Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via non-unitary similarity transformations

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Similarity transformation of the Hubbard Hamiltonian using a Gutzwiller correlator leads to a non-Hermitian effective Hamiltonian [1], which can be expressed exactly in momentum-space representation, and contains three-body interactions [2]. We apply this methodology to study the two-dimensional Hubbard model with repulsive interactions near half-filling in the intermediate interaction strength regime ($U/t = 4$).
We show that at optimal or near optimal strength of the Gutzwiller correlator, the similarity transformed Hamiltonian has extremely compact right eigenvectors, which can be sampled to high accuracy using the Full Configuration Interaction Quantum Monte Carlo (FCIQMC) method [3], and its initiator approximation.
Near-optimal correlators can be obtained using a simple projective equation, thus obviating the need for a numerical optimisation of the correlator. The FCIQMC method, as a projective technique, is well-suited for such non-Hermitian problems, and its stochastic nature can handle the 3-body interactions exactly without undue increase in computational cost. The highly compact nature of the right eigenvectors means that the initiator approximation in FCIQMC is not severe, and that large lattices can be simulated, well beyond the reach of the method applied to the original Hubbard Hamiltonian. Results are provided in lattice sizes upto 50 sites and compared to auxiliary-field QMC.
New benchmark results are provided in the off half-filling regime, with no severe sign-problem being encountered. In addition, we show that methodology can be used to calculate excited states of the Hubbard model and lay the groundwork for the calculation of observables other than the energy.

References

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