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Improved Full Configuration Interaction Monte Carlo for the Hubbard Model[1] HITESH CHANGLANI, ADAM HOLMES, FRANK PETRUZIELO, GARNET CHAN, C.L. HENLEY, C.J. UMRIGAR, Cornell University — We consider the recently proposed full configuration interaction quantum Monte Carlo (FCI-QMC) method and its "initiator" extension, both of which promise to ameliorate the sign problem by utilizing the cancellation of positive and negative walkers in the Hilbert space of Slater determinants. While the method has been primarily used for quantum chemistry by A.Alavi and his co-workers [1,2], its application to lattice models in solid state physics has not been tested. We propose an improvement in the form of choosing a basis to make the wavefunction more localized in Fock space, which potentially also reduces the sign problem. We perform calculations on the 4x4 and 8x8 Hubbard models in real and momentum space and in a basis motivated by the reduced density matrix of a 2x2 real space patch obtained from the exact diagonalization of a larger system in which it is embedded. We discuss our results for a range of fillings and U/t and compare them with previous Auxiliary Field QMC and Fixed Node Green's Function Monte Carlo calculations.

[1] George Booth, Alex Thom, Ali Alavi, J Chem Phys, 131, 050106,(2009)
[2] D Cleland, GH Booth, Ali Alavi, J Chem Phys 132, 041103, (2010)

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Hitesh Changlani
Cornell University

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