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Alternating-Basis Quantum Monte Carlo Method for Strongly Correlated Electrons

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Ultracold-atom simulators have provided important insights into charge and spin transport in the two-dimensional Hubbard model [1, 2]. However, theoretical tools to compute quantities directly measured in experiments, such as space- and time-resolved charge/spin densities following a quench of an external density-modulating field, are still scarce. Here, we devise the alternating-basis quantum Monte Carlo (ABQMC) method for interacting electrons on a lattice, which is uniquely suited to compute such quantities. Apart from out-of-equilibrium setups, the formalism is equally applicable in thermal equilibrium described by either canonical or grand-canonical ensemble. The method relies on the Suzuki–Trotter decomposition (STD) and owes flexibility to the representation of the kinetic and interaction terms in the many-body bases in which they are diagonal. We formulate a Monte Carlo update scheme that respects both the momentum and particle-number conservation laws, to restrict the configuration space. The sampling efficiency is further enhanced by ensuring that the ABQMC algorithm manifestly respects several symmetries of the Hubbard model [3, 4]. We find that the method's performance is heavily plagued by the fermionic sign problem, whose extent is primarly related to the number of time-slices in the STD. Nevertheless, the ABQMC equation of state (density vs. chemical potential curve) computed on square-lattice clusters containing up to 48 sites agrees remarkably well with reference methods. We also discuss how the (real-time) dynamics of the survival probability of pure density-wave-like states on 4x4 clusters depends on the filling and the initial density pattern.

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