

Abstract Submitted
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Calculation of nonequilibrium spectral functions in quantum dot systems using imaginary-time method JONG E. HAN, SUNY at Buffalo — Quantum mechanics for nonequilibrium many-body effects is formulated in the imaginary-time formalism. In quantum dot systems, we extend the chemical potentials of the source and drain leads by including the Matsubara voltage, which makes it possible to compute equilibrium and nonequilibrium steady-state within the same conventional imaginary-time technique. While the formal equivalence of the imaginary-time and real-time Keldysh methods can be established, the main problem has been the numerical analytic continuation of the self-energy of mapping the Matsubara voltage to the real voltage. In this presentation, we compare the calculations from the Hirsch-Fye discrete-time quantum Monte Carlo (QMC) and the continuous-time QMC method which significantly improves the high frequency self-energy. Through a comparison of the methods, the high-frequency problem of the discrete-time QMC results is much improved by correctly including the effects of discontinuity in the Green functions. With these modifications, the analytic continuation becomes much more reliable and we discuss various aspects of numerical procedures of fitting numerical self-energy in the Kondo model.

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