Variational reduced-density-matrix calculation of the one-dimensional Hubbard model

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Variational reduced-density-matrix theory is applied to calculating the ground-state energy and two-electron reduced density matrices (2-RDMs) of the one-dimensional Hubbard model for a range of interaction strengths. The 2-RDM is constrained to represent an *N*-particle wave function by two sets of *N*-representability conditions, known as the 2- and partial 3-positivity conditions. Variational optimization of the energy with the 2-RDM constrained by *N*-representability conditions is performed using a first-order semidefinite-programming algorithm that was developed for treating atoms and molecules [D. A. Mazziotti, Phys. Rev. Lett. **93**, 213001 (2004)]. Accurate energies for a broad range of interaction strengths indicate that the variational 2-RDM method is a valuable tool for studying strongly correlated electrons.

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I. INTRODUCTION

When *N* particles in a quantum system interact pairwise, the *N*-particle wave function in the expectation value for the energy can be replaced with a two-particle reduced density matrix (2-RDM) [1]. While this two-particle parametrization of the energy suggests the possibility of a two-particle variational principle [1], variational minimization of ground-state energy of a many-particle quantum system with the 2-RDM yields an unrealistically low result [2]. The 2-RDM must be constrained to represent an *N*-electron density matrix where these constraints are known as *N-representability conditions* [3]. Significant progress on the *N*-representability problem for the 2-RDM has been made in two areas: (i) development of a systematic set of *N*-representability constraints for the 2-RDM [4–13], and (ii) formulation of the 2-RDM minimization as a special type of optimization known as *semidefinite programming* [8–11,14,15], and development of a first-order algorithm [13,16,17] that improves computational efficiency of the optimization by orders of magnitude. Applications have been made recently to molecular electronic energies and properties [9–11,13,18–20] including organic molecules [18] and potential energy surfaces [19] as well as quasispin models [6,8,12,21,22] and a study of the quantum phase transition in the Lipkin model [23]. The accuracy of the 2-RDM ground-state energies and properties at nonequilibrium molecular geometries [13,16–19] and near quantum phase transitions [23] demonstrates the suitability of the 2-RDM method with nonperturbative *N*-representability conditions [10,17] for the treatment of strong quantum correlation effects. In this paper, we explore the application of the variational 2-RDM to Hubbard-like Hamiltonians with a study of the one-dimensional Hubbard model.

The Hubbard model [24–26] is an approximation to a many-electron Hamiltonian in which all electron-electron interactions except same-site (or on-site) Coulomb repulsions are neglected. Although simple, the Hubbard model has been used to describe a wide variety of physics, including superconductivity in copper oxide systems [27] and magnetism in narrow-band systems [28]. In one dimension, a modification of the Hubbard model, known as the Pariser-Parr-Pople (PPP) model [29–31], has been applied extensively to approximate conjugated organic molecules while, more recently, the one-dimensional Hubbard model has been applied to study conducting polymers [32]. Both the Hubbard and the PPP models may be interpreted as extended Huckel models.

The one-dimensional Hubbard model has been studied two ways: (1) by analytic techniques, such as the Bethe ansatz [33], and (2) by numerical techniques. Lieb and Wu [34] first solved the one-dimensional Hubbard model exactly with the Bethe ansatz [25]. Exact numerical solution for a finite lattice, including the explicit wave function, may be obtained by large-scale diagonalization. From the wave function, various properties, such as the momentum distribution and correlation functions, can be studied. Because the analytic solution to the Hubbard model is only available in one dimension, numerical methods are important for understanding extensions of the Hubbard model to two or three dimensions or more general interactions.

Other than diagonalization, quantum Monte Carlo (QMC) and density matrix renormalization group (DMRG) methods have been applied extensively to the Hubbard model. With sufficient computational work both methods can converge (at least theoretically) to the exact solution. In practice, for the two-dimensional Hubbard model the computational cost associated with both methods has limited the applications of QMC and DMRG to 16×16 and 12×12 sites respectively [35,36]. At low temperatures, QMC suffers from the fermionic sign problem although it has the attractive feature of scaling as $\sim|\Lambda|^d$, where $|\Lambda|$ indicates system size and d is the dimension of the lattice. The numerical behavior of DMRG depends on the orbital ordering and thus has varied behavior for Wannier and Bloch representations, because unlike the Wannier basis, the Bloch representation does not have an obvious optimal ordering [37].

In this paper, we perform a finite lattice calculation of the one-dimensional Hubbard model with the variational 2-RDM method. Advantages in the RDM method include: (i) generation of a rigorous *lower bound* on the ground-state energy [10,17], (ii) invariance of the results with respect to unitary transformations of the basis set [38], and (iii) efficient use of

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TABLE I. Errors in the ground-state energies of the half-filled Hubbard model with $|\Lambda|=6$ from the variational 2-RDM method with the DQG and DQGT conditions. Exact full-configuration-interaction (FCI) energies are computed by Lanczos diagonalization. Energies are in dimensionless units.

	FCI		DQG		DQGT	
U	E_{FCI}	E_{CORR}	$E_{\mathrm{RDM}}-E_{\mathrm{FCI}}$	$\%E_{\mathrm{CORR}}$	$E_{\mathrm{RDM}}-E_{\mathrm{FCI}}$	$\%E_{\mathrm{CORR}}$
1	−6.601	−0.203	−0.0161	107.94	−0.0006	100.30
2	−5.409	−0.830	−0.0669	108.06	−0.0046	100.55
3	−4.433	−1.897	−0.1401	107.39	−0.0150	100.79
4	−3.669	−3.334	−0.2094	106.28	−0.0212	100.63
8	−2.048	−10.122	−0.2999	102.96	−0.0338	100.33
20	−0.853	−29.163	−0.1870	100.64	−0.0160	100.05
40	−0.429	−59.573	−0.1009	100.17	−0.0064	100.01
80	−0.215	−119.785	−0.0514	100.04	−0.0016	100.00

both spatial- and spin-symmetries in the *two-electron* basis set of the 2-RDM [13] for the potential treatment of very large systems. Calculations are performed with two sets of *N*-representability conditions on the 2-RDM: (i) the 2-positivity conditions [4,8,10], and (ii) partial 3-positivity conditions [8], including the T_2 condition [11–13]. The 2-RDM energies are compared to the exact energies from the Lieb-Wu equations (before taking the thermodynamic limit) for a broad range of interaction strengths.

II. THEORY

In this section, we define the Hubbard Hamiltonian, summarize the lower-bound variational principle for the ground-state energy as a function of the 2-RDM including the imposed *N*-representability constraints, and develop a measure of correlation for the Hubbard model by using the cumulant (or connected) part of the 2-RDM.

A. Lower-bound variational principle

The one-dimensional Hubbard Hamiltonian in a lattice-site basis set is given by

$$\hat{H}=-\sum_{i}^{|\Lambda|}\sum_{\sigma=\alpha,\beta}(\hat{a}_{i,\sigma}^{\dagger}\hat{a}_{i+1,\sigma}+\hat{a}_{i,\sigma}^{\dagger}\hat{a}_{i-1,\sigma})+U\sum_{i}^{|\Lambda|}\hat{a}_{i,\alpha}^{\dagger}\hat{a}_{i,\alpha}\hat{a}_{i,\beta}^{\dagger}\hat{a}_{i,\beta}, \tag{1}$$

where $\hat{a}_{i,\sigma}^{\dagger}$ and $\hat{a}_{i,\sigma}$ are the creation and annihilation operators, respectively, for a particle at site i with spin σ, and the symbol $|\Lambda|$ represents the number of lattice sites. Periodic boundary conditions are imposed on the lattice. The spin σ of the particle is either $+1/2$ (α) or $-1/2$ (β). In the calculations, the lowest singlet state of the *half-filled* Hubbard model is computed, where half-filled means that the number N of fermions equals the number of lattice sites $|\Lambda|$. Taking the expectation value of the Hamiltonian yields the energy

$$E=\sum_{i,j,k,l}^{|\Lambda|}({}^{1}T_{k,\alpha}^{i,\alpha}\otimes{}^{1}I_{l,\beta}^{j,\beta}+{}^{1}I_{k,\alpha}^{i,\alpha}\otimes{}^{1}T_{l,\beta}^{j,\beta}+{}^{2}U_{k,\alpha;l,\beta}^{i,\alpha;j,\beta}){}^{2}D_{k,\alpha;l,\beta}^{i,\alpha;j,\beta}, \tag{2}$$

where the elements of the one- and two-particle reduced Hamiltonian matrices, ${}^{1}T$ and ${}^{2}U$, respectively, are ${}^{1}T_{k,\sigma}^{i,\sigma}=-1$ if $i=k\pm1$ and ${}^{2}U_{k,\alpha;l,\beta}^{i,\alpha;j,\beta}=U$ if $i=j=k=l$, and

$${}^{2}D_{k,\alpha;l,\beta}^{i,\alpha;j,\beta}=\langle\psi|\hat{a}_{i,\alpha}^{\dagger}\hat{a}_{j,\beta}^{\dagger}\hat{a}_{l,\beta}\hat{a}_{k,\alpha}|\psi\rangle \tag{3}$$

is the two-particle reduced density matrix (2-RDM).

Direct variational minimization of Eq. (2) yields an energy that is unrealistically low because the 2-RDM must be constrained by *N*-representability conditions [3]. A systematic hierarchy of *N*-representability conditions, known as *p*-positivity conditions, has been developed. Coleman and Yukalov [3] and Garrod and Percus [4] originally showed that three different matrix forms of the 2-RDM must be constrained to be positive semidefinite. A matrix is *positive semidefinite* if and only if all of its eigenvalues are nonnegative. These conditions, which are called 2-positivity conditions, have been generalized by Erdahl and Jin [7] and Mazziotti and Erdahl [8] to *p*-positivity conditions which enforce the generalized uncertainty relations for all pairs of Hermitian $p/2$-body operators. Calculations on atoms and molecules [10,11,13] as well as quasi-spin models [8,12,23] show that the lower bound on the ground-state energy rapidly converges with increasing p.

The *p*-positivity conditions may be explained as follows. The *p*-particle RDM may be represented by $(p+1)$ distinct metric (or overlap) matrices M

$$M_{j}^{i}=\langle\Psi|\hat{C}_{i}\hat{C}_{j}^{\dagger}|\Psi\rangle, \tag{4}$$

where each $\hat{C}_i$ is a product of p creation and/or annihilation operators [8]. The three metric matrices of 2-positivity, denoted as the ${}^{2}D$-, ${}^{2}Q$-, and ${}^{2}G$-matrices, can be generated by choosing the operators $\hat{C}_i$ to be products of two creation operators, two annihilation operators, and one creation and one annihilation operator, respectively [8,17]:

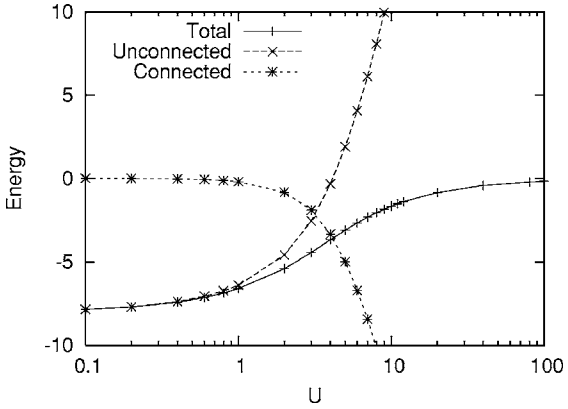

FIG. 1. The total, connected, and unconnected energies as functions of U for the 6-site half-filled Hubbard model. The connected (correlation) energy grows dramatically after $U=6$, while the total energy remains fairly constant due to significant cancelation of the connected and unconnected energies. Energies are computed from the connected part of the 2-RDM obtained from FCI.

$$ {}^2D^{i,j}_{k,l} = \langle\psi|\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}_l\hat{a}_k|\psi\rangle, \tag{5} $$

$$ {}^2Q^{i,j}_{k,l} = \langle\psi|\hat{a}_i\hat{a}_j\hat{a}^\dagger_l\hat{a}^\dagger_k|\psi\rangle, \tag{6} $$

$$ {}^2G^{i,k}_{l,j} = \langle\psi|\hat{a}^\dagger_i\hat{a}_k\hat{a}^\dagger_j\hat{a}_l|\psi\rangle, \tag{7} $$

where the indices refer to a finite basis set of spin orbitals. Each of these metric matrices must be positive semidefinite, which we indicate by ${}^2D \geqslant 0$, ${}^2Q \geqslant 0$, and ${}^2G \geqslant 0$. By rearranging the second-quantized operators in Eqs. (6) and (7), we can express ${}^2Q$ and ${}^2G$ in terms of ${}^2D$, and hence, the 2-positivity conditions for ${}^2Q \geqslant 0$ and ${}^2G \geqslant 0$ restrict the allowed values for ${}^2D$ in the variational expression for the energy in Eq. (2).

If we define the set of $\{\hat{C}_i\}$ to include all products of three creation and/or annihilation operators, we generalize the three 2-positivity metric matrices to obtain four 3-positivity metric matrices:

$$ {}^3D^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}^\dagger_k\hat{a}_n\hat{a}_m\hat{a}_l|\psi\rangle, \tag{8} $$

$$ {}^3E^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}_k\hat{a}^\dagger_n\hat{a}_m\hat{a}_l|\psi\rangle, \tag{9} $$

$$ {}^3F^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}_i\hat{a}_j\hat{a}^\dagger_k\hat{a}_n\hat{a}^\dagger_m\hat{a}^\dagger_l|\psi\rangle, \tag{10} $$

$$ {}^3Q^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}_i\hat{a}_j\hat{a}_k\hat{a}^\dagger_n\hat{a}^\dagger_m\hat{a}^\dagger_l|\psi\rangle. \tag{11} $$

Relating these matrices by linear mappings and restricting them to be positive semidefinite generates the 3-positivity conditions. Approximate 3-positivity conditions, originally proposed by Erdahl [5], are given by

$$ T_1 = {}^3D + {}^3Q \geqslant 0, \tag{12} $$

$$ T_2 = {}^3E + {}^3F \geqslant 0. \tag{13} $$

These special combinations of the 3-positive metric matrices cause the connected (or cumulant) [6,41–44] part of the metric matrices to cancel exactly, and hence, both the T_1 and the T_2 metric matrices can be evaluated with the 2-RDM only [12,13]. The T_1 and T_2 conditions were implemented recently for atoms and molecules [11,13,20] and the Lipkin model [12]. Because previous investigations have the found the T_1 condition to be less important than the T_2 condition [11], it will not be employed in the present paper, and the use of 2-positivity (DQG) and the T_2 condition will be denoted by DQGT.

The 2-RDM and each of the metric matrices are both spin- and symmetry-adapted [13,40]. The spatial symmetry adaptation is accomplished by the Bloch transformation $\hat{a}_k = \Sigma_r e^{ikr}\hat{a}_r, r \in \Lambda$. For $|\Lambda|=6$, the largest RDM block in the

TABLE II. Accuracy of the 2-RDM as a function of the interaction strength U for the lowest singlet state of the half-filled Hubbard model with $|\Lambda|=6$. Spin adaptation of the 2-RDM yields two distinct matrices ${}^2D_s$ and ${}^2D_a$ which are symmetric and antisymmetric respectively in the permutation of their indices [13,40]. The error in the 2-RDM is reported as the L_2 norm of the difference matrix from the approximate 2-RDMs and the exact 2-RDMs from Lanczos diagonalization (FCI).

	Antisymmetric			Symmetric		
		$\|{}^2D_{\mathrm{RDM}} - {}^2D_{\mathrm{FCI}}\|_2$			$\|{}^2D_{\mathrm{RDM}} - {}^2D_{\mathrm{FCI}}\|_2$	
U	$\|{}^2D_{\mathrm{FCI}}\|_2$	DQG	DQGT	$\|{}^2D_{\mathrm{FCI}}\|_2$	DQG	DQGT
1	0.9873	0.0039	0.0010	1.0042	0.0199	0.0049
2	0.9482	0.0137	0.0030	1.0056	0.0410	0.0044
3	0.8834	0.0225	0.0051	0.9910	0.0722	0.0163
4	0.8026	0.0344	0.0088	0.9589	0.1127	0.0241
8	0.5543	0.0641	0.0074	0.8265	0.2056	0.0166
20	0.3798	0.0921	0.0093	0.7383	0.2782	0.0252
40	0.3372	0.0969	0.0078	0.7226	0.2913	0.0204
80	0.3241	0.0981	0.0082	0.7185	0.2946	0.0208

TABLE III. Ground-state energies *per lattice site* $E/|\Lambda|$ of the half-filled Hubbard model with $|\Lambda|=10$ and $|\Lambda|=14$ from the variational 2-RDM method with the DQG and DQGT conditions. The energy errors are reported as energy error per lattice site, that is $(E_{\mathrm{RDM}}-E_{\mathrm{Exact}})/|\Lambda|$. The exact energies were obtained via numerical solution of the Lieb-Wu equations using MAPLE [46]. Energies are in dimensionless units.

	$\|\Lambda\|=10$			$\|\Lambda\|=14$		
		Error per site			Error per site	
U	E_{Exact} per site	DQG	DQGT	E_{Exact} per site	DQG	DQGT
1	−1.0614	−0.0040	−0.0002	−1.0511	−0.0046	−0.0004
2	−0.8638	−0.0162	−0.0009	−0.8539	−0.0185	−0.0024
3	−0.7046	−0.0326	−0.0021	−0.6963	−0.0362	−0.0041
4	−0.5834	−0.0458	−0.0052	−0.5777	−0.0491	−0.0077
5	−0.4933	−0.0533	−0.0075	−0.4895	−0.0561	−0.0094
6	−0.4255	−0.0568	−0.0085	−0.4226	−0.0594	−0.0099
7	−0.3730	−0.0579	−0.0085	−0.3707	−0.0603	−0.0097
8	−0.3315	−0.0576	−0.0082	−0.3295	−0.0599	−0.0089
10	−0.2704	−0.0547	−0.0069	−0.2688	−0.0570	−0.0074
20	−0.1390	−0.0372	−0.0027	−0.1381	−0.0391	−0.0028
100	−0.0281	−0.0087	−0.0002	−0.0279	−0.0093	−0.0001

Wannier representation is 36×36, but in the Bloch representation the largest RDM block is only 6×6. The $|\Lambda|$-fold reduction in matrix rank reduces the computational work by $\sim|\Lambda|^3$. The SU(2) pseudospin symmetry [39] was not used in the present calculations.

B. Correlation analysis

The correlation energy is usually defined as the exact energy in a given finite basis set, obtained from full configuration interaction, minus the Hartree-Fock energy. For strongly correlated systems, however, the Hartree-Fock calculation may not be meaningful. In this paper, we define the correlation energy as the energy from the connected (or cumulant) part ${}^2\Delta$ of the 2-RDM:

$$E=\mathrm{Tr}[{}^2K{}^2\Delta], \tag{14}$$

where ${}^2\Delta$ is defined by the cumulant expansion of the 2-RDM [6,41–44]:

$${}^2D^{i,j}_{k,l}={}^1D^i_k\wedge{}^1D^j_l+{}^2\Delta^{i,j}_{k,l} \tag{15}$$

$$=\frac{1}{2}({}^1D^i_k\otimes{}^1D^j_l-{}^1D^i_l\otimes{}^1D^j_k)+{}^2\Delta^{i,j}_{k,l}. \tag{16}$$

The wedge $\wedge$ denotes the antisymmetric tensor product known as the Grassmann wedge product [6]. Because the mean-field (or unconnected) energy calculated from ${}^1D\wedge{}^1D$ is not necessarily the variationally optimized solution from a Hartree-Fock computation, it will always be an upper bound on the Hartree-Fock energy. Consequently, the correlated (or connected) energy in Eq. (14) is a rigorous lower bound to the conventional value of the correlation energy.

III. COMPUTATIONAL METHODOLOGY

The energy minimization in Eq. (2) with a 2-RDM constrained by N-representability conditions generates a special optimization problem which can be solved by semidefinite programming [8–11,13–17], The 2-RDM semidefinite programming for the DQG conditions was performed with a second-order primal-dual interior-point algorithm implemented in SeDuMi [45], while the optimization for the DQGT conditions was performed with a first-order nonlinear algorithm implemented in RRSDP [16,17]. We calculated total energies for $|\Lambda|=6$, 10, and 14 using the variational 2-RDM method with two levels of N-representability conditions, the 2-positivity conditions (DQG) and the 2-positivity conditions plus the T_2 condition (DQGT). For six sites, correlation (or connected) energies were computed from the connected (or cumulant) part of the 2-RDM. Exact energies were obtained by numerical solution of the exact Lieb-Wu equations using MAPLE [46], while exact RDMs were obtained using the ARPACK [47] Lanczos diagonalization method in MATLAB [48].

IV. RESULTS

For the lowest singlet state of the half-filled Hubbard model with $|\Lambda|=6$, Table I shows the error in the ground-state energy as a function of the interaction strength U. The percentage of correlation energy achieved is always within 10% for the DQG constraints and 1% for the DQGT constraints, which highlights the nonperturbative character of the variational 2-RDM method with the positivity conditions. In general, the addition of the T_2 condition improves the lower bound on the ground-state energy by an order of magnitude. The largest absolute error is obtained when $U=8$,

where competition between kinetic effects and localization effects (U) is strong. As $U \to \infty$, where ordinary perturbation theory fails, the variational 2-RDM method with both DQG and DQGT constraints remain accurate. Figure 1 shows the total, connected, and unconnected energies as a function of U for the 6 site Hubbard model. The connected (correlation) energy grows dramatically after $U=6$, while the total energy remains fairly constant due to significant cancellation of the connected and unconnected energies. In addition to energies, the variational 2-RDM method with positivity conditions yields accurate 2-RDMs for the calculation of other ground-state properties. Table II shows the L_2-norm of the matrix difference between the exact and approximate 2-RDMs. Spin adaptation of the 2-RDM yields two distinct matrices ${}^2D_s$ and ${}^2D_a$, which are symmetric and antisymmetric, respectively, in the permutation of their indices [13,40]. As with the energies, the 2-RDMs calculated by DQGT are generally an order of magnitude more accurate than those of DQG.

With the variational 2-RDM method using the DQG and DQGT conditions, Table III examines the ground-state energies *per lattice site* $E/|\Lambda|$ of the half-filled Hubbard model with $|\Lambda|=10$ and $|\Lambda|=14$. The energy error per site is computed by $(E_{\mathrm{RDM}}-E_{\mathrm{Exact}})/|\Lambda|$ where the exact energies were obtained via numerical solution of the Lieb-Wu equations using MAPLE. The energy per site slightly increases as the number of sites per period $|\Lambda|$ is increased from 10 to 14. This increase reflects the contributions of the correlations with a length scale between 10 and 14. As for $|\Lambda|=6$ the maximum error for $|\Lambda|=10$ and $|\Lambda|=14$ is near $U=8$ where there is strong competition between the kinetic and static terms in the Hamiltonian. The steep increase in absolute error between $U=4$ and $U=8$ for DQGT suggests an increase in the importance of higher-order positivity conditions. As U becomes large, which corresponds to the t-J model, the energies from both DQG and DQGT become more accurate. The addition of the T_2 condition generally improves the lower bound on the ground-state energy by an order of magnitude.

V. CONCLUSIONS

Variational 2-RDM calculations employing positivity constraints known as the DQG and DQGT conditions have been shown to be accurate for the one-dimensional Hubbard model. Although an exact solution for the one-dimensional Hubbard model exists [34], these calculations suggest that the variational 2-RDM method is an excellent candidate for approximate numerical calculations on other strongly correlated lattice models. There exist few, if any, approximate numerical methods that are capable of treating strongly correlated models, such as the Hubbard model, accurately for a wide range of parameters. The potentially exact methods QMC and DMRG are incredibly powerful, but they often require significant computational resources and have well-known limitations.

Important aspects of the variational 2-RDM method are as follows: (i) a distinctive *lower bound* on the ground-state energy is generated, (ii) spin symmetry, which is often difficult for wave-function-based methods, is implemented readily on the *space of two electrons* [13,40], (iii) spatial symmetry permits the 2-RDM to be represented by many small matrix blocks for computational efficiency, and (iv) the positivity conditions are *size extensive*, meaning that the error in the ground-state energy scales linearly with system size. Previous 2-RDM calculations [49] have produced accurate results for zero-dimensional (Lipkin quasi-spin models [8,12,22]), quasi-one-dimensional (atomic chains [50]), and three-dimensional (molecules [18,19] and radicals [20]) quantum systems. The 2-RDM variational method and the N-representability conditions employed in this paper are applicable to a wide variety of quantum systems. Quantum lattice systems with more general kinetic and potential terms could be calculated without modification, and unlike algebraic and perturbative methods, the variational 2-RDM method is not limited to special cases, such as half-filling or special $U/|t|$ values. Because of this generality, variational 2-RDM methods provide an important new tool for studying lattice models, particularly those with strong correlations.

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