

Simulation of small quantum systems by Path Integral Numerical Methods

Voznesenskiy M.A.¹, Polyakov E.A.¹, Vorontsov-Velyaminov P.N.¹

¹ Physical faculty SPbSU, Saint-Petersburg, Russia,
e-mail: mikhail.voznesenskiy@gmail.com

We propose a new approach in obtaining the partition function of a system of several interacting particles (fermions) in external field within path integral Monte Carlo method based on direct averaging of exchange contributions over the positive weight determined by non-closed trajectories. This way the complete partition function is obtained at finite temperatures down to their low values. The new approach allows us to reach observably lower temperatures, compared to the previously proposed path-integral Monte Carlo method [1,2], thus permitting significantly to reduce the sign problem. The proposed approach yields an independent way to treat thermal properties of quantum systems, so the good agreement with previous data [1,2] allows us to test and state the validity of both approaches. The presented approach allows one to carry out calculations for low temperatures that make it possible to estimate the ground-state energy and low-temperature thermodynamics. A quantum dot model of several interacting electrons confined in a harmonic oscillator field was simulated. The interaction with environment (phonons, plasmons) was accounted for within harmonic heat bath approximation [3].

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