray spectroscopy [24].

IV. SUMMARY

We have calculated unified photorecombination cross sections and independent-processes photorecombination cross sections for U^{90+} in the vicinity of the KLL resonances. Our use of the isolated-resonance approximation appears to be valid. The magnitude of the interference effect between the direct and indirect processes, relative to the direct one, is much stronger for this case where radiation damping dominates over autoionization than found previously [18] for the reverse case. We have found that the photorecombination line $1s^2+e^- \rightarrow 1s^22s+h\nu$ in the presence of the $1s2s(1)2p(3/2)$ resonance shows a particularly strong interference effect and should be of interest to any recombination experiment attempting to observe the breakdown of the independent-processes approximation.

ACKNOWLEDGMENT

This work was supported by the Office of Fusion Energy, U.S. Department of Energy, under Contract No. DE-FG05-ER53217 with Auburn University.

[1] L. H. Andersen and J. Bolko, Phys. Rev. A **42**, 1184 (1990).
[2] L. H. Anderson, J. Bolko, and P. Kvistgaard, Phys. Rev. A **41**, 1293 (1990).
[3] G. Kilgus, J. Berger, P. Blatt, M. Grieser, D. Habs, B. Hochadel, E. Jaeschke, D. Krämer, R. Neumann, G. Neureither, R. Stokstad, E. Szmola, and A. Wolf, Phys. Rev. Lett. **64**, 737 (1990).
[4] W. G. Graham, K. H. Berkner, E. M. Bernstein, M. W. Clark, B. Feinberg, M. A. McMahan, T. J. Morgan, W. Rathburn, A. S. Schlachter, and J. A. Tanis, Phys. Rev. Lett. **65**, 2773 (1990).
[5] R. E. Marrs, P. Beiersdorfer, C. L. Bennett, M. H. Chen, D. A. Knapp, M. A. Levine, K. J. Reed, M. B. Schneider, and J. H. Scofield, J. Phys. (Paris) Colloq. **50**, C1-445 (1989).
[6] N. R. Badnell, M. S. Pindzola, and D. C. Griffin, Phys. Rev. A **41**, 3422 (1990).
[7] D. C. Griffin, M. S. Pindzola, and P. Krylstedt, Phys. Rev. A **40**, 6699 (1989).

[8] M. S. Pindzola, N. R. Badnell, and D. C. Griffin, Phys. Rev. A **42**, 282 (1990).
[9] M. S. Pindzola and N. R. Badnell, Phys. Rev. A **42**, 6529 (1990).
[10] Y. Hahn and B. Bellantone, Phys. Rev. A **40**, 6117 (1989).
[11] P. C. W. Davies and M. J. Seaton, J. Phys. B **2**, 757 (1969).
[12] R. H. Bell and M. J. Seaton, J. Phys. B **18**, 1589 (1985).
[13] Y. Hahn, Adv. At. Mol. Phys. **21**, 123 (1985).
[14] L. Armstrong, C. E. Theodosiou, and M. J. Wall, Phys. Rev. A **18**, 2538 (1978).
[15] S. L. Haan and J. Cooper, Phys. Rev. A **28**, 3349 (1983).
[16] G. Alber, J. Cooper, and A. R. P. Rau, Phys. Rev. A **30**, 2845 (1984).
[17] V. L. Jacobs, Phys. Rev. A **31**, 383 (1985).
[18] V. L. Jacobs, J. E. Rogerson, M. H. Chen, and R. D. Cowan, Phys. Rev. A **32**, 3382 (1985).
[19] V. L. Jacobs, J. Cooper, and S. L. Haan, Phys. Rev. A **36**, 1093 (1987).
[20] S. L. Haan and V. L. Jacobs, Phys. Rev. A **40**, 80 (1989).
[21] K. J. LaGattuta, Phys. Rev. A **36**, 4662 (1987).
[22] K. J. LaGattuta, Phys. Rev. A **38**, 1820 (1988).
[23] K. J. LaGattuta, Phys. Rev. A **40**, 558 (1989).
[24] P. Beiersdorfer, R. E. Marrs, J. R. Henderson, D. A. Knapp, M. A. Levine, D. B. Platt, M. B. Schneider, D. A. Vogel, and K. L. Wong, Rev. Sci. Instrum. **61**, 2338 (1990).
[25] Proceedings of the Workshop on Highly Charged Ions: New Physics and Advance Techniques, Berkeley, 1989 [Nucl. Instrum. Methods B **43**, 265 (1989)].
[26] B. M. Penetrante, J. N. Bardsley, M. A. Levine, D. A. Knapp, and R. E. Marrs, Phys. Rev. A **43**, 4873 (1991).
[27] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Systems* (Plenum, New York, 1977).
[28] R. J. W. Henry and L. Lipsky, Phys. Rev. **153**, 51 (1967).
[29] P. G. Burke and W. D. Robb, Adv. At. Mol. Phys. **11**, 143 (1975).
[30] K. A. Berrington, P. G. Burke, M. LeDourneuf, W. D. Robb, K. T. Taylor, and Vo Ky Lan, Comput. Phys. Commun. **14**, 367 (1978).
[31] N. S. Scott and K. T. Taylor, Comput. Phys. Commun. **25**, 347 (1982).
[32] P. H. Norrington and I. P. Grant, J. Phys. B **20**, 4869 (1987).
[33] M. J. Seaton and P. J. Storey, *Atomic Processes and Applications,* edited by P. G. Burke and B. L. Moiseiwitsch (North-Holland, Amsterdam, 1976).
[34] K. Sakimoto, J. Phys. B **24**, 3049 (1991).
[35] K. Sakimoto, M. Terao, and K. A. Berrington, Phys. Rev. A **42**, 291 (1990).
[36] S. N. Nahar and A. K. Pradhan, Phys. Rev. A **44**, 2935 (1991).
[37] A. Giusti-Suzor and P. Zoller, Phys. Rev. A **36**, 5178 (1987).