



复旦大学数学科学学院 数学综合报告会

报告题目: Dynamic mode decomposition of nonequilibrium Green's function for quantum many-body systems

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报告摘要:

Simulating quantum many-body systems away from equilibrium is computationally challenging. To make it easier, a practical way is to examine the Green's function based on the many-body perturbation theory. However, the Kadanoff-Baym equations (KBEs) which describe the dynamics of the two-time non-equilibrium Green's function (NEGF) form a set of coupled nonlinear integro-differential equations difficult to solve. In fact, to propagate the system until time T , typical numerical methods will take $O(T^3)$ computational time. To deal with this problem, I applied DMD, which is a data-driven model order reduction technique, to simulate the long-time dynamics of the NEGF by using snapshots computed within a small time window. This technique was first applied to the time-diagonal of the two-time Green's function, and then to the off-diagonal elements by decomposing the Green's function into a number of one-time functions. The effectiveness of DMD is demonstrated on a two-band Hubbard model system. In the equilibrium limit, the DMD analysis yields results that are consistent with those produced from a linear response analysis. In the nonequilibrium case, the extrapolated dynamics produced by DMD is more accurate than a special Fourier extrapolation scheme. A potential pitfall of the standard DMD method comes from the insufficient spatial/momentum resolution of the discretization scheme. For the model system, this problem can be overcome by using a variant of DMD known as the higher order DMD (HODMD).

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