Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Calculating thermodynamics properties of quantum systems by a non-Markovian Monte Carlo procedure[1] YANIER CRESPO HERNANDEZ, International Centre for Theoretical Physics (ICTP), ALESSANDRO LAIO, GIUSEPPE SANTORO, ERIO TOSATTI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), CONDENSED MATTER TEAM — We present a history-dependent Monte Carlo scheme for the efficient calculation of the free energy of quantum systems inspired by Wang-Landau and metadynamics. In the two-dimensional quantum Ising model, chosen here for illustration, the accuracy of free energy, critical temperature, and specific heat is demonstrated as a function of simulation time and successfully compared with the best available approaches. The approach is based on a path integral formulation of the quantum problem and can be applied without modifications to quantum Hamiltonians of any level of complexity. The combination of high accuracy and performance with a much broader applicability is a major advance with respect to other available methods.

[1]Supported by a MIUR/PRIN contract and benefited from the environment provided by the CNR/ESF/EUROCORES/FANAS/AFRI project.

Yanier Crespo Hernandez
International Centre for Theoretical Physics (ICTP)

Date submitted: 29 Nov 2011 Electronic form version 1.4