

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Iterative Monte Carlo for Quantum Dynamics¹ VIKRAM JADHAO,
NANCY MAKRI, University of Illinois at Urbana-Champaign — We present a fully
quantum mechanical methodology for calculating complex-time correlation functions
by evaluating the discretized path integral expression iteratively on a grid selected
by a Monte Carlo procedure [1]. Both the grid points and the summations performed
in each iteration utilize importance sampling, leading to favorable scaling with the
number of particles, while the stepwise evaluation of the integrals circumvents the
exponential growth of statistical error with time.

[1] V. Jadhao and N. Makri J.Chem.Phys. 129, 161102 (2008)

¹This work is supported by the National Science Foundation under Award Nos. ITR
04-27082, CHE 05-18452, and CRIF 05-41659

Vikram Jadhao

Date submitted: 21 Nov 2008

Electronic form version 1.4