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Scattering of proton by Lithium atom with electron exchange

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Synopsis , We present formalism of Time-dependent Exchange Perturbation Theory (TDEPT) built to all orders of perturbation, for arbitrary time dependency of perturbation and apply it to the problem of proton scattering on Lithium atom where we calculate the differential and the total cross-sections

In this work, we develop a dedicated perturbation theory, named exchange perturbation theory (EPT), which takes into account the indistinguishability of electrons participating in multi-centre molecular / atomic collisions to any order of perturbation. It is worth noting that the development of EPT requires careful study of the wave functions associated with electrons assigned to different atomic centres. The overlapping of these wave functions is responsible for the exchange effects that play a crucial role in both adiabatic and dynamic scattering events.

In the following, we consider the collision associated with the redistribution of electrons, as for example the collisions of proton scattering on Lithium atom: $\mathrm{Li} + p \rightarrow \mathrm{Li}^{+} + \mathrm{H}$, accompanied by charge transfer.

The formalism of the time-dependent exchange perturbation theory is developed in an invariant form [1] . The obtained expression for the differential cross section is

$$\frac{d\sigma_{fi}}{d\Omega} = j^{-1}\frac{dw_{fi}}{d\Omega} = \frac{\mu_i \mu_f k_f}{\left(2\pi\hbar^2\right)^2 k_i}\left|\left\langle \Psi_f^0 \left| \hat{T} \right| \Phi_i^0 \right\rangle\right|^2 .$$

The transition operator $\hat{T}$ given in the form

$$\hat{T} = V_0^{\mathbb{N}} + V_0^{\mathbb{N}}\left(\frac{f_0^2}{P}\right)^{-1}\left(E_i - H + i\eta\right)^{-1} V_0^{\mathbb{N}},$$

where H is the total Hamiltonian of the system and where $V_0^{\mathbb{N}} = \left(\frac{f_0^2}{P}\right) V_0$ is a renormalized perturbation operator. The initial state is described by the vector $\left|\Phi_i^{0(0)}\right)$, corresponding to the initial electron permutation between the centers, the antisymmetric vector $\left|\Psi_f\right\rangle$ of the final state is obtained by applying the normalized Young operator onto the wave function $\hat{A}\left|\Phi_f\right)$ with respect to all electron permutations between the centers.

As the initial permutation (p = 0) we assume the following arrangement: three electrons of the Lithium atom and the incident proton. We label the electrons as 1, 2 and 3. Figure 1 illustrates the arrangement of the particles. $\vec{R}$ is vector originating at proton and pointing to Lithium atom.

The total cross section σ_{fi} is summarized in Table 1, where the cross section values, obtained in this work are compared to those obtained from the experiments.

Table 1. Summary of total cross section values

v(cm)	E (eV)	k *a.u.*	σ(cm^2) Li-H$^+$	σ(cm^2) LiHe^{2+}	σ (cm^2)
$7.5\cdot10^5$	1.95	15	$7\cdot10^{-14}$	$6\cdot10^{-14}$	$6\cdot10^{-14}$
$2.5\cdot10^6$	21.6	50	$2\cdot10^{-14}$	$17\cdot10^{-15}$	$2.\cdot10^{-14}$

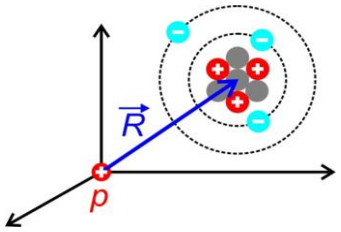

Figure 1. Arrangement of the particles in the proton - Lithium atom collision

References

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