Optical-potential study of electron-impact excitation of He^+

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(Received 21 January 1991)

Excitation of He^+ by electron impact is studied in the energy range 4.4–14.71 Ry using a six-state close-coupling expansion together with an optical potential representing higher bound and continuum states. An 18-state basis set emphasizing long-range pseudostates is used for calculations below 100 eV, and a 17-state basis containing more compact pseudostates is used at higher energies. Total excitation cross sections for transitions from the 1s, 2s, and 2p states are also calculated using the optical theorem. A detailed comparison is made with a recent 15-state close-coupling calculation and with experiment, where possible. In general, inclusion of the optical potential significantly reduces the excitation cross sections.

I. INTRODUCTION

Calculations of electron-impact excitation of He^+ have thus far made use of either the close-coupling approach or some high-energy approximation, whose validity criteria do not cover an energy region roughly bounded by the ionization energy from below and two or three times that energy from above.[1–3] There is a particular need for theoretical data in the intermediate-energy region because of a rather curious relationship between theory and experiment in the case of the $1s \rightarrow 2s$ transitions. As demonstrated by Seaton,[1] the relative measurements of Dolder and Peart[4] are in agreement with both high- and low-energy calculation when appropriately normalized, but the low-energy normalization yields cross sections higher by a factor of 1.8. There have been two calculations at intermediate energies dealing with the excitation of the $n=2$ state only, which used two[5] and three[6] additional pseudostates, apart from the exact $n=1$ and 2 states. In this work, we study the transitions among the $n=1$, 2, and 3 states by means of a six-state close-coupling approximation supplemented by an optical potential constructed from a large pseudostate basis set, including positive energy states representing the continuum. The use of an optical potential makes it possible to determine total cross sections for excitation plus ionization; the cross section for ionization can be roughly es-

TABLE I. Parameters and energies (Ry) of basis II. Energies E_i^l refer to the combination defined by Eq. (1).

n_i^l	ζ_i^l	E_i^l
	$l=0$	
0	1.0	−1.0
0	0.5	−0.25
1	0.5	−0.111 11
1	0.87	−0.059 75
0	1.4	0.013 34
0	0.333 33	0.257 38
1	0.333 33	1.218 77
2	0.333 33	7.802 52
	$l=1$	
1	1.0	−0.25
1	0.5	−0.111 11
2	1.0	−0.050 48
1	0.8	0.108 79
1	0.333 33	0.691 67
2	0.333 33	3.448 70
	$l=2$	
2	1.0	−0.111 11
3	1.0	0.107 22
2	0.333 33	1.318 34

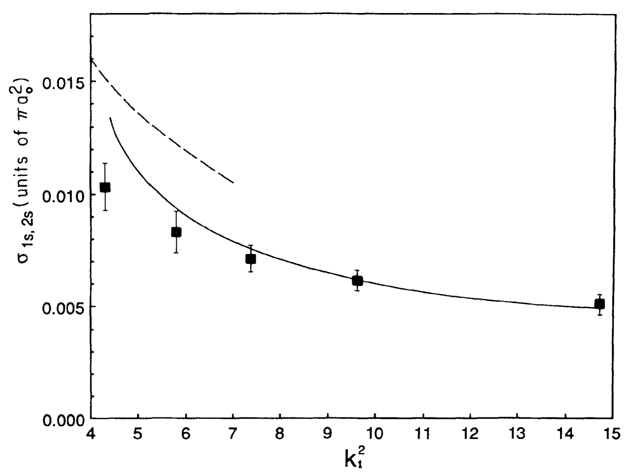

FIG. 1. Cross section for the $1s \rightarrow 2s$ transition. Solid line, present calculation; dashed line, Ref. 8; solid squares, experiment (Ref. 11).

TABLE II. Excitation cross sections (units of πa_0^2).

d Transition	k_1^2 (Ry) 4.4	4.8	5.2	5.6	6.0	7.35	11.03	14.71
$1s \to 2s$	0.0134	0.0117	0.0112	0.0095	0.0086	0.0079	0.0056	0.0049
$1s \to 2p$	0.0597	0.0619	0.0633	0.0650	0.0655	0.0679	0.0626	0.0584
$1s \to 3s$	0.004 10	0.003 3	0.002 8	0.002 1	0.001 8	0.001 4	0.000 99	0.000 89
$1s \to 3p$	0.011 4	0.009 9	0.009 7	0.009 9	0.010 8	0.011 2	0.009 9	0.009 4
$1s \to 3d$	0.005 2	0.005 1	0.003 9	0.003 6	0.003 0	0.002 3	0.001 5	0.001 1
$1s \to n > 1$	0.131	0.138	0.148	0.149	0.148	0.165	0.171	0.157
$2s \to 3s$	0.447	0.392	0.354	0.314	0.284	0.221	0.130	0.097 5
$2s \to 3p$	0.872	0.887	0.926	0.999	1.029	0.901	0.741	0.598
$2s \to 3d$	1.065	1.079	1.039	0.970	0.919	0.758	0.490	0.343
$2s \to n > 2$	4.63	4.54	4.42	4.02	3.95	2.95	2.04	1.45
$2p \to 3s$	0.092 2	0.066 8	0.060 2	0.056 5	0.053 4	0.040 3	0.026 7	0.020 7
$2p \to 3p$	0.578	0.464	0.404	0.372	0.329	0.253	0.146	0.107
$2p \to 3d$	1.963	2.068	2.122	2.246	2.194	1.979	1.547	1.220
$2p \to n > 2$	5.62	5.32	5.26	4.99	4.77	3.53	2.51	1.52

timated by subtraction. The only published work dealing with transitions to the $n = 3$ states seems to be that of Hummer and Storey,[7] who used a six-state close-coupling method which is clearly inadequate for this purpose. Quite recently, Aggarwal *et al.*[8] have completed a 15-state close-coupling calculation using the R-matrix method. The results of this calculation will be compared with ours in this paper. Astrophysical applications of He^+ excitation calculations are discussed in Ref. 7.

II. CALCULATION

The optical-potential formalism we employ has been described in detail earlier.[9,10] On the basis of previous experience,[11] we have used two different pseudostate basis sets for calculations in the lower (< 100 eV) and higher-energy regions. The former (basis I), was exactly the same 18-state basis used in Ref. 9, with appropriate changes to take account of the change in the nuclear charge. This basis was originally constructed for use in the resonance region between the $n = 2$ and 3 states and has extended orbitals appropriate for the low-energy region. The other (basis II), was essentially an extension of basis II of Ref. 11 to include the $n = 3$ states exactly, and had 17 states in all. Expressing the jth pseudostate of angular momentum l as

$$R_{jl}(r) = \sum_i C_{ji}^l r^{n_i^l} e^{-\zeta_i^l r} , \qquad (1)$$

the parameters used in basis II are given in Table I. This

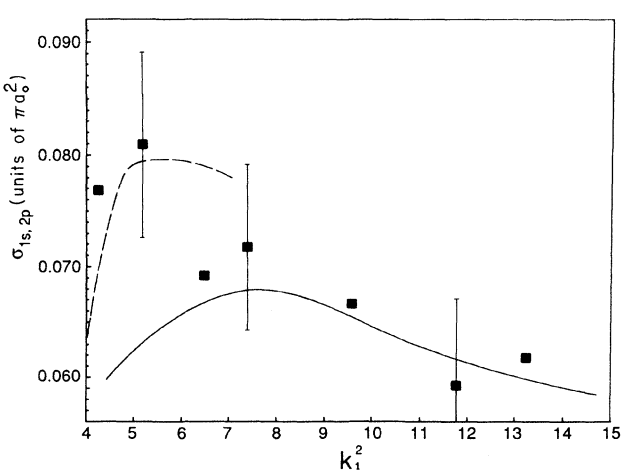

FIG. 2. Cross sections for the $1s \to 2p$ transition. Solid and dashed lines as for Fig. 1. Solid squares, experiment (Ref. 12).

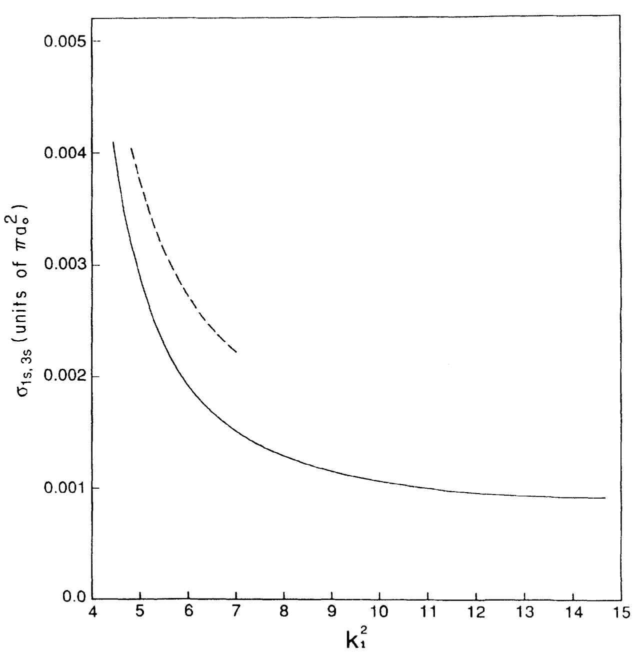

FIG. 3. Similar to Fig. 1, for the $1s \to 3s$ transition.

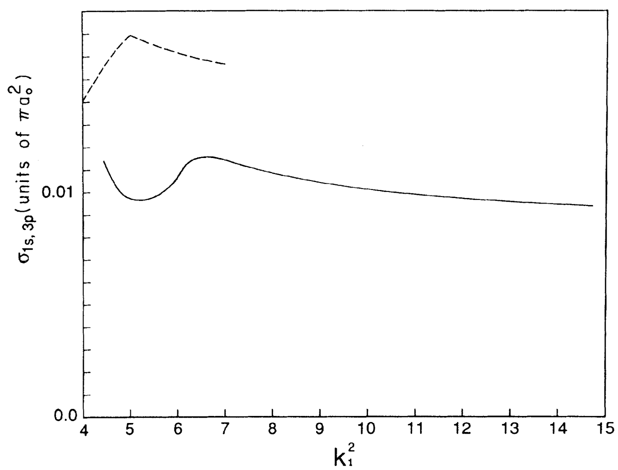

FIG. 4. Similar to Fig. 1, for the $1s \rightarrow 3p$ transition.

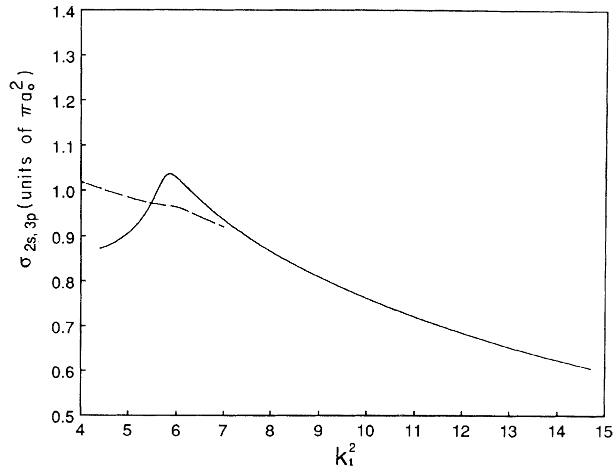

FIG. 7. Similar to Fig. 1, for the $2s \rightarrow 3p$ transition.

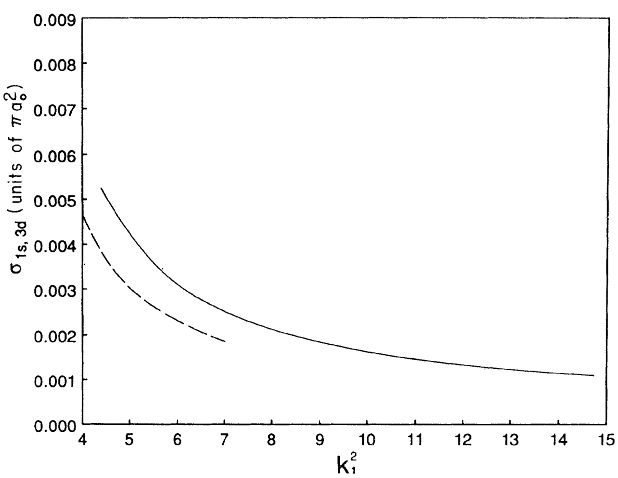

FIG. 5. Similar to Fig. 1, for the $1s \rightarrow 3d$ transition.

basis emphasizes short-range pseudostates describing higher-energy interactions between the incident and bound electrons.

Calculations proceeded as described in Ref. 10, with the $n = 1$, 2, and 3 states in the P space and the rest in the Q space. The maximum value of the total angular momentum L for which computations were carried out was $L_{\max} = 25$, except at 200 eV, where $L_{\max}$ was 32. Further, exchange was neglected for $L > 20$. Beyond $L_{\max}$, the partial excitation cross sections were extrapolated assuming[10] that for a given transition, $\sigma_{L+1}/\sigma_L = f(k^2)$. (The reasonableness of this was established by a few additional calculations.) The contribution from this region was significant only for the allowed transitions between the excited states at high energies, the maximum being 34% for $2s \rightarrow 3p$ at $k_1^2 = 14.71$ Ry.

As in the case of electron-hydrogen scattering, we can use the optical theorem[9,10] to estimate the total cross sec-

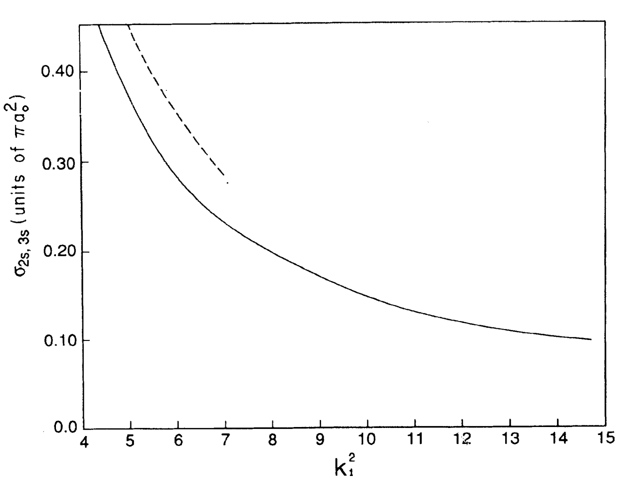

FIG. 6. Similar to Fig. 1, for the $2s \rightarrow 3s$ transition.

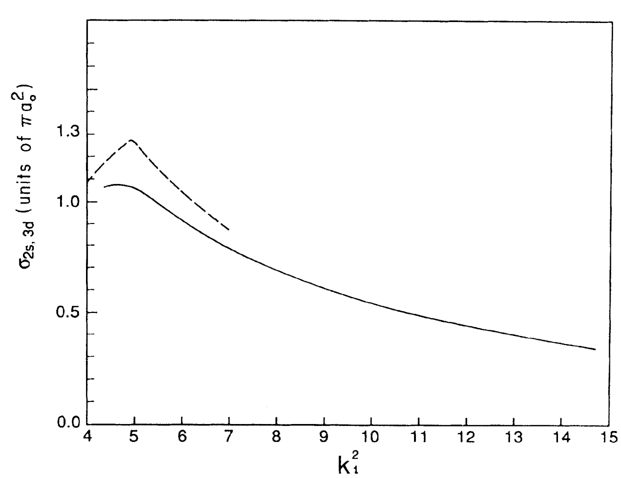

FIG. 8. Similar to Fig. 1, for the $2s \rightarrow 3d$ transition.

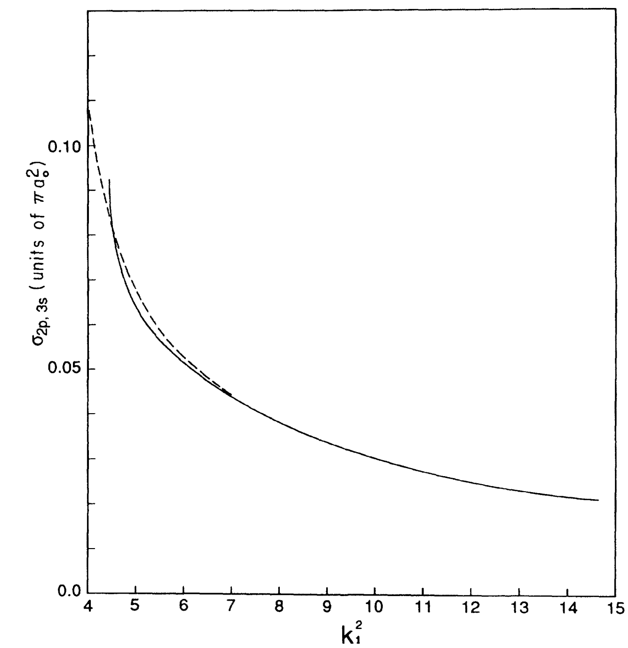

FIG. 9. Similar to Fig. 1, for the $2p \rightarrow 3s$ transition.

tions for all transitions from a given state. However, for He^+, in addition to the transitions $2s \rightleftarrows 2p$, elastic scattering is also divergent and has to be subtracted to yield a finite result. In this paper we report total cross sections for transitions to all higher states from $1s$, $2s$, and $2p$.

III. RESULTS AND DISCUSSION

Table II summarizes the results of our calculations in the energy range $k_1^2=4.4-14.71$ Ry with respect to the ground state of He^+. (For transitions from $n=2$ states this corresponds to $k_2^2=1.4-11.71$.) At $k_1^2=14.71$, the

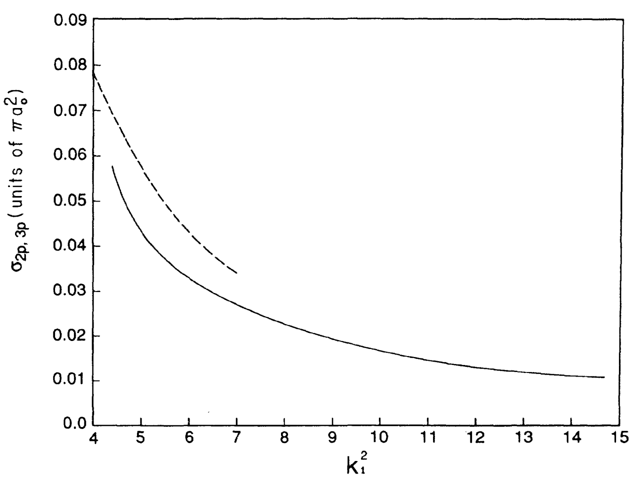

FIG. 10. Similar to Fig. 1, for the $2p \rightarrow 3p$ transition.

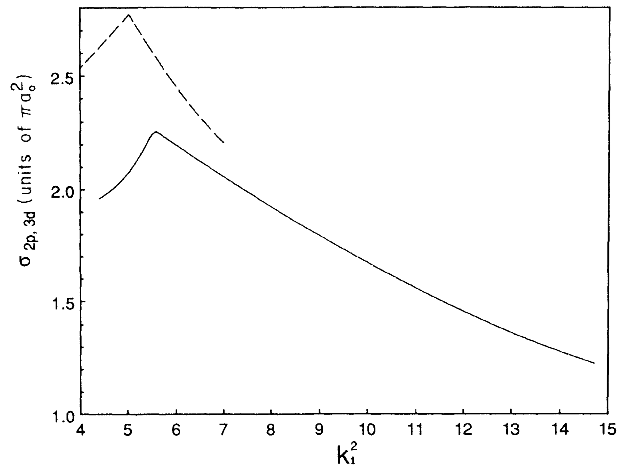

FIG. 11. Similar to Fig. 1, for the $2p \rightarrow 3d$ transition.

second-order potential calculation of Bransden and Noble[12] agrees exactly (to the number of digits published) with ours for the $1s$-$2s$ transition, while their value is higher for the $1s$-$2p$ transition, being 0.067 (units of πa_0^2). As mentioned earlier, the 15-state close-coupling calculations of Aggarwal *et al.*[8] are the best available for comparison in the energy range $k_1^2=4-7$ and their results are displayed along with the present results, in Figs 1–11. In general, since the optical-potential model calculation takes account of the higher bound states as well as the continuum, at least approximately, one would expect the

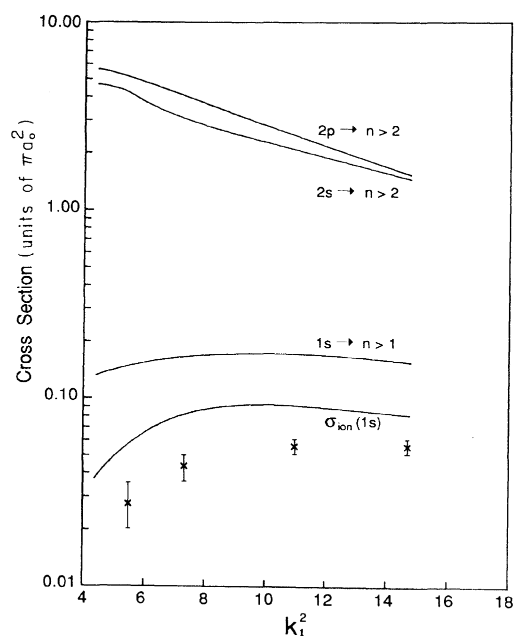

FIG. 12. Total cross sections for excitation from $1s$, $2s$, and $2p$. σ_{ion} $(1s)$ is an estimate of the total cross section for ionization from $1s$.

excitation cross sections to be smaller as compared to a pure close-coupling calculation, especially at energies above the ionization threshold. This is indeed seen to be the case, except for the $1s \rightarrow 3d$ transition (and also the $2s \rightarrow 3p$ in a small energy range). We have verified by a separate six-state close-coupling calculation at $k_1^2=6$ that the above-mentioned cross sections are lower in this case and agree very well with the corresponding benchmark results reported by Aggarwal *et al.*[8] In general, our results are smaller by 25% or more in comparison with those of Ref. 8, $\sigma_{2p\text{-}3s}$ being an exception.

Comparison with experiment is possible only for the $1s \rightarrow 2s,2p$ transitions. We see from Fig. 1 that the experimental data of Dolder and Peart[4] (normalized at high energy) are in agreement with the present results at 100 eV and above, but fall below them at lower energies. This discrepancy, *vis-à-vis* accurate low-energy calculations, has been discussed in some detail by Seaton.[1] Since our results join smoothly with the close-coupling results at $k_1^2=4$, only improved measurements are likely to produce agreement between theory and experiment in this energy region.

In the case of the $1s$-$2p$ transition (Fig. 2), the relative cross sections measured by Dashchenko *et al.*[13] have been renormalized to our calculated value at 200 eV. Again, there is reasonable agreement between theory and experiment above $k_1^2=6$ Ry; however, the dispersion in the experimental data is quite substantial.

Finally, in Fig. 12 are presented the total cross sections for excitation from the $1s$, $2s$, and $2p$ states, calculated as described in the Introduction. Also presented are total "ionization" cross sections σ_{ion} for $\text{He}^+(1s)$, estimated by subtracting the cross sections for the $1s \rightarrow n=2,3$ transitions. The experimental data are from Ref. 14. σ_{ion} provides an upper bound on the ionization cross section at all energies and a reasonable estimate at sufficiently high energies. In the case of hydrogen,[10] for example, σ_{ion} at 100 eV is 0.747 (units of πa_0^2) as compared to the experimental[15] value of 0.614. However, it is clear from Fig. 12 that close agreement with experiment may be expected for He^+ only at energies well above 200 eV.

ACKNOWLEDGMENTS

This work was supported in part by the National Science Foundation under Grant No. PHY 88 20507. We are indebted to Dr. K. M. Aggarwal for useful discussions and numerical data on his R-matrix calculations.

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