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Many-electron approach to atomic photoionization: Rydberg series of resonances and partial photoionization cross sections in helium, around the $n=2$ threshold

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Transition probabilities involving the continuous spectrum of many-electron atoms exhibit a variety of resonance phenomena and deviations from independent-particle model predictions. We present a general theory of photoionization which (i) utilizes function spaces for initial and final states which are state specific and are based on numerical as well as on analytic basis sets. The valence, Rydberg, scattering, and virtual orbitals are optimized by different methods. (ii) In addition, our theory is formulated within a configuration-interaction, reaction-matrix, and multichannel quantum-defect approach suitable for the treatment of the continuous and of the discrete Rydberg spectrum via the use of numerical frozen-core Hartree-Fock channel orbitals. In this work we have calculated the cross sections for the simultaneous photoionization and photoexcitation to the $n=2$ shell of He$^+$. Our results for the ratio of the cross section at the degenerate He$^+$ thresholds $2s$ and $2p$ agree with those of published close-coupling calculations and disagree with those of a many-body perturbation theory. We also compute values for energies very close to and at the threshold, previously not available. The autoionization widths and quantum defects of the Rydberg series $2snp$, $2pnd$, and $2pns$ are also in agreement with previous close-coupling calculations.

I. INTRODUCTION

The photoabsorption process yields information which may sometimes be interpreted in terms of simple single-particle models and sometimes may not. The second case is the most interesting one because it reveals details of the electronic structure and dynamics and requires the application of advanced many-electron methods. As an application of the K-matrix theory of the continuous and discrete spectrum presented in Ref. 1 and of the state-specific theory for the calculation of excited-state wave functions,[2-4] we have studied the phenomenon of photoionization of He with simultaneous excitation to the He$^+$ $n=2$ shell, in the energy region at, above, and below threshold.

The choice of this phenomenon was based on the following considerations.

(1) The complexities which are present in the problem (Rydberg series of resonances, threshold degeneracies, etc.) constitute a sufficient numerical test of our K-matrix, configuration interaction in the continuum (CIC) theory.[1] Since the ground state can be computed very accurately, the overall accuracy of the calculation depends on the rigor and the numerical efficiency of our CIC method.

(2) In recent years a number of experiments and theories have been applied to this process.[5-11] The strong qualitative disagreement between the results of a perturbation[7] and a close-coupling theory[5,6] close to threshold presented a worthwhile opportunity for applying our theory. Our results agree with the close-coupling results of Refs. 5 and 6.

The results which are presented in this paper are based on the theory of Ref. 1 whose main characteristics are the following.

(a) It uses the multichannel K-matrix formalism and unifies in a self-consistent manner the configuration-interaction treatment in the discrete and in the continuous spectrum.

(b) In the case of the Coulomb potential, this has led to the derivation of multichannel quantum-defect theory (MQDT) without the use of irregular Coulomb or unbound functions. Instead, numerical zeroth-order Hartree-Fock functions are allowed to be considered and no separation of configuration space into inner and outer space is necessary. The fundamental questions of smoothness and analyticity are solved via appropriate transformation of the expansion coefficients rather than from consideration of the properties of the Coulomb functions, as in the standard MQDT.[12]

(c) The inclusion of closed channels in the unified K-matrix theory and the development of smoothing techniques, which allow for *interpolation* of information on the energy axis, whether in the continuous or the discrete spectrum. This constitutes a significant advance over the *extrapolation* procedures from the continuous to the discrete spectrum proposed in Seaton's MQDT.[12]

In the following sections we develop our proposal for the many-electron treatment of photoionization. It is applicable to atoms of arbitrary electronic structure and complements other advanced theories (e.g., Refs. 13 and 14). The theory and methods for the solution of the multichannel continuous spectrum apply equally well to the treatment of autoionization.[15]

II. MANY-ELECTRON APPROACH TO ATOMIC PHOTOIONIZATION

Before presenting the specific developments and applications for this work, we outline our many-electron approach to the problem of photoabsorption. As regards discrete-continuum transitions, we have already presented results from simplified photoionization calculations on the F atom,[16] (which predict a broad resonance about 22 eV above the ground state with a width of 3.1 eV), as well as from the accurate treatment of the phenomenon of radiative autoionization in simple systems, where there is no interchannel coupling.[17]

As in the case of photoabsorption in the discrete spectrum, for which one of the present authors, Theodorakopoulos and Beck have developed a many-electron approach for transition probabilities in atoms and molecules—either at the property-oriented FOTOS (first-order theory of oscillator strengths) level (e.g., Refs. 3 and 18–20) or at the highly correlated level (e.g., Refs. 21 and 22)—our theory is state specific. This implies that we put emphasis on the separate and optimized calculation of the wave functions of initial and final symmetry-adapted states.

For the initial square-integrable function we make the separation

$$\psi=\phi_{\mathrm{FS}}+\phi_{\mathrm{corr}} \cdot \tag{1}$$

ϕ_{FS} is the Fermi-sea zeroth-order function obtained numerically at the multiconfigurational Hartree-Fock (MCHF) level[2,3,23] and ϕ_{corr} represents the remaining correlation.[2]

The final scattering-state wave function is composed, in general, of the following parts: (1) Rydberg and continuum channel orbitals obtained in the term-dependent, single-configuration, frozen-core Hartree-Fock approximation. In this basis set, Brillouin-type intrachannel mixing is zero.[24] (2) The $(N-1)$-electron, correlated core to which the previously obtained channel orbitals are coupled. (3) N-electron valence- or inner-shell excited configurations in the discrete or in the continuous spectrum. (4) N-electron correlations vectors whose radial functions are kept orthogonal to the open-channel core orbitals. For this class of functions, although optimization of nonlinear exponents within a phase-shift variational bound method[25] can be adopted in principle, practical considerations lead us to suggest that, given choices (1)—(3), fixed expansions are sufficient.

The mixing of the various parts can be carried out, in principle, within a CIC approach.[1] Nevertheless, reliable inclusion of electron correlation in the discrete and in the continuous spectrum presents a formidable problem. Our proposal to this effect includes the following conceptual and computational steps.

(a) Choose the important correlation effects according to the state-specific analyses of electronic structure already in the literature (e.g., Refs. 2–4).

(b) Choose the function spaces outlined above.

(c) Define and use a "Fermi sea in the continuum" concept where the total K matrix is obtained only in the presence of a few important configurations and then the resulting scattering functions are coupled with the fully correlated $(N-1)$-electron core for the calculation of cross sections.

The final step implies that the scattering functions u_{iE} have the form

$$u_{iE}=\left[\sum_k b_k\phi_k^{N-1}\right]W_i(E)\,, \tag{2}$$

where b_k are the CI coefficients of the most important core configurations and W_i are the channel orbitals.

The object of this paper is to present an application of our theory[1] to the calculation of $^1P^\circ$ highly excited state properties of He arising from photoionization plus excitation to the He$^+$ $n=2$ shell. The corresponding doubly excited main configurations are of the type $2sn(\epsilon)p$, $2pn(\epsilon)s$, and $2pn(\epsilon)d$. The mixing of such configurations gives rise to slowly convergent R^1 integrals, which account for the "dipole-potential" contributions whose importance has been predicted and examined in the case of H$^-$.[26] Of course, a full CI theory accounts for multipole couplings automatically. In He, the dipole-potential contributions are small and the choice of the zeroth-order HF orbitals in the Coulomb field of He$^+$ $n=2$ is good. However, if we studied H$^-$, the zeroth-order orbitals to be used in CI would be obtained in the dipole field.

Once the initial- and final-state wave functions are available, one can compute the photoionization cross section. On the other hand, a transformation of the K matrix[1] permits the calculation of the energies, the reduced widths, and the mixing coefficients of Rydberg series of resonances independently of the calculation of the cross section. This is done as follows.

In a basis where the submatrix $\mathscr{K}^{oo}$ is diagonal, the reaction matrix on the energy shell takes the form[1,27]

$$\overline{\mathscr{K}}^{(r)}=U^{\dagger}I\overline{\mathscr{K}}^{oc}\left[\frac{1}{\pi}\tan[\pi(\nu+\mu)]-\overline{\mathscr{K}}^{cc}-\overline{\mathscr{F}}^{cc}\right]^{-1}\overline{\mathscr{K}}^{co}IU\,, \tag{3}$$

where U is the unitary matrix that diagonalizes

$$I=[1+(\pi\overline{\mathscr{K}}^{oo})^2]^{-1/2} \tag{4}$$

and

$$\overline{\mathscr{F}}^{cc}=-\pi^2\overline{\mathscr{K}}^{co}I\overline{\mathscr{K}}^{oo}I\overline{\mathscr{K}}^{oc}\,. \tag{5}$$

The indices o and c refer to the open and closed channels, respectively. The overbars refer to the smooth K matrices. The quantity $\tan[\pi(\nu+\mu)]$ is a diagonal matrix containing the zeroth-order quantum defects μ and the parameter ν which is related to the total energy by $E=-1/2\nu^2$. The μ which appears in the expression of the reaction matrix incorporates the information provided by the use of frozen-core Hartree-Fock orbitals as zeroth-order functions rather than hydrogenic ones on which the standard MQDT (Ref. 12) is based. The resonances occur at the solutions of the equation

$$(\overline{\mathscr{K}}^{cc}+\overline{\mathscr{F}}^{cc})c=\frac{1}{\pi}\tan[\pi(\nu+\mu)]c \tag{6}$$

with reduced widths

$$\gamma=c\overline{\mathscr{K}}^{co}IU \tag{7}$$

and mixing coefficients c.

III. NUMERICAL APPLICATION

A. Photoionization of He to the He^+ $n=2$ threshold

We have calculated the partial photoionization cross sections for the process

$$\mathrm{He}(1s^2)+h\nu \rightarrow \mathrm{He}^+(2s,2p)+e^-$$

for the energy range above the $n=2$ threshold $E(\mathrm{a.u.})=[0,1.5]$.

The ground state of He was constructed using the $1s^2$ Hartree-Fock (HF) solution as zeroth-order wave function, to which correlation vectors were added[2] until the energy reached the value of -2.9032 a.u. The exact nonrelativistic energy is[28] -2.9037 a.u.

The continuum-state functions were expressed in terms of configurations of type $1sn(\epsilon)p$, $2ns(\epsilon)p$, $2pn(\epsilon)s$, and $2pn(\epsilon)d$. Fixed-core HF functions were used, thus eliminating intrachannel coupling. Rydberg orbitals with principal quantum number up to nine were explicitly included in the expansion. Orbital energies ran up to 3.0 a.u. for the $1s$ continuum and up to 1.5 a.u. for the $2s$ and $2p$ continuum (the two thresholds differ by 1.5 a.u.). The calculation of the reaction matrix off the energy shell—and hence of the final wave function—presents certain numerical difficulties which we shall discuss below.

The first difficulty has to do with the evaluation of the principal-value integrals. It was bypassed by Altick and Moore[29] through the application of a form of Filon's quadrature.[30] More specifically, the interaction as well as the K matrices are fitted to polynomials and the principal-value integrals are performed analytically. The upper part of the Rydberg series is treated as an appendage to the continuum. In this way, the integral Lippmann-Schwinger equations are reduced to algebraic ones, which are then solved by standard methods.

The second difficulty has to do with the numerical evaluation of interchannel matrix elements which contain terms of the form

$$\int_R^\infty dr \frac{1}{r^{k+1}} W_{k_1}(r) W_{k_2}(r), \quad k>0 .$$

These terms result from $R^k(\phi_{c_1},W_{k_1};\phi_{c_2},W_{k_2})$ integrals where ϕ_{c_1},ϕ_{c_2} are core orbitals. They are evaluated by the asymptotic series method of Belling.[31] Specifically, the orbitals of the continuous spectrum are calculated numerically up to the radius R. At this radius the core orbitals are practically zero. For larger values of r, the WKB approximation is used.[32] Hence, the R^k integrals are calculated numerically up to this radius, while the remaining terms of the above form are evaluated by the summation of asymptotic series.

For some energies, the summation of the asymptotic series is impossible. In this case we split the integral from R to ∞ into two parts. The one goes from R to R_1 and the other from R_1 to ∞. R_1 is chosen so that the asymptotic series in the interval $[R_1,\infty)$ can be summed. The first part is calculated numerically by again employing the WKB approximation for the scattering orbital.

The third difficulty results again from integrals of this type. Specifically, these are responsible for the nonsmoothness of the matrix elements of the interactions and of K whenever the wave numbers k_1 and k_2 are equal. That is, the matrix element as a function of k_1 lies on a different curve for $k_1<k_2$ than for the values of $k_1>k_2$. The two curves meet at the point $k_1=k_2$ so that the matrix element is continuous but its derivative has a discontinuity at this point. This behavior must be taken into account when we perform the interpolations and the integrations, as it is not permissible to interpolate along points of nonsmoothness.

Having computed the K matrix, we evaluate the dipole matrix elements. Filon's quadrature is employed again for the evaluation of the principal-value integrals. In the end, the dipole matrix elements are transformed to the ones corresponding to final state functions fulfilling the ingoing boundary conditions. This is obtained through the transformation

$$\psi_E^- = \psi_E (1 - i\pi\mathcal{K})^{-1} , \tag{8}$$

where $\mathcal{K}$ is the reaction matrix on the energy shell.[1]

The partial cross sections are given by the formula

$$\sigma_i(\omega) = \frac{4\pi\alpha}{3}\hbar\omega \, |\langle\psi_0|D|\psi_{iE}^-\rangle|^2 , \tag{9}$$

where $\hbar\omega=E-E_0$ and α is the fine-structure constant.

The resulting partial photoionization cross sections are shown in Fig. 1 together with those calculated by Jacobs and Burke.[6] Their calculations start at a value of 0.05 a.u. above the $2s$ threshold. Both sets of curves show the same behavior, although ours are slightly transposed to

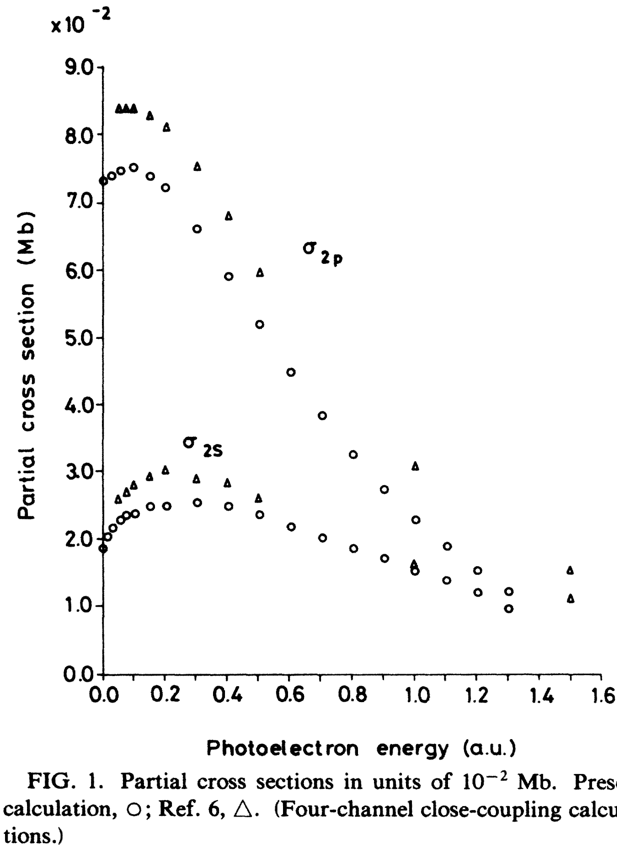

FIG. 1. Partial cross sections in units of 10^{-2} Mb. Present calculation, ○; Ref. 6, △. (Four-channel close-coupling calculations.)

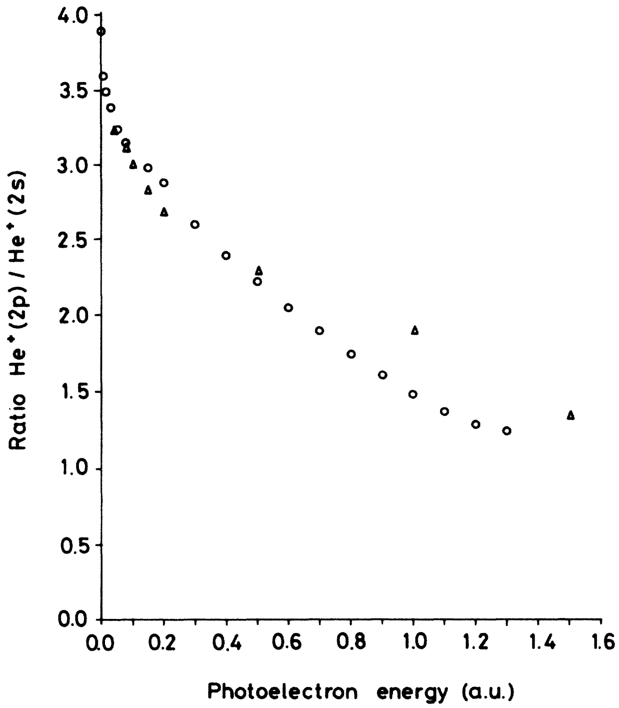

FIG. 2. Ratio of He^+ ions in $2p$ and $2s$ states. Present calculation, ○; Ref. 6, △. (Four-channel close-coupling calculations.) More recent calculations (Ref. 5) (nine-channel R-matrix calculations) do not alter this curve significantly.

lower values. Nevertheless, the curves of the ratio coincide for values close to the threshold, as shown in Fig. 2. Our calculations give a ratio equal to 3.9 at the threshold. We note that our curve exhibits a sharp increase at very small energies. This energy region is not included in the calculation of Refs. 5 and 6. We believe that the threshold value is an even more sensitive test of the flexibility of theory to account for short-range correlation effects and the influence of the long-range $2s$-$2p$ dipole coupling.[26]

B. Calculation of quantum defects, reduced widths, and mixing coefficients of the three Rydberg series of resonances below the $n=2$ threshold

In this section we employ the results of Ref. 1 in order to calculate the K matrix for the energy -0.005 a.u. below the $2s$ threshold. The first step is to consider the high-energy part of a Rydberg series as an appendage to the continuum. We then proceed to solve the eigenvalue problem of Eq. (6) and obtain the quantum defects and the mixing coefficients. The reduced widths are given by Eq. (7).

These quantities are calculated from a reaction matrix which is computed at *negative energies*. This is in contrast to the usual applications of MQDT (Ref. 12) where this matrix is a result of extrapolation from energies above threshold. (See also Fano's papers, Ref. 33.) In order to avoid the generalized eigenvalue problem present in Eq. (6) and to take the advantage of the degeneracy of the $2s$ and $2p$ thresholds, we perform the transformation from the fixed-core HF basis functions to Coulombic ones,

$$-\pi K^{\text{Coul}} = [\sin\delta - \pi(\cos\delta)K^{\text{HF}}] \times [\cos\delta + \pi(\sin\delta)K^{\text{HF}}]^{-1}\,, \qquad (10)$$

where δ is a diagonal matrix containing the zeroth-order phase shift of the $1s$ channel and the zeroth-order quantum defects of the three Rydberg series multiplied by π.

We close by noting that the theory and its numerical implementation is capable of treating accurately situations with higher thresholds (e.g., $n=3$) and with the presence of spectroscopic configurations of the type $3s3p$, $3p3d$, etc. Ojha's[11] recent analysis suggests that closed channels corresponding to such configurations affect the width of the *pd* series by an order of magnitude.

As can be seen from Table I, our results are very close to the values quoted by Bely[34] and Burke and McVicar.[35] The widths given are the reduced ones. The numbers quoted by Bely[35] are the result of extrapolation from values of the K matrix above threshold. In order to cope with the nonsmoothness caused by the dipole terms he uses the appropriate basis functions accounting for this effect. His numbers refer to states with $n=10$ and below. Burke and McVicar[36] obtain their result by direct numerical integration of the close-coupling equations. They reach levels up to $n=5$, as this method is progressively more difficult for higher values of n.

Finally, Table II gives the values of the mixing coefficients. The numbers in parentheses refer to the same quantities at the series limit, i.e., on the threshold. We observe that the coefficients of the series assigned $(+)$ by Cooper *et al.*[36] remain almost constant, a result also found by Burke *et al.*[37]

TABLE I. Quantum defects and reduced widths of the three Rydberg series. The assignment of Ref. 36 is given in parentheses.

Rydberg series	Present results μ	Present results Γ (a.u.)	Bely (Ref. 34) μ	Bely (Ref. 34) Γ (a.u.)	Burke and McVicar (Ref. 35) μ	Burke and McVicar (Ref. 35) Γ (a.u.)
$2pnd$	0.676	2.38×10^{-6}	0.674	1.6×10^{-6}	0.674	2.31×10^{-6}
$2snp$ $(-)$	0.740	6.2×10^{-5}	0.725	6.75×10^{-5}	0.725	6.60×10^{-5}
$2pns$ $(+)$	0.132	8.3×10^{-3}	0.134	8.25×10^{-3}	0.150	7.93×10^{-3}

TABLE II. Mixing coefficients of the three Rydberg series at the energy −0.005 a.u. below the $N=2$ threshold. The same quantities at the threshold energy are given in parentheses.

zeroth order corr	$2snp$		$2pns$		$2pnd$	
$2pnd$	−0.26	(−0.43)	0.60	(0.63)	0.76	(0.65)
$2snp\ (-)$	0.86	(0.78)	−0.22	(−0.10)	0.46	(0.61)
$2pns\ (+)$	0.44	(0.45)	0.77	(0.77)	−0.45	(−0.45)

IV. SYNOPSIS

Given that the bound-state many-electron problem is by now understood well, the calculation of transition probabilities for processes such as photoionization and autoionization requires the knowledge of correlated scattering states.

In this paper we have implemented the theory of Ref. 1 where we have generalized the configuration interaction in the continuum formalism of Fano and Prats[38] and Ramaker and Schrader[27] to include closed channels and have developed it into a practical approach applicable to problems of resonance-resonance interactions and of perturbed or unperturbed Rydberg series of resonances. Compared to the previously applied approaches of coupled integro-differential equations and MQDT,[12] this theory, through the introduction of smooth wave functions and reaction matrices which are related to MQDT,[1] has the advantage of replacing extrapolation with interpolation, a more accurate numerical procedure. Furthermore, through the use of nonorthonormal basis functions, it permits an economical (state-specific) description of the various parts comprising the final state wave function. No separation of configuration space into inner and outer regions is necessary.

The applicability of the present theory has been demonstrated by the successful study of the subtle phenomenon of the simultaneous photoionization and photoexcitation processes in He.[5–11]

Finally, we point out that the structure of the formalism allows similar applications to arbitrary systems with many electrons and a multiconfigurational zeroth-order description.

Note added in proof. A recent paper by Salomonson *et al.*[39] presents theoretical results on the same problem which are in agreement with ours.

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