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Numerical investigations of the sign problem in full configuration interaction quantum Monte Carlo JAMES J. SHEPHERD, Rice University, USA, JAMES S. SPENCER, Imperial College London, UK, GUSTAVO E. SCUSE-RIA, Rice University, USA — We explore the sign problem in full configuration interaction quantum Monte Carlo in a systematic manner. A large data set generated for the 1D k-space Hubbard model is used to demonstrate that, under certain conditions, the amount of information required to store the exact-on-average wave function has sub-linear cost with the number of Hilbert space states. It is our hope that this data set will be of use to people looking to improve both FCIQMC and its initiator adaptation. The sign problem is then discussed in connection with seniority zero configuration interaction and pair coupled cluster theories. Reference: Phys. Rev. B 90, 155130 (2014).

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