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The ground state of the Hubbard model

E.O. Aiyohuyin, A.A. Oni-Ojo
Department of Physics,
University of Benin, Benin City, Nigeria.

Abstract

The Hubbard Hamiltonian was diagonalized using Valatin-Bogojiubov transformations. The following results were obtained:

$$U_i^2 = \frac{\left(\varsigma_i^2 - 2\Delta_i^2\right)}{2\left(\varsigma_i^2 - \Delta_i^2\right)} \pm \sqrt{\frac{(2\Delta_i^2 - \varsigma_i^2)^2 + 4\left(\varsigma_i^2 - \Delta_i^2\right)\left(\Delta_i^2\right)}{4\left(\varsigma_i^2 - 2\Delta_i^2\right)^2}}$$

$$V_i^2 = 1 - U_i^2$$

V_i and U_i are numbers defined for positive values of i. The energy of the quasiparticle vacuum was found to be

$$E_0 = \sum_{<iJ>} (t_{ij} - \lambda) V_i^2 + U \sum_i V_i^4$$

And the number of particles in the ground state was found to be N_o

$$N_0 = \sum_i \left\{ 1 - \frac{\left(\varsigma_i^2 - 2\Delta_i^2\right)}{2\left(\varsigma_i^2 - \Delta_i^2\right)} \pm \frac{\sqrt{\left(2\Delta_i^2 - \varsigma_i^2\right)^2 + 4}\left(\varsigma_i^2 - \Delta_i^2\right)\Delta_i^2}{2\left(\varsigma_i^2 - \Delta_i^2\right)} \right\}$$

where $\varsigma_i = (\lambda - t_{ij})$, $\Delta_i = -\Sigma U U_i V_i$, t is the hopping parameter, U is the on-site interaction, λ is the Lagrange multiplier.

1.0 Introduction

The Hubbard Hamiltonian describes electrons on a lattice with one orbital per site. The Hamiltonian has the form: $H = \sum_{<ij>,\sigma} t_{ij} a_{i\sigma}^{+} aj\sigma + \sum_i u n_{i\uparrow} n_{i\downarrow}$ where t_{ij} is the hopping matrix element between different sites. Electrons on the same site are the only ones that interact. $n_{i\sigma} = a_{i\sigma}^{+} a_{i\sigma}$ is the occupation number operator.

In Fock space, all systems with an arbitrary number of particles in them, get diagonalized simultaneously. This is why Fock space calculations are more powerful then configuration space. Once our physical problem is expressed in the term of a diagonalization of a certain matrix one can resort to any approximate method that is justifiable mathematically. One of the most powerful methods of approximating the eigenvalues of H involves the transformation to a scheme that mixes states of different numbers of particles.

Bogoljubov and Valatin suggested the following canonical transformation from a_i to the operators α_i through

$$\alpha_i = U_i a_i - V_i a_{-i}^+,\ \alpha_{-i} = U_i a_{-i} + V_i a_i^+ i > 0 \tag{1.1}$$

Here *Ui* and *Vi* are numbers defined only for positive values of *i.*

$$\alpha_i^+ = U_i a_i^+ - V_i a_{-i},\ \alpha_{-i}^+ = U_i a_{-a}^+ + V_i a_i i > 0 \tag{1.2}$$

The α_I operators satisfy the anticommutation relations $\left[\alpha_{ia}^+, \alpha_{j\sigma'}\right]_+ = \delta_{ji}\delta_{a\sigma'}$, U_i and V_i satisfy $U_i^2 + V_i^2 = 1$. It is observed that since the α_i's obey Fermion anticommuntation rules the numbers operator in "α space" $\alpha_i^+ \alpha_i$ will have eigenvalue 1 or 0. Equations (1.1) and (1.2) can be inverted to express the a_i's in terms of the $\alpha_i's$:

$$a_i = U_i \alpha_i + V_i \alpha_{-i}^+,\ a_{-i} = U_i \alpha_{-i} - V_i \alpha_i^+ i > 0 \tag{1.3}$$

$$a_i^+ = U_i \alpha_i^+ - V_i \alpha_{-i},\ a_{-i}^+ = U_i \alpha_i^+ + V_i \alpha_{-i} i > 0 \tag{1.4}$$

2.0 Calculations

The non interacting part of the Hubbard Hamiltonian is diagonalized first.

$$H_0 = \sum_{<ij>\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} \tag{2.1}$$
$$= \sum_{<ij>} t_{ij} \left(U_i^2 \alpha_i^+ \alpha_{-i} - U_i V_i \alpha_i^+ \alpha_i^+ - V_i U_i \alpha_{-i} \alpha_{-i} + V_i^2 \alpha_{-i} - \alpha_i^+\right)$$

To solve for the energy of the system described by H_o subject to the condition that the average number of particles is fixed one has to introduce the Lagrange multiplier λ multiplying the number operator $\hat{N}$, where $\hat{N} = \sum_{<ij>}^{n} a_i^+ a_j$. We are thus looking for the eigrenvalues and eigenfunctions of

$$H - \lambda \hat{N} = \sum_{<ij>} \left(t_{ij} - \lambda\right)\left(U_i^2 \alpha_i^+ \alpha_{-i} - U_i V_i \alpha_i^+ \alpha_i^+ - V_i U_i\ \alpha_{-i} \alpha_{-i} + V_i^2 \alpha_{-i} \alpha_i^+\right)$$
$$= \sum \left(t_{ij} - \lambda\right)\left\{\left(U_i^2 - V_i^2\right)\alpha_i^+ \alpha_{-i} + V_i^2 - U_i V_i \alpha_i^+ \alpha_i^+ - V_i U_i\ \alpha_{-i} \alpha_{-i}\right\} \tag{2.2}$$

where λ is to be fixed by the prescribed expectation value of $\hat{N}$. $N = \left\langle \hat{N} \right\rangle$

The operators $\alpha_i^+ \alpha_i^+$ and $\alpha_{-i} \alpha_{-i}$, however, do not commute with $\hat{N}_\alpha$. Hence to diagonalize H-λ $\hat{N}$, we choose U_i and V_j such that the last two terms in equation (2.2) vanish. This leads to the result

$$U_i V_i = 0 \text{ for all } i\text{'s} \tag{2.3}$$

Taking equation (2.3) with the condition $V_i^2 + U_i^2 = 1$. We have that if

$$V_i = 0,\ U_i = 1 \text{ or } U_i = 0,\ V_i = 1$$

The lowest eigenstate of H - λ $\hat{N}$ is the quasi-particle vacuum 10 > α. It satisfies

$$\left(H - \lambda \hat{N}\right)\left| 0 \right\rangle_\alpha = \sum_{\langle ij \rangle_\sigma} \left(t_{ij} - \lambda\right) V_i^2 \left| 0 \right\rangle_\alpha$$

The lowest eigenvalue of H - $\lambda \hat{N}$ is obtained by setting $V_i = 1, U_i = 0$ *if* $t_{ij} < \lambda$, V_i =0, U_i = 1, if

$t_{ij} > \lambda$. The value of λ can be determined by the condition $\alpha\left\langle 0\left|\hat{N}\right|0\right\rangle_\alpha = \sum_i V_i^2 = N_o$. Let us now go over to the Hubbard Hamiltonian $H = \sum_{\langle ij\rangle_\alpha} t_{ij} a_{i\sigma}^+ a_{j\sigma} + U\sum_i a_{i\sigma}^+ a_{i\sigma} a_{i\sigma}^+ a_{i\sigma}$ (2.4)

Introducing the transformations of equations (1.3) and (1.4) we have $H = A + H_{11} + H_{20} + H'$

where $A = \sum_{\langle ij\rangle} t_{ij} V_i^2 + U\sum_i V_i^4$

$$H_{11} = \sum_{<ij>} t_{ij}\left(U_i^2 - V_i^2\right)\alpha_i^+\alpha_{-i} + \sum_i U\left(U_i^4\alpha_i^+\alpha_i + U_i^2V_i^2\alpha_{-i}^+\alpha_{-i} - U_i^2V_i^2\alpha_i^+\alpha_i - V_i^4\alpha_{-i}^+\alpha_{-i}\right)$$

$$H_{20} = -\sum_{<ij>} t_{ij}\left(U_iV_i\alpha_i^+\alpha_i^+ + V_i\,U_i\alpha_{-i}\alpha_i\right) + \sum_i U(U_i^3\,V_i\alpha_i^+\alpha_{-i}^+ - V_i\,U_i^3\alpha_i^+\alpha_i^+ - 2V_i^3U_i\alpha_i^+\alpha_{-i}^+$$

$$- U_i^3V_i\alpha_{-i}\alpha_i + V_i\,U_i^3\alpha_i\,\alpha_i + 2V_i^3U_i\alpha_{-i}\alpha_i - V_i^3U_i\alpha_{-i}\alpha_{-i} + V_i^3U_i\alpha_i\,\alpha_{-i} + V_i^3U_i\alpha_{-i}^+\alpha_{-i}^+$$

$$- V_i^3U_i\alpha_{-i}^+\alpha_i^+\Big)$$

H' is proportional to terms containing four α's operators and is neglected in this work.

To ensure that there is a fixed number of real particles in the quasiparticle ground state one imposes the condition.

$$\left\langle\hat{N}\right\rangle = \sum_{\langle ij\rangle}\left(V_i^2 - V_i^2\alpha_i^+\alpha_{-i} + U_i^2\alpha_i^+\alpha_{-i} - U_iV_i\alpha_i^+\alpha_i^+ - V_iU_i\alpha_{-i}\alpha_{-i}\right) = N_o \qquad - \qquad (2.6)$$

This can be achieved by diagonalizing H-$\lambda \hat{N}$, and choosing the lagrange multiplier λ, so that equation (2.6) is satisfied. One is thus led to the problem of diagonalizing the operator $H = A' + H_{11}' + H_{20}' + H'$, where A' = A - $\lambda\sum_i V_i^2$, $H_{11}' = H_{11} - \lambda\sum_{\langle ij\rangle}\left(U_i^2\alpha_i^+\alpha_{-i} - V_i^2\alpha_i^+\alpha_{-i}\right)$

$H_{20}' = H_{20} - \lambda\sum\left(U_iV_i\alpha_i^+\alpha_i^+ + V_iU_i\alpha_{-i}\alpha_i\right)$. The diagonalization of $H_0' = A' + H_{11}' + H_{20}'$ amounts to choosing U_i *and* V_i such that $H_{20}' = 0$

$$H'_{20} = \sum_{\langle ij\rangle}\left\{\left(\lambda - t_{ij}\right)U_iV_i - \sum_i U\,U_i^2U_iV_i\right\}\alpha_i^+\alpha_i^+$$

$$+ \sum_{\langle ij\rangle}\left\{\left(\lambda - t_{ij}\right)U_iV_i - \sum_i U\,V_i^2U_iV_i\right\}\alpha_{-i}\alpha_{-i} + \sum_i\left\{UU_i^2 - 2U\,V_i^2\right\}U_i\,V_i\alpha_i^+\alpha_{-i}^+ \qquad (2.7)$$

$$+ \sum_i UV_i^2U_iV_i\alpha_{-i}\alpha_{-i} + \sum_i UU_i^2U_iV_i(\,\alpha_i\alpha_i - \alpha_{-i}a_i) + \sum_i UV_i^2U_iV_i\left(\alpha_{-i}^+\alpha_{-i}^+ - \alpha_{-i}^+\alpha_i^+\right)$$

3.0 Introducing the notations

$$\varsigma_i = (\lambda - t_{ij})$$

$$\Delta_i = -\sum_i UV_i U_i \tag{3.1}$$

and noting the mutual independence of the operators for different valyes of *i*, we see that $H'_{20} = 0$ leads to the equations:

$$\varsigma_i U_i V_i + \Delta_i V_i^2 = 0 \tag{3.2a}$$

$$\varsigma_i U_i V_i + \Delta_i U_i^2 = 0 \tag{3.2b}$$

$$\left(UU_i^2 - 2UV_i^2\right)UV_i = 0 \tag{3.2c}$$

$$U_i V_i^2 = 0 \tag{3.2d}$$

If we assume that for some values of i, that the product $U_i V_i^2 \neq 0$, from equation (3.2a) and the condition $U_i^2 + V_i^2 = 1$ we obtain

$$U_i^2 = \frac{\left(\varsigma_i^2 - 2\Delta_i^2\right)}{2\left(\varsigma_i^2 - \Delta_i^2\right)} \pm \sqrt{\frac{(2\Delta_i^2 - \varsigma_i^2)^2 + 4\left(\varsigma_i^2 - \Delta_i^2\right)\left(\Delta_i^2\right)}{4\left(\varsigma_i^2 - 2\Delta_i^2\right)^2}}$$

and $$V_i^2 = 1 - U_i^2 \tag{3.3}$$

The remaining part of the Hamitonian A′ + H′$_{11}$ is then diagonal in the α-scheme. The quasiparticle vacuum |0 > α has the energy

$$E_o = {}_\alpha\langle 0|\left(A' + H'_{11}\right)|0\rangle_\alpha = \sum_{\langle ij\rangle}\left(t_{ij} - \lambda\right)V_i^2 + U\sum_i V_i^4 \tag{3.4}$$

To determine the determine the Lagrange multiplier λ we use

$$N_O = \sum_i \left(1 - \frac{\left(\varsigma_i^2 - 2\Delta_i^2\right)}{2\left(\varsigma_i^2 - \Delta_i^2\right)} \pm \sqrt{\frac{(2\Delta_i^2 - \varsigma_i^2)^2 + 4\left(\varsigma_i^2 - \Delta_i^2\right)\left(\Delta_i^2\right)}{4\left(\varsigma_i^2 - 2\Delta_i^2\right)^2}}\right) \tag{3.5}$$

4.0 Conclusion

The many electron problem has been studied using the Hubbard model. The powerful tool of Bogojiubov-Valatin canonical transformation has been used to derive the ground rate energy which has a remarkable simple form. Equations (3.1), (3.3) and (3.5) have remarkable resemblance to the celebrated superconducting solutions of BCS, where the Bogoljubov transformation was first used.

This gives credence to the belief that the physics of high-T_c superconductivity may yet be found in the Hubbard model or variants of it.

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