

Im

## Oberseminar Analysis

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**TU Dresden, Fakultät Maschinenwesen**

einen Vortrag zum Thema

### **Transport in systems with helical confinement: space-adiabatic approximation**

Abstract:

Chiral molecules filter electrons passing through them dependent on their spin. Occurring in a wide range of chiral structures and experiments with polarization up to 100%, the effect is usually attributed to an interplay of geometry and spin-orbit coupling and is therefore called chiral-induced spin selectivity (CISS). We attempt to contribute to the theoretical understanding of the effect by considering a minimal model: an electron moving through a helical confinement potential (realized by Dirichlet boundary conditions) with spin-orbit coupling (SOC). We give a rigorous proof that for strong confinement (i. e. in the adiabatic limit), a 1-dimensional approximation to the exact Hamiltonian of the system exists. To this end we adapted space-adiabatic perturbation theory to include the SOC term from the Pauli equation. This provides an estimate for the deviation of the ex-act and approximate time evolution operators in terms of confinement strength. Despite restricting the electron movement completely to the helix, the effective model still contains terms depending on extrinsic properties of the curve (i. e. its embedding into the ambient space) in accordance with classical adiabatic results. To probe its physical content, Landauer transport calculations were performed on a discretized version of the model. The results are compared to an atomistic tight-binding model for helicene pointing out how a detailed understanding of confinement processes might help remedy the shortcomings of existing models for CISS.

Datum: **Montag, 29. November 2021 (!)**

Zeit: **10:00 Uhr (!)**

Der Vortrag findet über das Videokonferenzsystem „Zoom“ statt.

Ansprechpartner: Prof. Dr. Ralph Chill

Der virtuelle Raum ist über folgenden Link erreichbar:

<https://tu-dresden.zoom.us/j/89887698744?pwd=TVR3djhXNkV2U1ZFMTJ3czBOd3c4dz09>

Meeting ID: 898 8769 8744, Passcode: @8%qq2

Alle Interessenten sind herzlich eingeladen.