Path integral estimation of complex-time correlation functions

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We present a method based on the Path Integral Monte Carlo formalism for the calculation of ground-state time correlation functions in quantum systems [1]. The key point of the method is the consideration of time as a complex variable whose phase δ acts as an adjustable parameter. By using high-order approximations for the quantum propagator, it is possible to obtain Monte Carlo data all the way from purely imaginary time to δ values near the limit of real time. As a consequence, it is possible to infer accurately the spectral functions using simple inversion algorithms. We test this approach in the calculation of the dynamic structure function $S(q,\omega)$ of two one-dimensional model systems, harmonic and quartic oscillators, for which $S(q,\omega)$ can be exactly calculated. We notice a clear improvement in the calculation of the dynamic response with respect to the common approach based on the inverse Laplace transform of the imaginary-time correlation function. Extensions to systems of up to ten particles are also discussed.

[1] R. Rota, J. Casulleras, F. Mazzanti, and J. Boronat, J. Chem. Phys. **142**, 114114 (2015).