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Double Charge Transfer, $He^{++}+He$†

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A model, previously discussed, in which electron correlation in helium is neglected, is used to calculate the double-charge-transfer cross section for He^{++} in He. The model yields a double-charge-transfer probability which is the product of two single-charge-transfer probabilities. The single-transfer probability is calculated by a Born approximation and a modified Born approximation. The one existing experiment is in satisfactory agreement with the latter.

INTRODUCTION

THE cross section for the double-charge-transfer reaction $He^{++}+He \rightarrow He+He^{++}$ has been measured by Allison[1] and calculated by Gerasimenko and Rosentsveig.[2] Allison's cross-section results were extracted from the equilibrium fractions of charge states of a beam and probably have large errors associated with them. The cross section is for capture into all bound states of He. The calculation[2] is a straightforward first Born approximation for capture into the ground state in which the He wave function was approximated by an uncorrelated product. The agreement between theory and experiment is satisfactory, considering the crudeness of both.

In a recent paper[3] the double-charge-transfer reaction was considered, and it was shown that the usual first Born approximation is a very bad approximation for this reaction and that it should vanish when electron correlation is neglected. The fact that it does not vanish is due to an unphysical lack of orthogonality between the Born approximations for initial and final states so that a "constant potential" causes a transition. A formalism was presented in which the first Born approximation vanished when electron correlation was neglected. It was further shown that the usual first Born approximation gives a high-energy behavior for the cross section $\sigma \propto E^{-7}$. The second Born, which is the first surviving term in the no-correlation model, gives $\sigma \propto E^{-11}$, and correlation contributes a term $\sigma \propto E^{-10}$ from the corrected first Born term.

In a second paper[4] the no-correlation model was applied to the double transfer reaction $H^+ + H_2 \rightarrow H^- + 2H^+$. The agreement with experiment was reasonably good in view of the low energy at which it was applied. We have therefore used this model to calculate the cross section for the $He^{++}+He$ double-transfer reaction where results at somewhat higher energies are available.

At the outset we make the approximation of using the impact parameter model in which the nuclei are assumed to behave classically and that their accelerations vanish. The approximation is known to be good at the energies in question. Our starting point is then the time-dependent Schrödinger equation for the electrons

$$\{i(\partial/\partial t)-H(t)\}\psi=0, \tag{1}$$

where

$$H=-\nabla_1^2-\nabla_2^2+\frac{2}{|\mathbf{r}_1-\mathbf{r}_2|}-4\left[\frac{1}{|\mathbf{r}_1-\tfrac{1}{2}\mathbf{R}|}+\frac{1}{|\mathbf{r}_1+\tfrac{1}{2}\mathbf{R}|}+\frac{1}{|\mathbf{r}_2+\tfrac{1}{2}\mathbf{R}|}+\frac{1}{|\mathbf{r}_2-\tfrac{1}{2}\mathbf{R}|}\right], \tag{2}$$

and where

$$\mathbf{R}=\mathbf{b}+\mathbf{V}t \tag{3}$$

is the internuclear coordinate. Units are used in which distances are measured in Bohr radii and time in units of $\hbar/\mathrm{Ry}$. The laboratory energy of the projectile is given by $E=V^2\times 25$ keV.

† Work done under the auspices of the U. S. Atomic Energy Commission.

[1] S. K. Allison, Rev. Mod. Phys. **30**, 1137 (1958).

[2] V. I. Gerasimenko and L. N. Rosentsveig, Zh. Eksperim. i Teor. Fiz. **31**, 684 (1956) [English transl.: Soviet Phys.—JETP 4, 509 (1957)].

[3] M. H. Mittleman, Proc. Roy. Soc. (London) **277**, 206 (1964).

[4] M. H. Mittleman, Phys. Rev. **137**, A1 (1965).

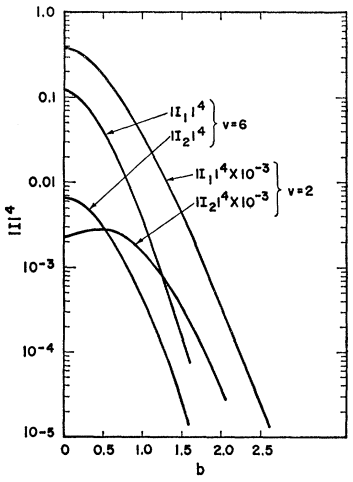

FIG. 1. Double transfer probabilities versus impact parameter for $V=2, 6$.

We now make a no-correlation approximation and replace the Hamiltonian by

$$H=-\nabla_1^2-\nabla_2^2+V(\mathbf{r}_1-\tfrac{1}{2}\mathbf{R})+V(\mathbf{r}_1+\tfrac{1}{2}\mathbf{R}) +V(\mathbf{r}_2+\tfrac{1}{2}\mathbf{R})+V(\mathbf{r}_2-\tfrac{1}{2}\mathbf{R}). \quad (4)$$

Ideally, V should be chosen as a Hartree-Fock potential for He, but we shall not be so ambitious. Instead we shall approximate the ground state of He by a product wave function

$$\phi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_2)=\phi(r_1)\phi(r_2) \quad (5)$$

and choose

$$V(r)=\int d^3x|\phi(x)|^2\left(\frac{2}{|\mathbf{x}-\mathbf{r}|}-\frac{4}{r}\right). \quad (6)$$

That is, V is the static potential on an electron due to the nucleus and the other electron. With the approximate Hamiltonian, Eq. (4), it is easy to show[3] that if the total wave function starts as an uncorrelated product it will remain so and that the double transfer probability $P_2(b)$ will be a product of two single transfer probabilities:

$$P_2(b)=[P_1(b)]^2. \quad (7)$$

Our problem then becomes one of calculating the single transfer probability from

$$(i(\partial/\partial t)-h)X=0, \quad (8)$$

where the single-particle Hamiltonian is

$$h=-\nabla^2+V(r-\tfrac{1}{2}R)+V(r+\tfrac{1}{2}R). \quad (9)$$

We chose the simplest possible representation of the He orbitals

$$\phi(r)=\alpha^{3/2}\pi^{-1/2}e^{-\alpha r}, \quad (10)$$

where α is determined variationally; $\alpha=27/16$.

We have obtained $P(b)$ from Eq. (10) in two approximations, the usual first Born approximation and a modified[5] first Born approximation. The modification

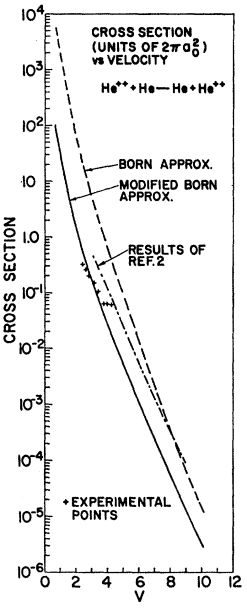

FIG. 3. Cross section (units of $2\pi a_0^2=1.76\times10^{-16}$ cm^2) versus velocity ($E=V^2\times25$ keV).

corrects for the lack of orthogonality of initial and final states.

The probability amplitudes are given below; for the usual Born approximation

$$I_1(b)=-i\int dtd^3re^{i(d\mathbf{R}/dt)\cdot\mathbf{r}/2} \times\phi(\mathbf{r}+\tfrac{1}{2}\mathbf{R})\phi(\mathbf{r}-\tfrac{1}{2}\mathbf{R})V(\mathbf{r}+\tfrac{1}{2}\mathbf{R}) \quad (11)$$

and for the modified first Born approximation

$$I_2(b)=-i\int dtd^3re^{i(d\mathbf{R}/dt)\cdot\mathbf{r}/2} \times\phi(\mathbf{r}+\tfrac{1}{2}\mathbf{R})\phi(\mathbf{r}-\tfrac{1}{2}\mathbf{R})[V(\mathbf{r}+\tfrac{1}{2}\mathbf{R})-U(R)], \quad (12)$$

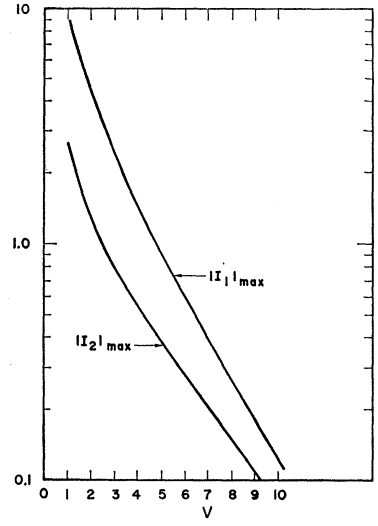

FIG. 2. Maximum amplitudes for double transfer versus V.

[5] M. H. Mittleman, Phys. Rev. **122**, 1930 (1961).

where

$$U(R)=\int d^3x V(\mathbf{x}-\mathbf{R})\phi^2(x). \quad (13)$$

The cross sections were obtained from

$$\sigma=2\pi\int_0^\infty bdb|I(b)|^4. \quad (14)$$

The multiple integrations implied by Eqs. (11), (12), and (14) were carried out with the aid of an IBM 7094 computer using a total time of about 15 min.

Figure 1 is a plot of the two-particle transfer probability versus impact parameter as obtained from Eqs. (11) and (12) for two different velocities. It is seen that the probability becomes greater than unity for sufficiently small velocity and impact parameter and the calculation loses all validity. It should be noted that $|I_2|^4<|I_1|^4$, so that the modified theory can be extended to lower energies than the usual first Born theory. In Fig. 2 the maximum value of $|I|$ is plotted versus velocity for the two theories. Since these probabilities must be less than one, a limit on the range of validity at the low-energy end can be obtained from the curve. Finally, Fig. 3 gives the cross section in units of $2\pi a_0^2(=1.76\times10^{-16}$ cm^2) versus velocity ($E_{\text{lab}}=V^2\times25$ keV) for the two results obtained here and the usual first Born approximation of Gerasimenko and Rosentsveig.[2] The experimental points of Allison[1] are also shown. Note that all three calculations are for ground-state capture only while the experiments are for total capture. Thus the theories should all lie below the experiment.

Of the two theories presented here the modified one appears to be better. However, we believe that the experiment is not sufficiently good to choose between our modified theory and the first Born approximation of Ref. 2. It is only internal consistency that seems to favor ours. It is desirable that the experiments be redone more directly.

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Electron–Alkali-Atom Interaction Potential and Elastic-Scattering Cross Section*†

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The potential energy between an incident electron and a neutral alkali atom has been calculated using first-order perturbation theory in the adiabatic approximation. The results are shown to be expressible in terms of a multipole expansion suitably generalized to allow for the penetration of the target-atom wave function by the incident electron. The monopole and dipole contributions have been calculated in detail for cesium. For large separations, the monopole contribution to the potential is small compared to the dipole contribution but becomes increasingly significant at smaller separations. For infinite separation, the calculations can be interpreted to yield the atomic polarizability, and the result for cesium (61.0 Å^3) is in reasonable agreement with experimental results. With this interaction potential, the elastic scattering of low-energy electrons from neutral cesium is treated in the adiabatic approximation with exchange. For purposes of comparison, the nonexchange approximation is also treated.

I. INTRODUCTION

THE elastic scattering of low-energy electrons by neutral atoms may be treated in terms of an effective potential which represents the interaction between the incoming electron and the target atom. This effective potential can be considered as made up of several component parts. At high energies, the dominant component of the scattering potential is a shielded Coulomb field due to penetration by the incident electron into the electron "cloud" of the target atom. However, at low incident energies, the small polarization forces arising at large separations make an important contribution to the scattering. This polarization component of the potential results from the distortion of the target atom due to the proximity of the incident particle and reacts back on the incident particle as one of the scattering forces. It must vanish for zero separation, since, in this limit spherical symmetry prevails and no nonzero multipole moments can be induced. On the other hand, for asymptotically large separations, the polarization potential varies with the inverse fourth power of the separation and, in this regard, the atom is

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