

## Karlsruher PDE-Seminar

# The approximation of solutions to the Schrödinger equation by anisotropic Gauß functions

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The electronic Schrödinger equation describes the motion of  $N$  electrons under Coulomb interaction forces in a field of clamped nuclei. The solutions of this equation, the electronic wavefunctions, depend on  $3N$  variables, three spatial dimensions for each electron. Approximating them is therefore a grand challenge. We propose to approximate these wavefunctions by linear combinations of anisotropic Gauß functions. We show that the original, singular wavefunctions can, up to a negligibly small error, be approximated with only insignificantly more effort than their convolutions with a Gaussian kernel of sufficiently small width and that basically arbitrary orders of convergence in the number of the terms involved can be reached.

**Termin:** Donnerstag, 12. Februar 2015, 17:30 Uhr

**Ort:** 1C-03, Allianz-Gebäude 05.20

**Gastgeber:** Die Dozenten des Schwerpunkts Partielle Differentialgleichungen