Excitation of Be^{+} by electron impact

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Calculations of the collision strength for excitation of the $2p$ state of Be^{+} are performed at incident energies of 2, 5, and 8 Ry. A modified five-state close-coupling expansion is used in which three pseudostates $\overline{3s}$, $\overline{3p}$, and $\overline{3d}$ are retained in addition to target states $2s$ and $2p$. Pseudostates are chosen so that, for a given incident electron energy, there is a minimum in the dominant partial-wave collision strength with respect to variation of the range parameter. Collision strengths are obtained which lie a few percent closer to the measurements of Taylor, Phaneuf, and Dunn than do the five-state calculations of Hayes *et al.*

The two major limiting factors on the accuracy achieved by a close-coupling approximation are the number of states included in the close-coupling expansion and the choice of ionic states to be used in the expansion.

A close-coupling expansion which is limited to the initial and final state of the ion is expected to be accurate for optical excitation cross sections at energies well above threshold since coupling to all other states is weak compared with the strong coupling of the initial and final states. The high-energy part of the optical excitation cross section[1] is proportional to $f/\Delta E$, where f is the ionic oscillator strength and ΔE is the energy splitting between the initial and final states. At low and intermediate energies, the cross section[2] is more sensitive to the polarizability of the ground state which is proportional to $f/(\Delta E)^2$.

In a recent study on $2s \rightarrow 2p$ excitation in Be^{+} by electron impact, Hayes *et al.*[3] used a variety of calculational techniques, the most sophisticated of which was a five-state close coupling including exchange effects. One check on the convergence of the results with the number of target states included in the expansion was performed at an incident energy of 16.3 eV. They found a reduction in the $2s \rightarrow 2p$ cross section due to the inclusion of the $n=4$ levels in a nonexchange calculation of 2% compared to 10% due to inclusion of $n=3$ levels in a similar nonexchange calculation.

We would like to point out that the apparent convergence of the close-coupling expansion is probably true with respect to inclusion of further bound states. However, the continuum states may be important since they contribute 40% to the oscillator strength sum rule.[4]

Convergence to an incorrect limit may be seen for the radial limit case study by Burke and Mitchell[5] on H. In their Fig. 2, for the $1s$-$2s$ excitation cross section, we note the apparent convergence on including eigenstates $1s$, $2s$ and $3s$ in the close-coupling expansion. However, when pseudostates are employed instead of a $3s$ state,

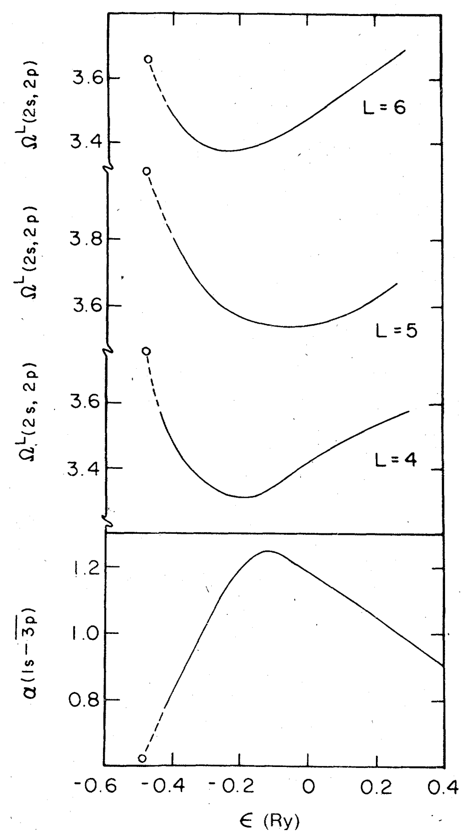

FIG. 1. Partial wave collision strengths $\Omega^L(2s,2p)$ for $L=4$, 5, and 6 vs pseudostate energy for incident electron energy of 2 Ry. Lower curve represents dipole polarizability $\alpha(2s \rightarrow \overline{3p})$ vs ϵ. Open circles represent five-state close-coupling calculations.

convergence occurs to a different (lower) limit.

Previously, on a study of $1s$-$2s$ and $1s$-$2p$ excitation of He^+ by electron impact, Henry and Matese[6] found that with a judicious choice of pseudostate, excitation cross sections could be lowered significantly at intermediate energies. The pseudostates were chosen so as to optimize overlap with the bound states and the low-lying continuum states of the same symmetry, and for this choice of pseudostate, a minimum in the partial wave cross section was found.

For Be^+, we choose three pseudostates $\overline{3s}$, $\overline{3p}$, and $3d$ which are degenerate in energy and are orthogonal to the lower orbitals of the same symmetry. In addition, target states $2s$ and $2p$ are included in the close-coupling expansion. The orbitals $1s$, $2s$, and $2p$ are taken from Weiss.[7] The resulting integro-differential equations are solved by a noniterative integral equation method.[8] High partial waves are calculated in a Coulomb-Bethe approximation.[9]

We have examined the behavior of partial wave contributions to the collision strength $\Omega(2s, 2p)$ at an incident electron energy of 2 Ry for Be^+. The dominant contributions from $L=4$, 5, and 6 are plotted in Fig. 1 as a function of pseudostate threshold energy ϵ(Ry), where $\epsilon=0$ refers to positioning of the pseudostates at the ionization threshold of Be^+. The open circles represent five-state calculations in which $2s$, $2p$, $3s$, $3p$, and $3d$ states are retained. These $n=3$ levels are nondegenerate.

A minimum in each partial wave cross section occurs at approximately $\epsilon=-0.2$ Ry. Thus, a choice of pseudostate with $\epsilon=-0.2$ Ry is made for

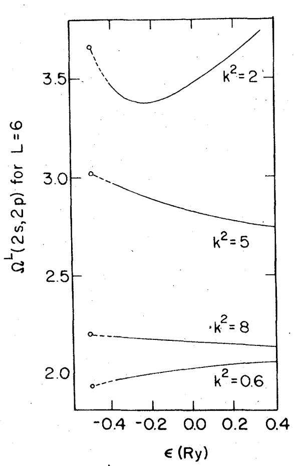

FIG. 2. Partial wave collision strength $\Omega^L(2s, 2p)$ for $L=6$ vs pseudostate energy for incident electron energies of 0.6, 2, 5, and 8 Ry.

all partial waves in which the modified five-state close-coupling calculation is performed. Also shown in Fig. 1 is the contribution to the dipole polarizability of the ground $2s$ state which comes from the pseudo-$\overline{3p}$ state. This quantity maximizes near the same pseudostate threshold energy as that which optimizes the $2s\rightarrow 2p$ cross section. Thus, we note that for this intermediate energy, the contribution to the ground-state dipole polarizability from p states other than $2p$ is a useful measure of the optimum pseudostate which leads to improved values for the collision strength.

Figure 2 gives the $L=6$ partial wave contribution to $\Omega(2s, 2p)$ for incident energies 0.6, 2, 5, and 8 Ry. As the incident energy is increased, we find that the position at which the collision strength optimizes moves to higher pseudostate energies. This reflects the fact that the pseudostate should have greater overlap with continuum states for higher incident energies. Simultaneously, the curves flatten, i.e., become more independent of choice of pseudostate. Again, as the energy increases, the effect of states other than the initial and final state will disappear. We infer that the collision strength optimizes for incident energies of 5 and 8 Ry since two-state close-coupling results have values of 3.01 and 2.20 for $L=6$, respectively. A two-state calculation may be considered equivalent to a five-state close-coupling calculation in which ϵ is infinite. The two-state results are larger than the results given for $\epsilon=0.4$ Ry.

No variational principle exists presently to show that the optimum representation for our functional form of a pseudostate is given at the extremum of a minimum collision strength for $2s\rightarrow 2p$ excitation. However, Fig. 2 exhibits the correct physical qualitative features and so we choose our pseudostate parameters such that for each incident electron energy, there is a minimum in the dominant partial wave collision strength with respect to variation of the range parameter. Then we calculate all partial wave contributions to the collision strength for that incident energy.

Total collision strengths at incident energies of 2.0, 5.0, and 8.0 Ry are compared in Table I with two-state (2*CCX*) and five-state (5*CCX*) close-coupling calculations of Hayes *et al.*[3] Figure 3, in which the product of cross section times energy E is plotted versus $\ln E$, compares the calculations with measurements of Taylor *et al.*[10] The dashed curve represents 2*CCX* results and the solid curve gives the present calculations.

Replacement of target eigenstates $3s$, $3p$, and $3d$ by pseudostates $\overline{3s}$, $\overline{3p}$, and $\overline{3d}$ does not lead to a more accurate calculation at low energy such as 0.6 Ry. The criterion for the pseudostate

TABLE I. Collision strengths $\Omega(2s, 2p)$ for Be^+.

k^2 (Ry)	2.0	5.0	8.0
Hayes *et al.* (Ref. 3) 2*CCX*	39.6	55.1	63.5
Hayes *et al.* (Ref. 3) 5*CCX*	37.9		
Present calculation	36.1	53.0	61.6

parameters of a minimum in the dominant partial wave collision strength suggests that pseudostates similar to $n=3$ eigenstates are optimal choices. However, the restriction of degeneracy for our pseudostates of different symmetry leads to a poorer result than that obtained with eigenstates. At low energies, *if* correlation effects are important, then it will be necessary to include many pseudostates or correlation terms in the close-coupling expansion in order to achieve convergence of the calculations for the collision strength. However, note that the close-coupling results of Hayes *et al.*[3] may have converged in this low-energy region, and the discrepancy between theory and measurements of Taylor *et al.*[10] may be experimental in origin.

At intermediate energies, collision strengths are obtained which lie between the calculations of Hayes *et al.*[3] and measurements of Taylor *et al.*[10] The lower values obtained in the present calculation are due to replacement of the $n=3$ target

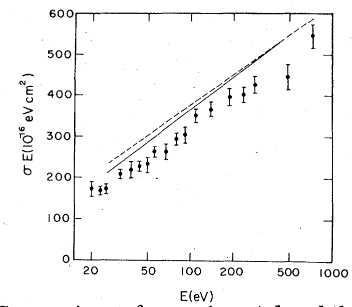

FIG. 3. Comparison of experimental and theoretical values of the product σE for Be^+ $2s$-$2p$ excitation. Dashed curve: Hayes *et al.* (Ref. 3) 2*CCX*; solid curve: present results; solid circles with error bars, Taylor *et al.* (Ref. 10).

eigenstates by pseudostates. We anticipate that a more complete close-coupling expansion would further lower the collision strengths. Our results do not lie within the experimental error bars of Taylor *et al.*, but the results do represent an improvement over conventional close-coupling calculations since the pseudostates allow for absorptive effects. Further, the experimental results include cascade effects, whereas the theoretical results do not.

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