Abstract Submitted
for the TSF05 Meeting of
The American Physical Society

Feynman-Kac Path Integral Convergence Enhancement by Rational Curve Fitting JOHN HOPKINS, BRUCE MILLER, Texas Christian University — By creating a mapping between a quantum system and a classical polymer chain of p beads, the Feynman-Kac path integral provides a well-established formalism for representing the system density matrix. In the limit of large p, it is accurately represented by an integral over all possible paths of the Euclidean action. Few cases can be worked out analytically, so the integral is usually performed numerically using Monte Carlo techniques. Limits must be taken for large numbers of Monte Carlo samples and large p. Systematic errors associated with large p make it is desirable to determine this limit without the direct calculation of integrals for large p. We have numerical evidence that a rational function curve-fitting technique applied to integrations for several relatively small p values gives reasonable answers for the large p limit for a simple system where the analytic solution is known–a single quantum particle in a one-dimensional periodic lattice of atoms. This algorithm is similar to other convergence enhancing techniques, such as the Bulirsch-Stoer algorithm for finding numerical solutions to differential equations.

John Hopkins
Texas Christian University

Date submitted: 14 Sep 2005 Electronic form version 1.4