# Heteroisotopic Feshbach resonances in collisions of cold Ca and $Ca^+$

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**Synopsis** We investigate ultracold collisions of heteroisotopic pairs of Ca with $Ca^+$ mediated by an external magnetic field. Based on the nuclear spin of Ca, namely $I = 7/2$ for $^{43}$Ca and $I = 0$ for other isotopes, we identify different scattering dynamics and characterize magnetic Feshbach resonances in $^{43}Ca+^{43}Ca^+$ and $^{43}Ca+^{(40,42)}Ca^+$ collisions. Our results suggest that interisotopic Feshbach resonances could be used to control charge-exchange in ultracold atom-ion mixtures of Ca and its ion.

Recent progress in experiments involving small ensembles of trapped ultracold atoms and ions cooled below the critical mass ratio is for the first time allowing direct studies of atom-ion collisional dynamics and controlled chemistry at temperatures in the milli- and microkelvin regime[1]. In addition, such hybrid systems are suitable for studying atom-ion interactions, many-body physics of cold neutral samples doped with charges, quantum simulation, and quantum information processing. Such studies rely on detailed descriptions of atom-ion interactions and the means to control them via external electromagnetic fields. As in case of neutral atoms[2], Feshbach resonances allow the pairwise atom-ion interactions to be tuned over a wide range and offer means to control charge exchange rate in collisions.

In this study, we theoretically investigate the properties of magnetic Feshbach resonances and their impact on charge-exchange rates in collisions of Ca with $Ca^+$. Specifically, we consider cold collisions between $^{43}$Ca (nuclear spin $I = 7/2$) and $^{(40,42)}Ca^+$ ($I = 0$) in a magnetic field. A key component of our model are non-Born-Oppenheimer couplings between the potential energy curves of different symmetry due to the mass polarization term present for the collisions between different isotopes [3]. These couplings give rise to magnetic Feshbach resonanances between different isotopes that could be used to resonanly enhance charge-exchange rate in a collision between the particles in selected hyperfine states.

We find and characterize Feshbach resonances by numerically solving a system of time-independent coupled-channel equations for the collision energy $E = 10\ \mu$K, where the atom-ion interactions are described by *ab-initio* electronic interaction potentials smoothly extended to the long-range region [4]. The electronic potentials for $^{43}Ca+^{42}Ca^+$ with all corrections included are given in Fig. 1. The resulting scattering length for the incoming hyperfine channel $(\alpha\beta)$=(23) as a function of the magnetic field $B$ is shown in Fig. 1 (inset) (see Refs. [1, 5] for details related to the notation). A Feshbach resonance occurs at about 70 G. The charge-exchange rate at ultracold temperature is related to the scattering length as $K_{cx}(B) = 4\pi \mathrm{Im}(a)/\mu$, implying that a large variation of the rate is possible. Similar results are found in other channels. While the exact positions of the resonances are impossible to predict without an accurate spectroscopic study, the Feshbach resonances appear to be much broader than for $Be+Be^+$[5], suggesting $Ca+Ca^+$ as a more suitable candidate system for further investigation.

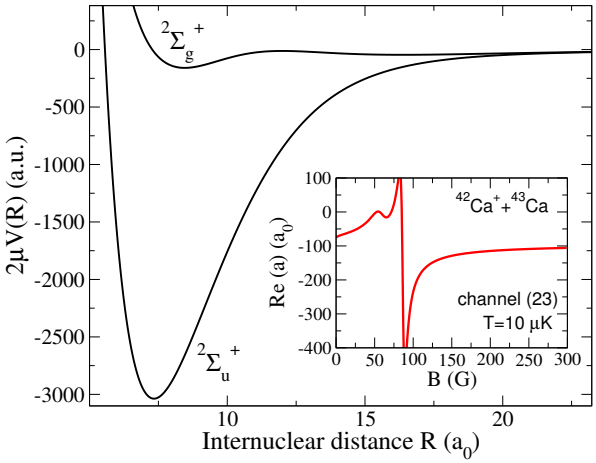


**Figure 1**. Electronic potential energy curves for $(^{43}Ca^{42}Ca)^+$ with non-Born-Oppenheimer couplings included. Inset: Scattering length as a function of the $B$ field for the scattering channel $(\alpha\beta) = (23)$. Feshbach resonance occurs at about 70 G.

## References

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