Diagrammatic Monte Carlo sampling of the dual-fermion expansion for the Hubbard model

JAN GUKELBERGER, University of Sherbrooke, EVGENY KOZIK, King’s College London, HARTMUT HAFERMANN, Huawei Technologies Co. Ltd. — The dual-fermion approach provides a formally exact prescription for calculating the properties of a correlated electron system in terms of a diagrammatic expansion around dynamical mean-field theory (DMFT). The approach can address the full range of interactions, is exact in both the weak- and strong-coupling limits, and naturally incorporates long-range correlations beyond the reach of current cluster extensions to DMFT. Practical implementations have so far been limited to leading-order or ladder-type approximations to the expansion. In this work we compute the dual-fermion expansion for the Hubbard model to higher orders by means of a diagrammatic Monte Carlo algorithm which stochastically samples all diagram topologies. This approach allows a systematic check for the convergence of the series and hence provides a route towards a fully controlled treatment of correlated electrons.