Single and double electron capture in the independent-electron approximation at high velocities

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Cross sections have been computed for single and double electron transfer from the ground state of a helium atom to the ground state of an α particle at high velocities by means of the independent-electron approximation with the Bates–Born version of first-order perturbation theory. Results are in reasonable agreement with experiment for both single and double electron capture.

While experimental data on the capture of more than one electron within a single ion-atom collision are plentiful, theoretical calculations are relatively scarce. In principle calculation of such a many-electron transition is difficult, becoming rapidly more difficult as the number of participating electrons increases. An elementary way to deal with this many-body problem is to use the independent-electron approximation, where what happens to any one electron does not influence any other electron. In this paper we simply test this idea by considering the capture of both electrons from the K shell of helium into the ground state of a colliding α particle.

The independent-electron approximation[1] may be derived using three conditions: (i) the projectile is well localized, i.e., the size of the projectile wavelength is small compared to atomic dimensions; (ii) asymptotically the system may be described by a product of single-particle wave functions, e.g., by using the uncorrelated Hartree-Fock approximation; and (iii) the total scattering wave function evolves as a product wave function during the collision. The first approximation permits us to treat probability amplitudes for scattering from various impact parameters incoherently and is well satisfied by heavy projectiles. The result of (ii) and (iii) is that the probability amplitude, corresponding to the projection of the full scattering wave function onto a particular final state, is a product of single-electron amplitudes. Each such single-electron amplitude may be computed using methods for single-electron transitions. Thus a many-electron amplitude is expressed as a product of single-electron amplitudes. We require only that correlations be small; it is not necessary that the interaction of the projectile with the target be small.

Briefly then, in mathematical form, we begin with the full Hamiltonian

$$H=-\frac{\nabla^2}{2M}+\frac{Z_1Z_2}{R}-\sum_{j=1}^{Z_2}\frac{Z_1}{|\vec{\mathrm{R}}-\vec{\mathrm{r}}_j|}+\sum_{j=1}^{Z_2}\left(-\frac{\nabla_j^2}{2}-\frac{Z_2}{r_j}+\sum_{k>j}|\vec{\mathrm{r}}_k-\vec{\mathrm{r}}_j|^{-1}\right)$$
$$=K+V+H^T,$$

where

$$V=\frac{Z_1Z_2}{R}-\sum_j\frac{Z_1}{|\vec{\mathrm{R}}-\vec{\mathrm{r}}_j|}=\sum_j\frac{Z_1}{R}-\frac{Z_1}{|\vec{\mathrm{R}}-\vec{\mathrm{r}}_j|}=\sum_j V_j.$$

Assumption (ii) corresponds to replacing the $|\vec{\mathrm{r}}_k-\vec{\mathrm{r}}_j|^{-1}$ terms by an effective one-electron potential. Then $H^T\simeq\sum_j H_j^T$ corresponding to $\Phi(r_1\cdots r_n)\simeq\Pi_j\phi_j(r_j)$ and

$$H=K+\sum_j(V_j+H_j^T),$$

so that the evolution operator factors, i.e.,

$$\Omega(t,t_0)=\exp[iH(t-t_0)]=\exp\left[i\left(K+\sum_j V_j+H_j^T\right)(t-t_0)\right]$$
$$=\exp[iK(t-t_0)]\prod_j\exp[i(H_j^T+V_j)(t-t_0)]$$
$$=\prod_j\Omega_j,$$

provided that

$$[K,(H_j^T+V_j)]=[K,V_j]\simeq 0,$$

corresponding to reordering operators in the exponential. Then the probability amplitude factorizes, i.e.,

$$A^{if}=\langle\Psi^i\,|\,\Phi^f\rangle=\prod_j\langle\psi_j^i|\,\phi_j^f\rangle=\prod_j a_j^{if}$$

and

$$\sigma_{if}=2\pi\int_0^\infty|A^{if}|^2BdB=2\pi\int_0^\infty\prod_j|a_j^{if}|^2B\,dB.$$

Of course a method is still required for computing the single-electron probability amplitude a_j^{if}. Here we have chosen to compute a_j^{if} using the method introduced by Bates[2] and by Bassel and Gerjuoy[3] based on first-order perturbation theory for systems with nonorthogonal states. We use this method to compute electron capture at moderately high velocities where two coupled-channel calculations have met with some success in reproducing single-electron-capture cross sections. At high velocities,[4] where back coupling $|S|^2$ and δ contributions are small, the two-coupled-channel calculation reduces[2] to our Bassel and Gerjuoy form for single-electron capture. At 600 keV our single-electron capture cross section lies above the coupled-channel calculation of Tunnell and Lin[5] by about 30%. We attribute most of this difference to backcoupling, since the probability amplitudes are not small, and possibly to our neglecting δ. In this case $|S|^2$ contributes about 10%.

In our calculation we use the experimental value for the binding energy of the atomic electron and use a hydrogenic wave function with a screened nuclear charge of 1.618. The Bassel and Gerjuoy scattering amplitude was evaluated algebraically,[6] then transformed to the probability amplitude a_j^{if}.

Our single $1s$-$1s$ capture results are presented in Fig. 1 along with observed results[7] for capture to all levels. At high velocities, i.e., when the projectile velocity is much greater than the velocity of the orbiting electron, the capture probabilities and cross sections vary[8] as n^{-3}, where n is the principle quantum number of the final state. In this way we estimate[9] that at most 80% of the observed results correspond to $1s$-$1s$ transitions. At lower velocities we expect relatively more capture to excited states. Consequently, our calculations, which omit capture to excited states, should lie further below the total capture data at low velocities than at high velocities. This is consistent with results in Fig. 1. Also, at the lower velocities backcoupling effects and contributions from $|S|^2$ and δ may be significant. Therefore we do not expect our calculations to be valid below 300 keV. Furthermore, it is difficult to estimate contributions from second Born terms[10] at all velocities considered.

Results for double $1s$-$1s$ capture are presented in Fig. 2. Again the agreement with observed data[11] is reasonable. The capture to excited states not included in the theory affects both electrons. Thus the cross section for capture only to the ground state is expected[9] to be below the data for capture of each electron to all projectile levels by 40% or more, rather than 20% or more—depending on velocity, as in the case of single capture. We also note that we have used the single unperturbed binding energy for each electron assuming fast collisions. Increasing the binding energy, corresponding to readjustment of the one electron after capture of the other, lowers our cross sections.

Our results for double-electron capture tend to

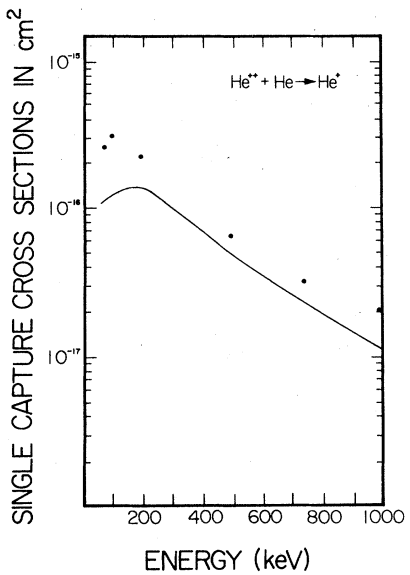

FIG. 1. Single-electron-capture cross sections versus projectile energy. Data taken from Ref. 7. Capture into excited states is not included in the calculation.

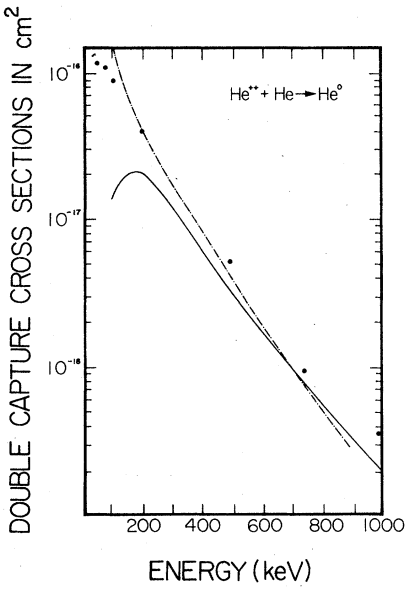

FIG. 2. Double-electron-capture cross sections versus energy. Data taken from Ref. 11. Dot-dash calculation due to Lin, Ref. 12. Capture into excited states is not included in the calculations.

compare favorably at high velocities with other calculations,[12-14] where the full two-electron wave function is approximated using three state, two center atomic expansions. At the lower velocities, however, these coupled-channel calculations fit closer to the data. Since our single and double capture lie beneath the data in a consistent way, we attribute the low-velocity discrepancy to the inadequacy of our single-electron-capture amplitude rather than a breakdown of the independent-electron approximation.

In summary, we have tested a simple way to compute multiple-electron-capture cross sections. Predictions for double-electron capture using the independent-electron approximation are presently accurate within the uncertainty of the theory for amplitudes for capture of a single atomic electron.

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$$\delta = \int_{-\infty}^{t} \frac{h_{ii} - h_{jj} - S_{ij}h_{ji}tS_{ji}h_{ij}}{1 - |S|^2}\, dt$$

corresponds to a perturbation of the atomic eigenenergies.

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