Spectral Theory and Dynamics of Quantum Systems

GRADUIERTENKOLLEG 1838

Stuttgart-Tübinger Doktorandenseminar

7. November 2016

Universität Stuttgart, Campus Vaihingen, Pfaffenwaldring 57
Raum 8.122

Programm	
14.00 – 14.25	**Andreas Wünsch:** Selfadjointness and Domain of the Nelson Hamiltonian
14.30 – 14.55	**Jan Köllner:** Spectral Estimates for the Stark Operator on Domains
15.00 – 15.25	**Bartosch Ruszkowski:** Hardy inequalities for a subelliptic operator
Kaffeepause	
16.00	**Mathematisches Kolloquium**
ab 17.30	**Nachsitzung**

Mathematisches Kolloquium:

Instanton Theory to Describe Atom Tunneling in Chemical Reactions

Prof. Johannes Kästner (Universität Stuttgart)

ABSTRACT: Quantum mechanical tunneling of atoms is emerging as an ubiquitous phenomenon in chemistry. Every chemical reaction that includes a hydrogen transfer can be expected to be influenced by tunneling at room temperature. While simulations can monitor tunneling directly, experimental approaches can only detect the consequences [1]. We use instanton theory, based on statistical Feynman path integrals, to find the most probable tunneling path and the reaction rate [2,3]. This is used to investigate the formation of H2 on the surface of carbonaceous dust grains in space as well as the deuteration of interstellar methanol. Large kinetic isotope effects in this and other reactions can be explained by the tunneling contribution.

[1] J. Meisner, J. Kästner, Angew. Chem. Int. Ed. 55, 5400-5413 (2016)
[2] J. Kästner WIREs Comput. Mol. Sci. 4, 158 (2014)
[3] J.B. Rommel, J. Kästner J. Chem. Phys. 134, 184107 (2011)

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