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Multi-Channel Quantum Scattering Calculation for Ultracold Ion-Atom Collisions

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We focus on the theoretical modelling of the dynamics of ion-neutral systems at ultracold temperatures (« 1K) in order to design ways for their full quantum control. Our aims are connected to experimental investigations of alkaline earth ion - alkali atom systems with hybrid traps. Due to the laser cooling scheme a metastable d-level of the alkaline-earth ion is considerably populated in these experiments, e.g. in case of 88Sr+ ion embedded in the cloud of ultracold 87Rb atoms [1] or 138Ba+ in 6Li cloud [2]. The large internal energy of the ion induces several inelastic processes like charge-exchange, spin-orbit change collisions or electronic excitation exchange.
We compute cross sections and rate coefficients for these processes within the framework of the quantum coupled-channel model considering the fine-structure of the colliding partners and the rotational coupling. Our calculations involve potential energy curves including the determination of R-dependent spin-orbit couplings (see Figs. 1, 2) following a diabatization approach [3].
Fig.1: Selected Hund's case (a) LiBa+ potential energy curves in the molecular frame. The red shadow shows the location of an avoided crossing of 21 Σ and 31 Σ responsible of the non-radiative charge exchange (NRCE) process (red arrow): Li(2s)+Ba+(5d) ⟶ Li++Ba(6s2,1S) .
Fig.2: The R-dependent spin-orbit couplings of the first 3 dissociation limits, based on Ω=0+/-, 1, 2, 3 the projection of the total angular momentum on molecular axis.

[1] R. Ben-Shlomi, R. Vexiau, Z. Meir, T. Sikorsky, N. Akerman, M. Pinkas, O. Dulieu, R. Ozeri, Phys. Rev. A 102 ,031301(R)
[2] P. Weckesser, F. Thielemann, D. Wiater, A. Wojciechowska, L. Karpa, K.Jachymski, M. Tomza, T. Walker, T. Schaetz, Nature 600, 429 (2021)
[3] X. Xing, R. Vexiau, N. Bouloufa, O. Dulieu et al, in preparation.

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