Excitation of He$^+$ by electron impact*

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A five-state close-coupling approximation in which $1s$, $2s$, and $2p$ eigenstates and $\overline{3s}$ and $\overline{3p}$ pseudostates of He$^+$ are included in the expansion, is used to calculate $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation of He$^+$ by electron impact in the intermediate energy range up to about three times ionization threshold energy. Pseudostates are chosen to maximize their overlap with bound states and low-lying continuum states of the same symmetry. Present results for $1s \rightarrow 2s$ excitation provide a link between accurate low- and high-energy results and agree with experiment above 70 eV.

I. INTRODUCTION

The poor agreement between experiment and theory for excitation of He$^+$ $1s \rightarrow 2s$ has been reviewed recently by Seaton.[1] Cross sections of Burke and Taylor[2] in a $1s$-$2s$-$2p$ plus 20-correlation-term calculation are a factor of 1.8 larger near threshold than the measurements by Dolder and Peart,[3] who performed a crossed-beam experiment, the results of which are normalized to high-energy theory.

We employ a five-state close-coupling approximation in which we retain the exact He$^+$ bound states $1s$, $2s$, and $2p$ and two pseudostates, $\overline{3s}$ and $\overline{3p}$. Calculations are performed in an intermediate energy range from 61.2 to 136 eV (the excitation threshold for $1s \rightarrow 2s$ and $1s \rightarrow 2p$ is at 40.8 eV).

The purpose of a pseudostate is to allow in some average manner for the infinity of bound and continuum states that are neglected in a truncated close-coupling expansion. If only $1s$, $2s$, and $2p$ are included in a close-coupling approximation, the truncation of the expansion results in an overestimate of inelastic cross sections. The coupling to higher states is important since these states contribute to correlation effects and to absorptive effects, i.e., loss of flux through higher excitation channels. Pseudostates used in low-energy scattering have been chosen so that long-range dipole polarization (correlation) effects are taken into account.[4] We propose to construct pseudostates for an intermediate-energy region so that overlap with omitted eigenstates is optimized.

II. PSEUDOSTATE

The reduced normalized radial functions for the pseudostates are chosen to have the form

$$P_{\overline{3s}}(r) = (a_1 + a_2 r + a_3 r^2) r e^{-\alpha_s r},$$

$$P_{\overline{3p}}(r) = (b_1 + b_2 r) r^2 e^{-\alpha_p r}.$$

The energy of the pseudostate $\overline{nl}$ is defined as

$$\epsilon_{\overline{nl}} = \langle \overline{nl} | \hat{H}_0 | \overline{nl} \rangle,$$

where $\hat{H}_0$ is the Hamiltonian for an isolated He$^+$ ion, and henceforth we define $\epsilon = \epsilon_{\overline{3s}} = \epsilon_{\overline{3p}}$.

The pseudostates are constructed orthonormal to lower states of the same symmetry, and we impose the constraint that the $\overline{3s}$ and $\overline{3p}$ states have the same threshold energy. With the above conditions, the only adjustable variable is the range parameter α_s or α_p, which can be related to $\epsilon_{\overline{nl}}$.
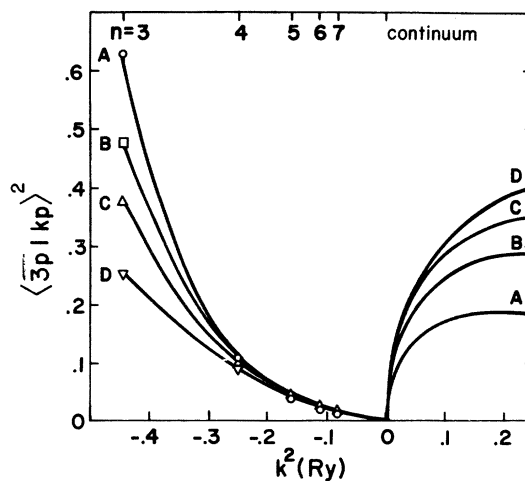

FIG. 1. Square of overlap of p pseudostates and p eigenstates versus eigenstate energy. Curve A, $\epsilon = -0.2$ Ry; B, $\epsilon = 0.0$ Ry; C, $\epsilon = 0.2$ Ry; D, $\epsilon = 0.6$ Ry.
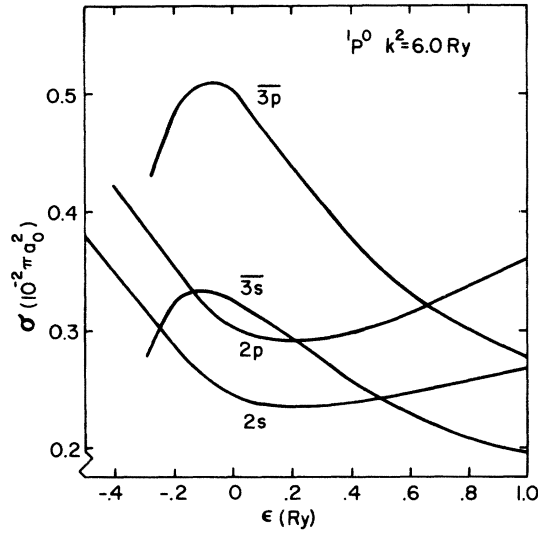
FIG. 2. $^1P^o$ partial-wave cross section versus pseudo-state energy for incident energy $k^2 = 6.0$ Ry. Curves $2s$, $2p$, $\overline{3s}$, and $\overline{3p}$ represent excitation to these states from the $1s$ state of He⁺.

We wish to construct pseudostates for an inter-mediate-energy range so that overlap with omitted eigenstates is optimized. We note that ionization and $1s \to 3p$ excitation are of comparable importance in the energy range under consideration. Further, for ionization at incident energies up to three times ionization threshold, the ejected electron will have energy of no more than a few eV. Thus, we choose a pseudostate which has optimum overlap with bound states and low-lying continuum states.
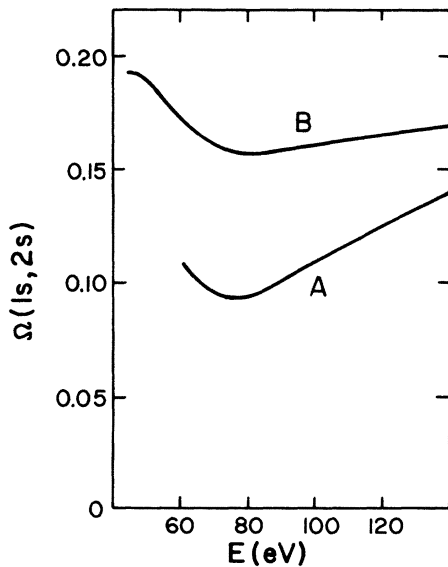

FIG. 3. Collision strength $\Omega (1s,2s)$ for He⁺ at inter-mediate energies. Curve A, present calculation; curve B, $1s$-$2s$-$2p$ close coupling of Burke et al. (Ref. 5).
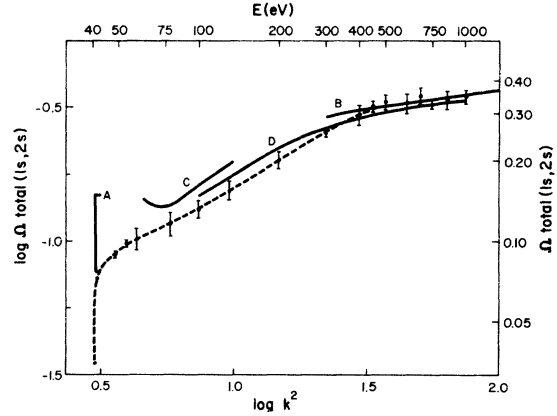

FIG. 4. Total collision strength for He⁺ $1s$-$2s$ on a logarithmic scale. Calculations are represented by (A) Burke and Taylor (Ref. 2); (B) Seaton (Ref. 1); (C) present results; (D) Bransden and Noble (Ref. 6). The filled circles are the measurements of Dolder and Peart (Ref. 3) normalized at high energies.

In Fig. 1, the squares of the overlap of a p pseudostate with p eigenstates of He⁺ are given versus eigenstate energy. Curves A, B, C, and D represent results for p pseudostates which have threshold energies of -0.2, 0.0, 0.2 and 0.6 Ry, respectively. For negative eigenenergies, only discrete values are possible, and the continuous curves serve to guide the eye. We note that overlap with low-lying continuum states is significantly larger for threshold energies in the range 0.2–1.0 Ry than the corresponding overlap for a pseudo-state which has threshold energy $\epsilon \leq 0$. Thus, we choose a pseudostate with threshold energy 0.2 Ry as our optimum representation.

In Fig. 2, cross sections are given as a function of pseudostate threshold energy ϵ for a dominant partial wave $^1P^o$ at an incident electron energy of
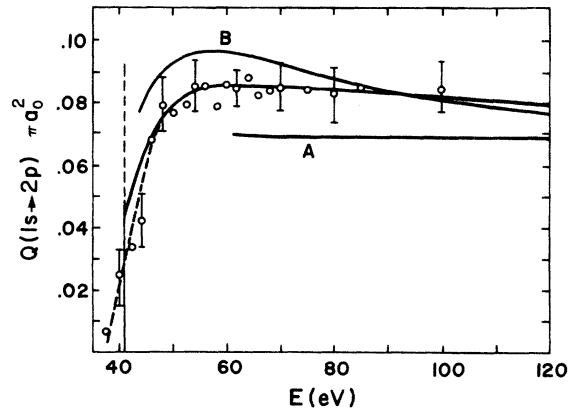

FIG. 5. Excitation cross section $Q(1s \to 2p)$ for He⁺ at intermediate energies. Curve A, present calculation; B, $1s$-$2s$-$2p$ close coupling (Ref. 5); ○, Dashchenko et al. (Ref. 7).

81.6 eV. Curves labeled $2s$, $2p$, $\overline{3s}$, and $\overline{3p}$ represent the partial excitation cross sections from the ground $1s$ state. Maximum absorptive effects (i.e., a maximum in $1s \rightarrow \overline{3s}$ and $1s \rightarrow \overline{3p}$) occur at $\epsilon = -0.1$ Ry, and a minimum occurs in $1s \rightarrow 2s$ and $1s \rightarrow 2p$ at $\epsilon = 0.2$ Ry. Further, the partial-wave $1s \rightarrow 2s$ cross section is fairly insensitive to the pseudostate energy over a broad range, i.e., within 10% of minimum value for $0.0 \leq \epsilon \leq 0.6$ Ry.

No variational principle exists presently to show that the optimum representation for this functional form of a pseudostate is given at the extremum of either a maximum cross section for pseudostate excitation or a minimum cross section for $1s \rightarrow 2s$ or $1s \rightarrow 2p$ excitation. However, we note that our choice for pseudostate parameters which gives optimum overlap with bound states and low-lying continuum states coincides with the minimum in the partial-wave cross section for $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation.

III. RESULTS

Collision strength versus energy for the direct $1s \rightarrow 2s$ excitation of He^+ by electron impact is given in Fig. 3. Present pseudostate results (curve A) are compared with the $1s$-$2s$-$2p$ approximation results of Burke et al.[5] (curve B). Inclusion of pseudostates which emphasize absorptive effects causes a significant decrease in the excitation cross section in the intermediate-energy range considered. We are unable to calculate collision strengths below 60 eV since we would encounter spurious effects due to the nonphysical pseudostate threshold at 57.1 eV.

Figure 4 shows results for the total collision strength $\Omega_{total}(1s, 2s)$ on a logarithmic scale for all energies between threshold and 1000 eV. Curve A represents the calculations of Burke and Taylor.[2] Curve B gives the high-energy results of Seaton[1] which include contributions from excitation to higher states followed by radiative cascade. Curve C gives our present pseudostate calculations. Recent second-order potential-model cal-

culations of Bransden and Noble[6] are given as curve D. Since this method involves a closure approximation, it is valid only above 100 eV. Both curves C and D include cascade contributions calculated with the formula of Seaton.[1] The measurements of Dolder and Peart[3] are give by filled circles. The measured cross section includes contributions from cascade, and the seven experimental points with $E > 450$ eV are in good agreement with the slope of the theory curve. The present calculation is in reasonable agreement with experiment for energies above 75 eV.

Cross section versus energy for the direct $1s \rightarrow 2p$ excitation of He^+ by electron impact is given in Fig. 5. Present pseudostate results (curve A) are compared with the $1s$-$2s$-$2p$ approximation results of Burke et al.[5] (curve B). Measurements by Dashchenko et al.[7] are given as open circles. The experimental results are normalized to a Coulomb-Born II calculation at 217 eV with the additional assumption that cascade contributions are negligible. The solid curve through the experimental points represents the normalized cross section after allowance has been made for the energy distribution of the incident electrons. Inclusion of pseudostates which emphasize absorptive effects causes a 25% decrease in the excitation cross section at 60 eV, and their influence decreases to 14% at 120 eV.

A consistent pattern is emerging from the theoretical calculations, and the present calculation provides an important link between the accurate low-energy and high-energy results. The present method, suggested for the choice of the pseudostate in the intermediate-energy range, appears successful in this application even with the very limited number of pseudostates employed.

ACKNOWLEDGMENTS

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