Quantum dynamics calculations on atom-diatom collisions: bosons versus fermions

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We have obtained new potential energy surfaces and carried out full quantum dynamics calculations for spin-polarized Li + Li$_2$ [1] and K + K$_2$ [2] collisions for both bosonic and fermionic isotopes. These are “reactive” scattering collisions because they include all possible arrangement channels. They are carried out in hyperspherical coordinates [3], which allow the full boson or fermion symmetry to be imposed. The potential energy surfaces are highly non-additive [4]. Our calculations give very high quenching rates for alkali dimers in excited vibrational states. For the low vibrationally excited states that we can handle at present, we do not see any suppression of inelastic scattering for fermionic atoms, even when the scattering length is large and positive. The low-temperature inelastic rate coefficients are typically above $10^{-10}$ cm$^3$ s$^{-1}$. We conclude that Pauli blocking occurs only for molecules formed in the highest vibrational state in the potential well. Our results have important implications for experiments aimed at transferring molecules to lower vibrational states. We expect that it will be necessary to transfer them directly to the ground vibrational state for them to be long-lived. Molecules produced in any intermediate vibrational state are likely to be ejected from the trap very quickly. We have also carried out calculations for mixed-isotope collisions involving alkali dimers [5]. For $^7$Li colliding with either $^6$Li$_2$ or $^6$Li$^7$Li, reactive scattering is possible even when the molecule is in its lowest rovibrational state because of the change in zero-point energy. For $^7$Li + $^6$Li$^7$Li, there is only one reactive channel and the reactive scattering rate is suppressed by a factor of 50 compares to the vibrational relaxation rates.