Abstract Submitted
for the DPP11 Meeting of
The American Physical Society

Configuration Path Integral Monte Carlo[1] MICHAEL BONITZ, TIM SCHOOF, SIMON GROTH, ALEXEI FILINOV, DAVID HOCHSTUHL, ITAP, Kiel University — A novel path integral Monte Carlo (PIMC) approach for correlated many-particle systems with arbitrary pair interaction in continuous space at low temperatures is presented. It is based on a representation of the N-particle density operator in a basis of (anti-)symmetrized N-particle states ("configurations" of occupation numbers) [1]. The path integral is transformed into a sum over trajectories with the same topology and, finally, the limit of M to infinity, (M is the number of high-temperature factors), is analytically performed. This yields exact expressions for the thermodynamic quantities and allows to perform efficient simulations for fermions at low temperature and weak to moderate coupling. Our method is applicable to dense quantum plasmas in the regime of strong degeneracy where conventional PIMC, e.g. [2], fails due to the fermion sign problem.

[1] T. Schoof, M. Bonitz, A. Filinov, D. Hochstuhl, and J.W. Dufty, Contrib. Plasma Phys. (2011), DOI 10.1002/ctpp.201100012;.
[2] "Introduction to computational methods for many-body physics," M. Bonitz and D. Semkat (eds.). Rinton Press, Princeton 2006, chapter 4.

[1]This work is supported by the Deutsche Forschungsgemeinschaft.

Michael Bonitz
ITAP, Kiel University

Date submitted: 13 Jul 2011 Electronic form version 1.4