The Real-time Dyson Expansion: Efficient Inclusion of Dynamical Correlations in Non-equilibrium Spectral Properties

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A key experimental technique for probing real-time non-equilibrium dynamics of electronic states is time-resolved photoemission spectroscopy. Predicting this time-resolved spectra theoretically represents a challenge, in particular in realistic systems. The Kadanoff-Baym equations provide one route to computing the two-time Green's function and thus the time-resolved spectrum,, however the resulting computation scales cubically in the number of time steps, thus quickly becoming prohibitively expensive. Using a mean-field approach fixes the problem of scalability with only a linear cost in the number of time steps. The cost of this reduced scaling is that mean-field methods neglect dynamical correlation effects and miss key spectral properties such as emergent spectral features. We present a new technique we have developed that allows for the inclusion of dynamical correlation effects while maintaining the same numerical scaling in the number of time steps as a mean-field approach. Further, the scheme generalizes a commonly applied equilibrium method that has had great success in practical ab-initio many-body perturbation theory. The method shows excellent agreement with exact results in test systems. Additionally we exemplify the scalability of the method on a periodic system and demonstrate clear evidence that our proposed scheme produces complex spectral features including excitonic band replicas, features that are not observed using static mean field approaches.