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Ground state energy of the Hubbard Hamiltonian: Perturbative results.

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Abstract

The ground state energy of the single-band Hubbard model on the one dimensional lattice is computed using perturbation theory. It is shown that for two electrons the results obtained gets better as the positive on-site coulomb interaction (U) and the number of sites N are increased provided the ratio $\left(\frac{U}{N}\right)$ ***is made small. In other words, contrary to expectations, perturbation theory is applicable even if U is chosen to be large provided N is also chosen large enough so that the ratio*** $\frac{U}{N}$ ***is small.***

I.0 Introduction

One of the major goals of condensed matter physics during the past decades has been to understand the role of electronic correlations in solids[1]. The underlying physical mechanism of this correlation is captured by the single-band Hubbard model[2],

$$H = -t\left[\sum_{\langle i,j\rangle\sigma} c_{i\sigma}^{+} c_{j\sigma} + h.c\right] + U\sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{1.1}$$

Here $c_{i\sigma}^{+}$, $c_{j\sigma}$ are the creation and annihilation operators respectively for an electron of spin σ in the Wannier state. $\langle i, j\rangle$ means the summation is only over nearest neighbour sites, $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$ are the number operators, *t* is the electronic hopping parameter between nearest neighbour sites *i* and *j*.*h.c* denotes Hermitian conjugation and U is the on-site interaction energy. The validity and convenience of perturbation theory in the context of the Hubbard model has been proved very recently [2] for small U values.

In this work we have shown that perturbation theory give correct result for the ground state energy when U and the number of lattice sites N are both large, provided the ratio $\left(\frac{U}{N}\right)$ is made small. This is an extension of the work of Galan and Verges (1991 [3]), Okanigbuan and Idiodi, (2006 [2]), where the perturbation theory works up to intermediate – *U* – values as large as *U* = 4. Firstly, we discuss the formulation and the present the results. Finally, we draw up some conclusions.

2.0 Fundamentals of the pertubative method

The idea of the present approach is to divide the Hamiltonian equation (1.1) in two parts, and consider the interaction part as a perturbation. $H = H_0 + H_1$ where

$$H_0 = -t\left[\sum_{\langle i,j\rangle\sigma} c^+_{i\sigma} c_{j\sigma} + h.c\right] \tag{2.1}$$

is the kinetic energy term, and

$$H_1 = U\sum_i n_{i\uparrow} n_{i\downarrow} \tag{2.2}$$

describes the interaction between electrons on the same site.

The perturbation calculation begins by constructing the one-electron Bloch wave functions that diagonalize H_0, and which are

$$\phi_{k\sigma} = \frac{1}{L}\sum_{R_j} e^{ik.R_j} c_{j\sigma} \tag{2.3}$$

$$\phi^+_{k\sigma} = \frac{1}{L}\sum_{R_j} e^{-ik.R_j} c^+_{j\sigma}\left|o\right\rangle \tag{2.4}$$

where R_j runs over all the cluster sites, and the allowed wave vectors k have the form

$$\vec{k}_i = \frac{2\pi l}{L}\hat{x},\ L = 1,\ l = 1,2,\Lambda\ ,$$

These states satisfy periodic boundary conditions and diagonilize H_0 with eigenenergies

$$\varepsilon(k_l) = -t\cos\frac{2\pi l}{L}, \tag{2.5}$$

for 2 electrons on 2 sites, and

$$\varepsilon(k_{_l}) = -2t\cos\frac{2\pi l}{L}, \tag{2.6}$$

For 2 electrons on N sites N > 2.

In the Hartree-Fock approximation the wave function for the ground state of the system can be written as

$$\Psi_0 = \left[\prod_{E_V \le E_F} A^+_V\right]\Psi_{Vac} \tag{2.7}$$

which contain creation operators referring to al filled levels below the Fermi level E_F. Using (8) one can construct many-body wave functions of the Hatree-Fock type.

$$\Psi_0 = \left[\prod_{n=1}^{M} \phi^+_{k_n\sigma_n}\right]\left|0\right\rangle \tag{2.8}$$

where M is the total number of electrons moving in the cluster and

$$\vec{k} = \sum_{n=1}^{M} k_n,\ \vec{\sigma} = \sum_{n=1}^{M} \sigma_n \tag{2.9}$$

In this way we classify many-body wave functions according to both wave vector $\vec{k}$ and spin $\vec{\sigma}$. The number of wave functions is restricted to those that provide the smallest kinetic energy T_0 for the 2 electrons.

$$T_0 = \sum_{n=1}^{2} \varepsilon(k_n) \tag{2.10}$$

The ground state energy matrix to second order in the perturbation U is given by

$$\left\langle \Psi^\alpha_{k\sigma}\left\|H\right\|\Psi^\beta_{k\sigma}\right\rangle = T_0 + \left\langle \Psi^\alpha_{k\sigma}\left\|H_1\right\|\Psi^\beta_{k\sigma}\right\rangle + \sum_\delta \frac{\left\langle \Psi^\alpha_{k\sigma}\left\|H_1\right\|\Psi^\delta_{k\sigma}\right\rangle\left\langle \Psi^\delta_{k\sigma}\left\|H_1\right\|\Psi^\beta_{k\sigma}\right\rangle}{T_0 - T^\delta_0}$$

(2.11)

The ground state wave function is given by

$$\Psi_{gs} = \sum_{\alpha} c_{\alpha} \Psi_{k\sigma}^{\alpha} + \sum_{\delta} D_{\delta} \Psi_{k\sigma}^{\delta} \tag{2.12}$$

where the zero-order coefficient c_α are obtained from the diagonalization of the second-order Hamiltonian matrix (equation 2.11) whereas first-order coefficients D_δ are given by

$$D_{\delta} = \sum_{\alpha} \frac{\Psi_{k\sigma}^{\delta} \| H_1 \| \Psi_{k\sigma}^{\alpha}}{T_0 - T_0^{\delta}} \tag{2.13}$$

3.0 Results

Using the perturbation method of II, we obtain ground state energies and wave functions for 2 electrons on N sites of 1D lattice N = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 40, 80. For N = 2, the ground state energy is given by

$$E_g = -2t + U \tag{3.1}$$

and the corresponding ground state wave function is

$$\Psi_{gs} = \tfrac{1}{2}\left[\left|1\uparrow 1\downarrow\right\rangle + \left|2\uparrow 2\downarrow\right\rangle + \left|1\uparrow 2\downarrow\right\rangle - \left|1\downarrow 2\uparrow\right\rangle\right] \tag{3.2}$$

For $N > 2$.

$$E_g = -4t + 2\frac{U}{N} \tag{3.3}$$

and the corresponding ground state wave function is

$$\Psi_{gs} = \tfrac{1}{N}\left[\sum_{i=1}^{N}\left|i\uparrow i\downarrow\right\rangle + \sum_{\substack{i,j=1 \\ i\neq j}}^{N}\left[\left|i\uparrow j\downarrow\right\rangle - \left|i\downarrow j\uparrow\right\rangle\right]\right] \tag{3.3}$$

N	Perturbation	Variation
2	2.0000	-0.8284
4	-2.0000	-3.4186
6	-2.6667	-3.6845
8	-3.0000	-3.8005
10	-3.2000	-3.8622
12	-3.3333	-3.8990
14	-3.4286	-3.9228
16	-3.5000	-3.9390
18	-3.5556	-3.9506
20	-3.6000	-3.9592
40	-3.8000	-3.9888
80	-3.9000	-3.9971

Table 3.1: Ground State Energy (Eg/t) as a function of *N*, for $U/4t = 1$

N	Perturbation	Variation
2	6.0000	-0.4721
4	0.0000	-3.2078
6	-1.3333	-3.5984
8	-2.0000	-3.7572
10	-2.4000	-3.8374
12	-2.6667	-3.8835
14	-2.8571	-3.9125
16	-3.00000	-3.9318
18	-3.1111	-3.9454
20	-3.2000	-3.9553
40	-3.6000	-3.9883
80	-3.8000	-3.9970

Table 3.2: Ground state energy (Eg/t) as a function of *N*, for $U/4t = 2$

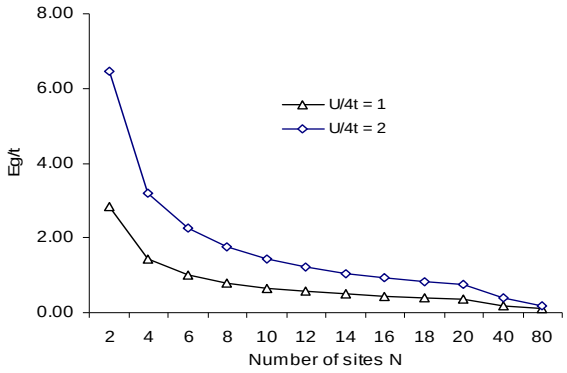

Figure 1 Difference in values of Eg/t as a function of N from Perturbation and Variation

Figure 3.1: Difference in values of Eg/t as a function of *N* between perturbation method and variational method

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4.0 Discussion

We have computed ground state energies for 2 electrons on N sites, when $\frac{U}{4t}=1$ and $\frac{U}{4t}=2$ using equations (3.1) and (3.3). Results obtained were compared with the result of Chen and Mei (1989 [4]).obtained using variational calculation.

In Table 3.1, when $\frac{U}{N}=2$, that is $\frac{U}{4t}=1$ and N =2 in units where the hopping integral t = 1, perturbation calculation gives 2.0000 for the energy while the value obtained from variational calculation is -0.8284. In Table 2, when $\frac{U}{N}=0.1$, that is $\frac{U}{4t}=2$ and N = 80, perturbation calculation gives -3.8000 for the energy while the value obtained from variational calculation is -3.9970. There is significant deviation in the values obtained by both methods when $\frac{U}{N}$ is large. Thus, perturbation calculation is favoured by small values of the ratio $\frac{U}{N}$. In Figure 3.1, we have plotted the difference in values of $\frac{E_g}{t}$ against the number of sites N for $\frac{U}{4t}=1$ and $\frac{U}{4t}=2$ respectively. It is shown in the graph that for large N, say 80, the energy difference is very small.

The total energy given by the Gutzwiller ansatz is $-4t\left(1-\frac{1}{N}\right)$ in the infinite –U limit, and the one given by the correlated ground state in the large –U limit asymptotically is $-4t\left(1-\frac{5}{N^2}\right)$ and they both agree with the one given by perturbation method $-4t+2\frac{U}{N}$ for very large N.

5.0 Conclusion

It is well known that perturbation theory breaks down when U is large. In this study, we have been able to show that even if U is large, provided we increase the number of sites N sufficiently enough such that $\frac{U}{N}$ is small we can still apply perturbation theory. The crucial parameter is not just U but $\frac{U}{N}$.

References

[1] Volthardt, D., Potthoff, M. and Eckstein, M. (2007) Phys Rev. B75 (125103-1)
[2] Okanigbuan, R. O. and Idiodi, J. O. A. (2006) J. Nig. Assoc. Math. Phys. 10 (583-594).
[3] Galan, J. and Verges, J. A. (1991) Phys. Rev. B44 (10093)
[4] Chen, L. and Mei, C. (1989) Phys. Rev. B39 (9006)
[5] Dagotto, E., Morico, A. and Barnes, T. (1989) Phys. Rev. B40 (6721)
[6] Pairault, S. Sencchal, D. and Tremblay, A. M. S. (2000) Eur. Phys. J. b16(85)
[7] Enaibe, A. E. and Idiodi, J. O. A. (2003). J. Nig. Assoc. Math Phys. 7 (275)
[8] Maska, M. M. (1989) Phys Rev. B51 (8759)