Pair State Analysis of the Hubbard Hamiltonian in One Dimension

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Introduction

Since electron interactions act pairwise, the energies of a many-body system can be found from a knowledge of the elements of the two-particle density matrix (2-RDM) [1, 2]. Early attempts, assuming a variational principle for the 2-RDM, resulted in energies significantly lower than the exact values. It was discovered that the 2-RDM obtained in this manner could not be obtained from a many-body wave function. The so-called *N*-representability problem is a set of conditions which are needed to ensure that the 2-RDM is consistent with the *N*-particle wave function [3]. Of the known *N*-representability conditions, the two-positivity conditions *P* and *Q* [3] as well as *G* [4] have received the most widespread use. Several authors have used semi-definite programming (SDP) algorithms to formulate the determination of the ground state energy and the 2-RDM with *N*-representability constraints, obtaining very good results for a variety of molecules [5, 6].

In this research, we use the one-dimensional Hubbard Hamiltonian, $\mathcal{H}$, to analyze the constrained optimization technique in detail. We compare the ground state energies obtained with the SDP approach with the exact energies and also analyze several properties of the exact and SDP results. By using the pair-state basis – eigenstates of the two-particle reduced Hubbard Hamiltonian, $\mathcal{H}'$ – we can both simplify the SDP equations and obtain additional insight into the method. Results are presented as a function of the U/t parameter, which is an indicator of the correlation strength.

The Method

In second quantization, any operator that consists solely of one- and two-body terms can be written as

$$\mathcal{A} = \sum_{ij} \langle i|a_1|j\rangle c_i^\dagger c_j + \frac{1}{2}\sum_{ijk\ell} \langle i,j|a_2|k,\ell\rangle c_i^\dagger c_j^\dagger c_\ell c_k. \tag{1}$$

Then it follows that the expectation value of A with respect to any many-body state is

$$\langle \mathcal{A} \rangle = \mathrm{Tr}\left(a_1\gamma\right) + \frac{1}{2}\mathrm{Tr}\left(a_2\Gamma\right) = \mathrm{Tr}\left(\mathcal{A}'\Gamma\right) \tag{2}$$

where the 1- and 2-RDM are defined as

$$\gamma_j^i = \langle\psi|c_i^\dagger c_j|\psi\rangle \text{ and } \Gamma_{k\ell}^{ij} = \langle\psi|c_i^\dagger c_j^\dagger c_\ell c_k|\psi\rangle \tag{3}$$

and $\mathcal{A}'$ is the reduced operator, defined as

$$\mathcal{A}' = \frac{1}{N-1}\sum_{ij}\langle i|a_1|j\rangle c_i^\dagger c_j + \frac{1}{2}\sum_{ijk\ell}\langle i,j|a_2|k,\ell\rangle c_i^\dagger c_j^\dagger c_\ell c_k. \tag{4}$$

The 1- and 2-RDM satisfy the following conditions:

1. **Hermiticity**
   $\Gamma_{k\ell}^{ij} = \Gamma_{ij}^{k\ell}$
2. **Antisymmetric Condition**
   $\Gamma_{k\ell}^{ij} = -\Gamma_{k\ell}^{ji} = -\Gamma_{\ell k}^{ij}$
3. **Trace Conditions**
   $\sum_i \gamma_i^i = N$ and $\sum_k \Gamma_{jk}^{ik} = (N-1)\gamma_j^i$

Semi-definite Programming

For our semi-definite programming problem, we used the general purpose SDPA code [7]. This code is capable of solving either the primal or dual formulation of SDP. In this case, we chose the dual form

$$\begin{aligned} &\text{maximize} && \mathbf{F}_0 \cdot \mathbf{Y} \\ &\text{subject to} && \mathbf{F}_i \cdot \mathbf{Y} = c_i \end{aligned}$$

where $\mathbf{F}_0$, $\mathbf{F}_i$, and $\mathbf{Y}$ are real symmetric matrices and c_i is a real constant. The notation $\mathbf{A}\cdot\mathbf{B}$ means $\sum_{ij} \mathbf{A}_{ij}\mathbf{B}_{ij}$. In addition, $\mathbf{Y} \geq 0$ (positive semi-definite). If we make the substitution that $\mathbf{F}_0 = -\mathcal{H}'$, where $\mathcal{H}'$ is the reduced Hubbard Hamiltonian [see below], then the maximization problem becomes a minimization one.

N-Representability Conditions

Unfortunately, the 1- and 2-RDM constraints are not enough to guarantee that the solution will be *N*-representable. Therefore, let us define the matrices *Q* and *G* as

$$Q_{k\ell}^{ij} = \langle\psi|c_i c_j c_k^\dagger c_\ell^\dagger|\psi\rangle \tag{5}$$

and

$$G_{k\ell}^{ij} = \langle\psi|c_i^\dagger c_j c_k^\dagger c_\ell|\psi\rangle. \tag{6}$$

The *P*, *Q*, and *G* conditions state that Γ, *Q*, and $G \geq 0$ (positive semidefinite). Due to the commutation relations for the fermion operators, the *Q* and *G* matrices are related to the 1- and 2-RDM by

$$Q_{k\ell}^{ij} = \delta_k^i\delta_\ell^j + \delta_k^i\gamma_\ell^j + \delta_\ell^j\gamma_k^i - \delta_k^j\gamma_\ell^i - \delta_\ell^i\gamma_k^j + \Gamma_{k\ell}^{ij} \tag{7}$$

and

$$G_{k\ell}^{ij} = \delta_\ell^j\gamma_k^i + \Gamma_{jk}^{i\ell}. \tag{8}$$

Here we have used the fact that *Q* has the same antisymmetry property as Γ and thus restricted the indices so that $i < j$ and $k < \ell$ (due to its form, such a restriction cannot be placed upon *G*). These relations for *Q* and *G* serve as additional constraints needed for *N*-representability. Also, it is important to note that these conditions are independent of the system being studied. With these definitions, we are now ready to define $\mathbf{Y}$

$$\mathbf{Y} = \begin{pmatrix} \boldsymbol{\Gamma} & & \\ & \mathbf{Q} & \\ & & \mathbf{G} \end{pmatrix}$$

The Hubbard Hamiltonian

For our model we chose the one-dimensional Hubbard Hamiltonian, which in second quantization is written as

$$\mathcal{H}(t,U) = -t\sum_{\langle i,j\rangle} c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}. \tag{9}$$

From this definition, the reduced Hubbard Hamiltonian is

$$\mathcal{H}' = \mathcal{H}\left(\frac{t}{N-1}, U\right) \tag{10}$$

and $\langle\mathcal{H}\rangle$ can be written as

$$\langle\mathcal{H}\rangle = \mathrm{Tr}\left(\mathcal{H}'\Gamma\right). \tag{11}$$

Finally, without loss of generality we have constructed our many-body base states such that

$$N_\uparrow - N_\downarrow = \begin{cases} 0, & N \text{ even} \\ 1, & N \text{ odd} \end{cases} \tag{12}$$

The Pair Representation

For the Γ and *Q* matrices, we will define the two-particle basis $\phi_{ij}^{(s,m)}$

$$\phi_{ij}^{(1,1)} = c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger \tag{13}$$

$$\phi_{ij}^{(1,-1)} = c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger \tag{14}$$

$$\phi_{ij}^{(1,0)} = \sqrt{\frac{1}{2}}\left(c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger\right) \tag{15}$$

$$\phi_{ij}^{(0,0)} = \sqrt{\frac{1}{2}}\left(c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger\right) \tag{16}$$

With these states as a basis, $\mathcal{H}'$, Γ, and *Q* are block diagonal. If the many-body state $|\psi\rangle$ we are interested in consists of an even number of electrons, these matrices consist of four blocks corresponding to the (s,m) pairs $(1,1)$, $(1,0)$, $(1,-1)$, and $(0,0)$. In the case of an odd number of electrons, there are only three blocks, each with a different *z*-component of spin, *m*.

Using these two-particle states, we can then diagonalize $\mathcal{H}'$ to find both its eigenstates $|\phi_a\rangle$ which satisfy the eigenvalue equation

$$\mathcal{H}'|\phi_a\rangle = E_a|\phi_a\rangle \tag{17}$$

and are also eigenstates of the total spin operator. These states $|\phi_a\rangle$ are what we are referring to when we mention the *pair representation*. As a many-body state we will use the ground state of $\mathcal{H}$, thus simplifying (11) to become

$$\epsilon_o = \sum_a \left(E_a\Gamma_a^a\right). \tag{18}$$

The 2-RDM appearing in this equation is now written in terms of the pair representation. Changing the 2-RDM used in the *Q* and *G* constraint relations given earlier to this basis is not difficult, since the two representation are easily related by

$$\Gamma_{k\ell}^{ij} = \sum_{aa'} \Gamma_{a'}^a \alpha_{ij}^{(a)} \alpha_{k\ell}^{a'} \tag{19}$$

where

$$|\phi_a\rangle = \sum_{i<j} \alpha_{ij}^a c_i^\dagger c_j^\dagger|0\rangle. \tag{20}$$

It is important to note that *G* can also be decomposed into smaller blocks, thus greatly reducing the number of constraints needed.

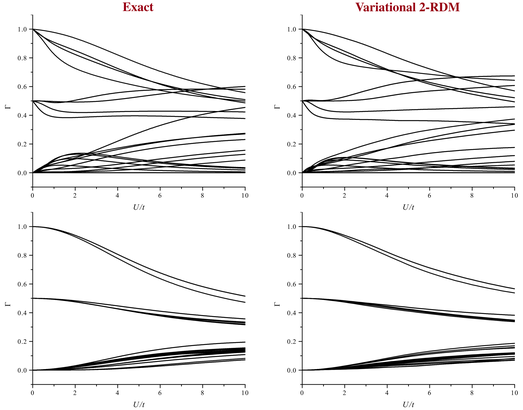

Figure 1: A comparison of the diagonal elements of Γ using exact diagonalization (*left*) and using the SDPA (*right*) for the case of 8 sites at half-filling and periodic boundary conditions. The $s = 0$ weight functions are shown on *top* while the $s = 1$ weight functions are plotted on *bottom*. In the case of the singlet states, at $U/t = 0$ only the lowest energy weight functions are nonzero. There are $\Lambda = N = N_s = 8$ high energy pair states, whose energies increase nearly linearly with U/t. The weight functions for these states are zero at $U/t = 0$ and approach 0 as $U/t \to \infty$. While the variational 2-RDM method appears to constrain these high energy states fairly well for all U/t, the lowest energy states show some considerable disagreement as U/t increases.

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Energy Comparison

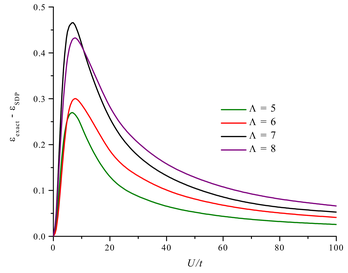

Figure 2: Differences between the dimensionless exact ground state energies of various periodic half-filled Hubbard systems to the variational 2-RDM method using the *P*, *Q*, and *G* conditions. The error is greatest when $7 \leq U/t \leq 8$, an observation which has been previously made [6]. As $U/t \to \infty$ the differences slowly decrease.

Comparison of Antiferromagnetism

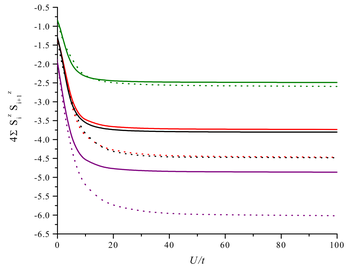

Figure 3: Comparison of the expectation value of the antiferromagnetic ordering operator $(4\sum_i S_i^z S_{i+1}^z)$ with respect to the exact ground state (solid lines) and the ground state obtained through the variational 2-RDM method (dotted lines) for various half-filled Hubbard systems. While Figure 2 shows that the error of the energies diminishes as U/t gets large, the error of this property is at a maximum in the same limit.

Comparison of Double Occupancy

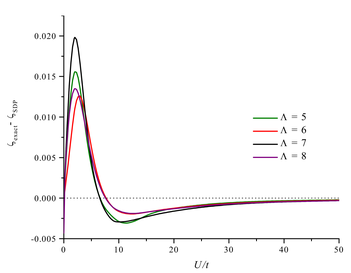

Figure 4: Difference between the expectation value of the double occupancy operator $\zeta = \frac{1}{N}\sum_i n_{i\uparrow}n_{i\downarrow}$ with respect to the exact ground state and the ground state obtained by the SDPA for various half-filled systems. At $2 \leq U/t \leq 3$, the deviation between the exact and SDP results is a maximum. As $U/t \to \infty$, the magnitude of this deviation approaches zero.

Conclusions

Using the *P*, *Q*, and *G* conditions for *N*-representability, we used the variational method for finding the 2-RDM to calculate the ground state energy of several half-filled one-dimensional Hubbard chains with periodic boundary conditions. As a two-electron basis, we used the pair states, which are eigenstates of the reduced Hubbard Hamiltonian.

Comparisons between the variational and exact energies as a function of the dimensionless Coulomb parameter U/t showed the greatest error when $7 \leq U/t \leq 8$. In the limit as $U/t \to \infty$, the variational and exact energies converged in all the cases we studied. However, a direct comparison of the weight functions shows that for several pair states there is significant deviation from the exact values with increasing U/t. These pair states (many of which have an energy that approaches 0 as U/t increases) do not have a large contribution to the energy calculation. However, this deviation suggests that while the energy calculations are converging in the strongly coupled limit, some of the properties of the wave functions are not.

When comparing the expectation values of an operator that measures double occupancy for the variational and exact wave functions, we found that they also converged in the large U/t limit. For $2 \leq U/t \leq 3$ the variational results gave the most disagreement.

However, and most interestingly, the antiferromagnetic ordering of the two wave functions does *not* converge in the strongly coupled limit. In fact, the difference between the two was a maximum in this limit for all the half-filled cases studied. This difference appears to be partially attributable to the weight functions for the pair states with energies near zero for large U/t.

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