Numerical Methods for the Approximation of Path Integrals with Applications in Quantum Statistical Mechanics

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Discretizations of the Feynman-Kac path integral representation of the quantum mechanical density matrix are investigated. Each infinite-dimensional path integral is approximated by a Riemann integral over a finite-dimensional Sobolev space, by restricting the integration to a subspace of all admissible paths. Using this process, a wide class of methods can be derived, with each method corresponding to a different choice for the approximating subspace. The traditional "short-time" approximation and "Fourier discretization" can be recovered from this approach, using linear and spectral basis functions respectively. As an illustration, a new method is formulated using cubic elements and is shown to have improved convergence properties when applied to model problems.
This talk consists of work completed in collaboration with Brian Laird (University of Kansas) and Ben Leimkuhler (University of Leicester).