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Complex instanton gas approximation for the Hubbard model away of half-filling

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We present recent advancements towards the alleviation of the sign problem for the Hubbard model away of half filling. We couple the thimble decomposition approach with certain approximations, which allow us to predict the structure of the thimble decomposition in advance, before actual Quantum Monte Carlo simulations.

First, we show that the saddle points for the Hubbard model with charge-coupled auxiliary field have simple and regular structure both at half filling and away of it. They are collections of instantons: objects, localized both in space and Euclidean time. Auxiliary fields inside instantons are real at half filling, but acquire non zero imaginary part at finite chemical potential thus leading to complex saddle points.

Instanton gas approximation, initially developed for the Hubbard model at half filing [Phys. Rev. B 107, 045143], is able to predict the share of particular thimble in the full partition function. We expand this approximation to (now complex) instantons away of half filling, showing that we can still predict both weights and phases of corresponding thimbles using relatively simple analytical expressions.

Using the results of this study, we can compute analytically the residual sign problem from the phases of various thimbles participating in the partition function. Formally, this phase shows rapid exponential decay with inverse temperature and system size, thus we can essentially prove a no-go theorem that straightforward thimble decomposition approach can not work for the Hubbard model away of half-filling for the auxiliary field coupled with charge density.

However, since the phases and the weights of the thimbles are known with high precision, we can perform resummation still allowing us to extract meaningful results for observables at least in Gaussian approximation to the thimble integrals around exact complex saddle points. We study charge density and superconducting order parameters depending on the chemical potential.

We also discuss possible further developments, in particular the connections between thimble decomposition and Constrained Path Quantum Monte Carlo.

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