



Michał Tomza

(University of Warsaw, Centre of New Technologies)

Quantum-chemical approach to ultracold atoms and molecules

In the first part I will present that isotope-exchange reactions between ground-state heteronuclear dimers consisting of two isotopes of the same atom provide the ground for testing models of the chemical reactivity. The number and energetics of open and closed reactive channels can be controlled by the laser and magnetic fields using a laser-induced isotope- and state-selective Stark shift control. The present proposal opens the way for studying the state-to-state dynamics of ultracold chemical reactions beyond the universal limit with a meaningful control over the quantum states of both reactants and products [1].

In the second part I will present the application of quantum-chemical coupled-cluster method to study the properties of a balanced two-component Fermi gas in a one-dimensional harmonic trap. We compute the energy, the chemical potential, the pairing gap, and the density profile of the trapped clouds, smoothly mapping the crossover between the few-body and many-body limits. The energy is found to converge surprisingly rapidly to the many-body result for every value of the interaction strength. Many more particles are instead needed to give rise to the nonanalytic behavior of the pairing gap, and to smoothen the pronounced even-odd oscillations of the chemical potential induced by the shell structure of the trap [2].

[1] M. Tomza, Phys. Rev. Lett. 115, 063201 (2015)

[2] T. Grining, M. Tomza, M. Lesiuk, M. Przybytek, M. Musiał, R. Moszynski, M. Lewenstein, P. Massignan, Phys. Rev. A 92, 061601(R) (2015)

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Universität Stuttgart, NWZII, Raum 3.123
Pfaffenwaldring 57, 70569 Stuttgart

