

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ab Initio Dynamical Correlations from Auxiliary-field quantum Monte Carlo: applications in the Hubbard model¹ ETTORE VITALI, HAO SHI, MINGPU QIN, SHIWEI ZHANG, William and Mary College — The possibility of calculating dynamical correlation functions from first principles provides a unique opportunity to explore the manifold of the excited states of a quantum many-body system. Such calculations allow us to predict interesting physical properties like spectral functions, excitation spectra and charge and spin gaps, which are more difficult to access from usual equilibrium calculations. We address the ab-initio calculation of dynamical Green functions and two-body correlation functions in the Auxiliary-field Quantum Monte Carlo method, using the two-dimensional Hubbard model as an example. When the sign problem is not present, an unbiased estimation of imaginary time correlation functions is obtained. We discuss in detail the complexity and the stability of the calculations. Moreover, we propose a new approach which is expected to be very useful when dealing with dilute systems, e.g. for cold gases, allowing calculations with a very favorable complexity in the system size.

¹Supported by NSF, DOE SciDAC, and Simons Foundation

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Date submitted: 06 Nov 2015

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