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Calculation of Photoabsorption Processes in Helium

A. Dalgarno, H. Doyle, and M. Oppenheimer
Harvard College Observatory and Smithsonian Astrophysical Observatory, Cambridge, Massachusetts 02138
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The cross section for photoionization is expressed as an integral over the dipole response function in a form that yields a unified procedure for calculating the background and the resonance contributions. Application is made to absorption by triplet metastable helium.

We have developed a simple procedure for the unified prediction of the background and resonance contributions to photoabsorption processes in atoms and molecules. The procedure is based upon an interchange theorem satisfied by the transition matrix element involved. If the transition from an initial state Φ_i to a final continuum state $\psi_f^+(E)$ of energy E is caused by an operator D, the matrix element that we need to evaluate is $\langle\Phi_i|D|\psi_f^+(E)\rangle$. We may write the outgoing final-state wave function $\psi_f^+(E)$ in terms of the Green's function G_E of the total system in the form

$$\psi_f^+(E)=(1+G_EV)\Phi(E),$$

where $\Phi(E)$ is the scattering solution in the absence of the interaction potential V between the separated systems. Then

$$\begin{aligned}\langle\Phi_i|D|\psi_f^+(E)\rangle&=\langle\Phi_i|D|\Phi(E)\rangle+\langle\Phi_iDG_E|V|\Phi(E)\rangle\\&=\langle\Phi(E)|D|\Phi_i\rangle^*+\langle\Phi(E)|V|G_ED\Phi_i\rangle^*.\end{aligned}$$

The function $G_ED\Phi_i=\chi_i(E)$ is the linear response function of the system Φ_i for the perturbation D, and it may be calculated approximately in various ways. For the dipole moment operator, the corresponding $\chi_i(E)$ occurs in the evaluation of the frequency-dependent dipole polarizability, which has been carried through for simple systems using time-dependent Hartree-Fock theory or the random-phase approximation and by variational configuration interaction methods.

We have used the latter method to explore the photoionization continuum and the resonance structures in the helium sequence associated with the photoabsorption processes

$$\begin{aligned}\mathrm{He}(1s2s)\,{}^{1,3}S+h\nu&\to\mathrm{He}(2s2p)\,{}^{1,3}P\\&\to\mathrm{He}^+(1s)\,{}^2S+e,\\\mathrm{He}(1s^2)\,{}^1S+h\nu&\to\mathrm{He}(2s2p)\,{}^1P\\&\to\mathrm{He}^+(1s)\,{}^2S+e.\end{aligned}$$

The function χ_i was represented by a discrete set of real Hylleraas correlated functions which were subjected to a unitary transformation to produce orthogonal eigenvectors θ_n such that $\langle\theta_n|H|\theta_n'\rangle=\epsilon_n\delta_{nn}'$. Then the matrix element is approximated by

$$\langle\Phi_i|D|\psi_f^+\rangle\sim\langle\Phi_i|D|\Phi(E)\rangle+\sum_{n=1}^{N}\frac{\langle\Phi_i|D|\theta_n\rangle\langle\theta_n|V|\Phi(E)\rangle}{E-\epsilon_n+i\Gamma_n/2},\qquad(1)$$

Γ_n being the width $2\pi|\langle\Phi(E)|V|\theta_n\rangle|^2\rho(E)$. One basis function θ_n is so chosen that it accurately represents the resonance configuration and the remaining $N-1$ functions provide an approximation to the continuous background. The procedure can be viewed alternatively as an extension of the root-stabilization method, the formal basis of the calculation deriving from the Feshbach construction of the optical potential. The second

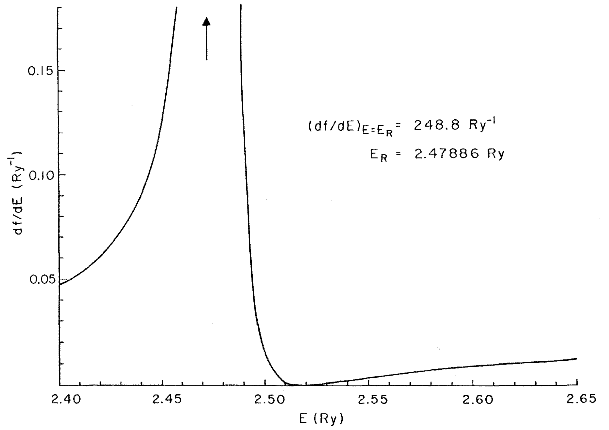

FIG. 1. The oscillator strength df/dE (Ry^{-1}) versus electron energy E (Ry) for He 2 $^3S \rightarrow sp\ ^3P$ around the $2s2p\ ^3P$ resonance.

term in (1) contains an approximate representation of the Green's function G_E.

At $E \approx \epsilon_n$, where ϵ_n is not a real resonance energy, Eq. (1) necessarily gives a spurious result. However, we may eliminate the function θ_n from the basis set, and then calculate the dipole matrix element at $E = \epsilon_n$. The energy E is separated from the remaining eigenvalues, and we obtain accurate values for the oscillator strength at ϵ_n. The positions of the eigenvalues can be moved by continuously varying the nonlinear parameters of the basis set within a physically reasonable range, and we may obtain accurate oscillator strengths throughout the background energy region. Where poles belonging to two different basis sets occur near the same energy, the calculated oscillator strengths generally agreed to within 2%. We also varied the number of functions in the set and verified that convergence was achieved, agreement being generally better than 1% for forty and fifty basis functions.

Results for the photoionization of metastable helium in the $1s2s\ ^3S$ state near the $2s2p\ ^3P$ resonance obtained using the basis set of Dalgarno and Drake[1] are shown in Fig. 1. They illustrate the interference between the background and the resonance configuration. The background oscillator strength $df/dE|_0 = 0.0203\ \mathrm{Ry}^{-1}$, while the Fano q value is -110.7; the width and position are $\Gamma = 0.0102$ eV and $E_{\mathrm{res}} = 2.4789$ Ry.[1] The values are in good agreement with close-coupling calculations[2] $df/dE|_0 = 0.0217\ \mathrm{Ry}^{-1}$, $q = -106.6$, $\Gamma = 0.0106$ eV, $E_{\mathrm{res}} = 2.481$ Ry.

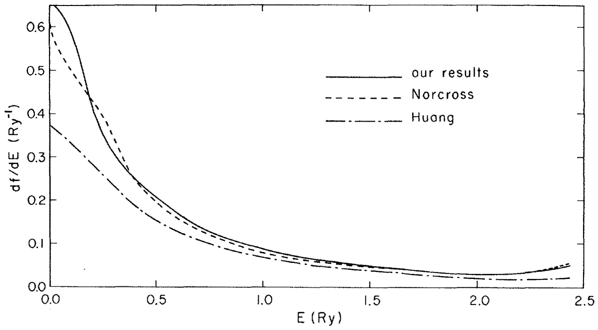

FIG. 2. The background oscillator strength df/dE (Ry^{-1}) versus electron energy E (Ry) for He 2 $^3S \rightarrow sp\ ^3P$.

The oscillator strengths for the 2 ^3S background are given in Fig. 2 along with previous calculations using the screened Born approximation[3] and the close-coupling method.[2] The screened Born approximation is the first term of Eq. (1), and it accounts for about half the oscillator strength at threshold. The figure shows that our oscillator strengths for 2 ^3S are significantly greater than the close-coupling values near threshold, but agree well above $E = 0.6$ Ry. In both the $1s^2\ ^1S$ and the $1s2s\ ^1S$ cases, the correction to the Born approximation is less than 15% and the background oscillator strengths for 1 ^1S and 2 ^1S are in harmony with previous work.[2,4] Our parameters $df/dE|_0 = 8.64 \times 10^{-3}\ \mathrm{Ry}^{-1}$, $q = 88.6$, $\Gamma = 0.0367$ eV, and $E_{\mathrm{res}} = 2.6146$ Ry for the 2 ^1S resonance configuration should be more accurate than the close-coupling values, for which the width is apparently too large. The accurate calculation of the $1s^2\ ^1S \rightarrow 2s2p\ ^1P$ resonance oscillator strength presents greater difficulties. Because it is a two-electron transition, the oscillator strength for 1 ^1S (unlike 2 ^1S) is extremely sensitive to the number of singly excited configurations in the expansion of the Green's function.

We shall present further discussion and calculations by this method in a forthcoming paper.

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