EQSE Diagonalization of the Hubbard Model

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Abstract
The application of enhanced quasi-sparse eigenvector methods (EQSE) to the Hubbard model is attempted. The ground state energy for the 4x4 Hubbard model is calculated with a relatively small set of basis vectors. The results agree to high precision with the exact answer. For the 8x8 case, exact answers are not available but a simple first order correction to the quasi-sparse eigenvector (QSE) result is presented.

1 Introduction

The enhanced quasi-sparse eigenvector (EQSE) method of solving quantum field theory Hamiltonians is the combination of quasi-sparse eigenvector (QSE) method [1] with a stochastic calculation for the contribution of the remaining basis states [2]. The Hubbard model was chosen as a laboratory for testing this method for several reasons. First, we believed the approach could yield results. The basis vectors can be specified in a few words of data and the Hamiltonian is sparse in momentum space. On the other hand, the ground state of the Hubbard model is known for its inclusion of an extraordinary number of Fock states [3] so the model presents a non-trivial challenge to the quasi-sparse approach. Finally, the Hubbard model is thought to be a physically relevant model for superconductivity [3]. While the description of the model is simple, solutions have been difficult and any promising new approach is worthwhile.

We work on a 2-dimensional spatial lattice with the Hubbard Hamiltonian

\[ H = -t \sum_{\sigma = \uparrow, \downarrow} (c_i^{\sigma} c_j \sigma + c_j^{\sigma} c_i \sigma) + U \sum_{<i,j>} (c_i^{\uparrow} c_i^{\uparrow} c_i^{\downarrow} c_i^{\downarrow}) \]
There are 2 species of electron so there are 4 possible states for each lattice site. Thus the 8x8 Hubbard model has $4^{64}$ dimensions. Even after using particle conservation to partition the space there are more than $10^{32}$ basis vectors. In this large space the Hamiltonian is clearly sparse but the equality of the off-diagonal elements contributes to an extraordinary number of Fock states in the ground.

It is thought that the D-wave correlator $C_{d_{x^2-y^2}}(r)$ is an important indicator of superconductivity [4].

2 Hamiltonian Momentum Lattice Formulation

After making space periodic we use the Fock states as our basis set. The Hamiltonian conserves momentum which helps limit the number of relevant basis states.

\[
H_{\text{kin}} = -2t \sum \left( \cos \frac{\pi n}{L} + \cos \frac{\pi n}{L} \right) a_{n,\sigma}^\dagger a_{n,\sigma}
\]

\[
V = \frac{U}{4L^2} \sum \delta_{k-l} \delta_{m-n} a_{kp}^\dagger a_{iq}^\dagger a_{mr} a_{ns}^\dagger
\]

\[
k - l + m - n = 0
\]
\[
p - q + r - s = 0
\]

There is a 16 member symmetry group generated by reflections in the $x$ and $y$ planes, $x \leftrightarrow y$ and $\downarrow \leftrightarrow \uparrow$. For the purpose of finding the ground state, we use only symmetrized basis states.

The first step in the calculation consists of picking a basis set of size $N$ and diagonalizing its submatrix of the Hamiltonian using the Lanczos method [5]. The $\frac{N}{2}$ basis vectors which least contribute to the ground are then discarded, replacements are chosen and the Hamiltonian is again diagonalized. When the ground energy $E_0$ obtained in this manner converges the QSE step is complete.

The EQSE is a first order correction to this result. We calculate it stochastically. Let $C$ be a set of basis vectors for the complement of the $N$-dimensional subspace. Then, choosing representative basis vectors $v \in C$ with probability $P(v)$.

\[
E = E_0 + \text{Average} \frac{FO(v)}{P(v)}
\]
\[
FO(v) = \frac{\langle 0 | H | v \rangle \langle v | H | 0 \rangle}{\lambda_v}
\]

where $|0\rangle$ is the ground state of the $N$ dimensional subspace. The expectation
is thus

\[ E = E_0 + \sum_{v \in C} P(v) \frac{FO(v)}{P(v)}. \]

### 3 Results

Results were obtained for the ground state energy, wavefunction and \(d\)-wave correlator. The computing time was about 2 days on a 350Mhz Pentium II. Where available, we compare with Husslein et al [4] results labeled Exact, Projector Quantum Monte-Carlo (PQMC), and Stochastic Diagonalization (SD) (which uses a different method of choosing the subspace than QSE).

| Coupling | States | QSE         | EQSE         | Exact         | SD  | PQMC |
|----------|--------|-------------|-------------|---------------|-----|------|
| U=2      | 50     | -.47471     | -.50127(5)  |               |     |      |
|          | 100    | -.47967     | -.50147(5)  | -.50194       | -.501|-.49 |
|          | 500    | -.49454     | -.50181(3)  |               |     |      |
|          | 1000   | -.50062     | -.50198     |               |     |      |
| U=4      | 50     | -1.5707     | -1.80635(5) |               |     |      |
|          | 100    | -1.6203     | -1.8113(4)  | -1.8309       | -1.829|1.8(2)|
|          | 500    | -1.7476     | -1.8242(3)  |               |     |      |
|          | 1000   | -1.8003     | -1.8302     |               |     |      |
| U=5      | 50     | -2.2450     | -2.6663(8)  |               |     |      |
|          | 100    | -2.3322     | -2.6724(7)  | -2.7245       | -2.723|2.9(3)|
|          | 500    | -2.5578     | -2.7073(4)  |               |     |      |
|          | 1000   | -2.6512     | -2.7208(2)  |               |     |      |
|          | 2000   | -2.685      | -2.7231     |               |     |      |
| U=6      | 50     | -2.963      | -3.615      |               |     |      |
|          | 100    | -3.103      | -3.635      |               |     |      |
|          | 1000   | -3.452      | -3.697      |               |     |      |
|          | 2000   | -3.595      | -3.723      |               |     |      |
The $d_{x^2-y^2}$ correlator was also obtained using the QSE algorithm. The 4x4 result again matched that of Husslein et al [4]. The EQSE calculation has not been completed and we therefore omit the data.
4 Conclusion

As we can see, the ground state for the 4x4 Hubbard model can be well described with about 1000 symmetrized states and the 50 state results yield remarkable accuracy when the first order correction is included. In the 8x8 case it is clear that even 4000 states are not sufficient to describe the ground state. The precision of the first-order values will be determined with the completion of higher order calculations.

Further advances will come in the refinement of the enhancement technique. Better importance sampling will speed convergence of second and higher orders contributions. Other extensions will be calculation of excited states of the Hamiltonian, correlation functions, binding energies and other quantities of interest.

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References

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