Variational Two-Particle Density Matrix Calculation for the Hubbard Model Below Half Filling Using Spin-Adapted Lifting Conditions

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(Received 7 November 2011; published 21 May 2012)

The variational determination of the two-particle density matrix is an interesting, but not yet fully explored technique that allows us to obtain ground-state properties of a quantum many-body system without reference to an N-particle wave function. The one-dimensional fermionic Hubbard model has been studied before with this method, using standard two- and three-index conditions on the density matrix [J. R. Hammond *et al.*, Phys. Rev. A **73**, 062505 (2006)], while a more recent study explored so-called subsystem constraints [N. Shenvi *et al.*, Phys. Rev. Lett. **105**, 213003 (2010)]. These studies reported good results even with only standard two-index conditions, but have always been limited to the half-filled lattice. In this Letter, we establish the fact that the two-index approach fails for other fillings. In this case, a subset of three-index conditions is absolutely needed to describe the correct physics in the strong-repulsion limit. We show that applying lifting conditions [J. R. Hammond *et al.*, Phys. Rev. A **71**, 062503 (2005)] is the most economical way to achieve this, while still avoiding the computationally much heavier three-index conditions. A further extension to spin-adapted lifting conditions leads to increased accuracy in the intermediate repulsion regime. At the same time, we establish the feasibility of such studies to the more complicated phase diagram in two-dimensional Hubbard models.

DOI: 10.1103/PhysRevLett.108.213001 PACS numbers: 31.15.aq, 03.65.Aa

The main problem in many-body quantum mechanics, which comprises nuclear physics, quantum chemistry, and condensed matter physics, is the exponential increase of the dimension of Hilbert space with the number of particles. The challenge has therefore been to develop approximate methods which describe the relevant degrees of freedom in the system without an excessive computational cost, i.e., with a polynomial increase. In one of these methods, the N-particle wave function is replaced by the two-particle density matrix (2DM), and over the last decade, a lot of progress has been made in this field [1–6]. For a Hamiltonian,

$$\hat{H} = \sum_{\alpha\beta} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta;\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \quad (1)$$

containing only pairwise interactions, the energy of the system can be expressed as

$$E(\Gamma) = \mathrm{Tr}\Gamma H^{(2)} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \Gamma_{\alpha\beta;\gamma\delta} H^{(2)}_{\alpha\beta;\gamma\delta}, \quad (2)$$

in terms of the 2DM:

$$\Gamma_{\alpha\beta;\gamma\delta} = \langle \Psi^N | a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma | \Psi^N \rangle, \quad (3)$$

and the reduced two-particle Hamiltonian,

$$H^{(2)}_{\alpha\beta;\gamma\delta} = \frac{1}{N-1} (\delta_{\alpha\gamma} t_{\beta\delta} - \delta_{\alpha\delta} t_{\beta\gamma} - \delta_{\beta\gamma} t_{\alpha\delta} + \delta_{\beta\delta} t_{\alpha\gamma}) + V_{\alpha\beta;\gamma\delta}. \quad (4)$$

Second-quantized notation is used where $a_\alpha^\dagger$ (a_α) creates (annihilates) a fermion in the single-particle state α.

In variational density-matrix optimization (V2DM), originally introduced by Löwdin, Mayer, and Coleman [7–9], one exploits this fact and uses the 2DM as a variable in a variational approach. From the resulting 2DM, all one- and two-body properties of the ground state can be extracted. This should not be implemented naively, however, as there are a number of nontrivial constraints that a 2DM has to fulfill in order to be derivable from an N-particle wave function. This is the N-representability problem [9], which was proven to belong, in general, to the QMA-complete complexity class [10]. In practical approaches, one uses a set of conditions which are necessary but not sufficient, and therefore lead to a lower bound on the ground-state energy. The most commonly used are the two-index conditions, called P (or D), Q, and G [9,11], and the computationally much heavier three-index conditions called T_1 and T_2 [12,13]. They all rely on the fact that for a manifestly positive Hamiltonian $\hat{H} = \sum_i \hat{B}_i^\dagger \hat{B}_i$, the expectation value of the energy has to be larger than zero. These conditions can be expressed as linear matrix maps of the 2DM that have to be positive semidefinite. Another type of constraint that has recently been developed is the subsystem or active-space constraints [14–16] in which linear conditions are imposed on only that part of the density matrix that is related to a subspace of the complete single-particle space. This allows one to increase accuracy (in the subspace) without having to use three-index conditions. Such V2DM methods have been used to study a

