Numerical Analysis and PDE

Quantum observables approximated by molecular dynamics in the canonical ensemble

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It is well known that quantum observables in the canonical ensemble can be approximated by molecular dynamics simulations, with constant number of particles, volume and temperature, if the temperature is small compared to the minimal difference of the second and first eigenvalue of the electron potential. In this talk I will show that molecular dynamics simulations can also be constructed so that quantum observables are well approximated for all temperatures. The analysis is based on Weyl's law.

This is joint work with Aku Kammonen, Caroline Lasser and Mattias Sandberg.