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Coupling quantum Monte Carlo and independent-particle calculations: self-consistent constraint for the sign problem based on density or density matrix[1] MINGPU QIN, HAO SHI, SHIWEI ZHANG, William Mary Coll — The vast majority of quantum Monte Carlo (QMC) calculations in interacting fermion systems require a constraint to control the sign problem. The constraint involves an input trial wave function which restricts the random walks. We introduce a systematically improvable constraint which relies on the fundamental role of the density or one-body density matrix. An independent-particle calculation is coupled to a constrained path auxiliary-field QMC calculation. The independent-particle solution is used as the constraint in QMC, which then produces the input density or density matrix for the next iteration. The constraint is optimized by the self-consistency between the QMC and independent-particle calculations. The approach is demonstrated in the two-dimensional Hubbard model by accurately determining the ground state when collective modes separated by tiny energy scales are present in the magnetic and charge correlations. Spin and charge-density wave orders are shown to exist at 1/8 doping, and their properties are characterized. Our approach also provides an ab initio way to predict effective interaction parameters for independent-particle calculations.

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Mingpu Qin
William
Mary Coll

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