niedersächsische
technische hochschule

Mathematisches Kolloquium

19.01.2012

15:00 Volker Bach, TU Braunschweig

Atoms, Molecules, and N-Representability

The notion of *N-representability* of a reduced density matrix in quantum chemistry and the derivation of the so-called G, P, Q, T_1, and T_2 conditions on the two-particle density matrix are reviewed. It is further shown that already the G and the P conditions lead to a correlation estimate from which the high accuray of the Hartree-Fock approximation for large atoms and molecules can be deduced.

16:15 Kaffee

17:00 Hans-Christoph Grunau, U Magdeburg

Up to bounded smooth corrections, biharmonic Green functions are positive

A classical example for a fourth order problem in mechanics is the linear clamped plate boundary value problem:

$$\begin{cases} \Delta^2 u = f & \text{in } \Omega, \\ u = |\nabla u| = 0 & \text{on } \partial\Omega. \end{cases}$$

In the two-dimensional case the domain $\Omega \subset \mathbb{R}^2$ may be considered as the horizontal equilibrium shape of a horizontally clamped thin elastic plate. The unknown u models then its vertical deflection under the vertical load f.
"Linear questions" like a priori estimates or existence results may be considered as well understood. This changes completely as soon as one poses the simplest "nonlinear question": What can be said about positivity preserving? Does a clamped plate bend upwards when being pushed upwards? It is known that the answer is "no" in general. However, there are still positivity issues like "almost positivity" to be discussed in terms of estimates for the corresponding Green function.
The lecture is based on joint work with F. Robert (Nancy) and G. Sweers (Cologne).

Ort Seminarraum A des Instituts für Mathematik, TU Clausthal

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