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Mobility of Holstein polaron from real and imaginary time quantum Monte Carlo calculations

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Electron-phonon (e-ph) interaction is responsible for majority of transport phenomena in condensed matter. In this work, we consider the short-range (localized) e-ph interaction described by the Holstein Hamiltonian. We develop numerically exact path integral Monte Carlo (PIMC) methods to obtain current-current correlation functions (CFs) and polaron mobility of one-dimensional Holstein model.

Generally, several challenges need to be overcome to reliably calculate dynamical properties using the PIMC methods. First one is the dynamical sign-problem of real time CFs which can be eliminated by doing calculations in imaginary time and then analytically continuing to real time. The other challenge is that there is not a reliable method for analytic continuation of numerically obtained values. We overcome these limitations by combining real time and imaginary time calculations with singular value decomposition method for analytical continuation.

For weaker e-ph interaction strengths we were able to calculate CFs in real time for a range of temperatures by using a Monte Carlo algorithm derived from momentum representation of electronic degrees of freedom and coordinate representation of phonons. For stronger interactions such an algorithm leads to a significant sign-problem for longer times and better results are obtained by using a different algorithm. This algorithm is derived from site representation of electronic degrees of freedom and coordinate representation of phonons. The phonon coordinates are then integrated out analytically and Monte Carlo summation over electronic states is performed. In the case of stronger interactions, where real time calculations cannot be used to obtain CFs at longer times, doing analytic continuation of both real time and imaginary time data gives much better results. The methods described enabled us to calculate polaron mobility for a range of temperatures and e-ph interaction strengths.

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