PHASE TRANSITIONS OF THE 1-D HUBBARD MODEL

E.O. Aiyohuyin[1], Amen Oni-Ojo[1]& Arthur Ekpekpo[2]
[1]Department of Physics, University of Benin, Benin City, Nigeria.
[2]Department of Physics, University of Benin, Abraka, Nigeria.

ABSTRACT
We show that the BCS Hamiltonian is a variant of the Hubbard model. The mean-field free energy of the system is derived. The pairing amplitude plays the role of the order parameter and it is used to study the phase transitions. The entropy and the heat capacity are obtained in this work.

1. INTRODUCTION

A many-body system with interactions is in general difficult to solve exactly. It is replaced by a 1-body problem with a chosen good external field. The external field replaces the interaction of all the other particles.

The formal basis for mean field theory is that the free energy of a system with Hamiltonian

$H = H_o + \Delta H$ has the upper bound [1].

$$F \leq F_o = \langle H \rangle_o - TS_o$$

Where S_o is the entropy and the average is taken over the reference Hamiltonian [2].

$$H = -t \sum_{\langle ij \rangle \sigma} \left(C^+_{i\sigma} C_{j\sigma} + C^+_{i\sigma} C_{j\sigma} \right) + U \sum_{j=1}^{N} n_{j\uparrow} n_{j\downarrow}$$

where $n_{j\sigma} = C^+_{j\sigma} C_{j\sigma}$ represents the number of electrons of spin σ at site j $C^+_{i\sigma}\left(C_{j\sigma}\right)$ creates (destroys) an electron of spin σ on site *i*.

The above Hamiltonian can be written in momentum space [4]. The following transformations are used

$$C_{j\sigma} = \frac{1}{\sqrt{N_s}} \sum_k C_{k\sigma} \; e^{i\vec{k}.\vec{R}_j}$$

$$C^+_{j\sigma} = \frac{1}{\sqrt{N_s}} \sum_k C_{k\sigma} \; e^{-i\vec{k}.\vec{R}_j}$$

consequently, the Hamiltonian becomes

$$H = \sum_{k\sigma} \in_k \; C^+_{k\sigma} C_{k\sigma} + \frac{U}{N_s} \sum_{q,k,k^1} C^+_{k-q\uparrow} C^+_{k+q\downarrow} C_{k'+q\downarrow} C_{k\uparrow}$$

The approximate free energy for a system containing pair wise interactions in its Hamiltonian [2].

$H = \sum_{(ij)} V_{ij}\left(\varsigma_i, \varsigma_j\right)$ is:

$$F_o = \sum_{(ij)} Tr_{ij} \; V_{ij}\left(\varsigma \;, \varsigma_j\right) P^{(i)}_o\left(\varsigma_i\right) P^{(i)}_o\left(\varsigma_j\right) \quad + kT \sum_{i=1}^{N} Tr_i \quad P^{(i)}_o\left(\varsigma_i\right) \log \, P^{(i)}_o\left(\varsigma_i\right)$$

where $P^{(i)}_o\left(\varsigma_i\right) = \frac{1}{Z_o} \, e^{-\beta h_i\left(\varsigma_i\right)}$ is the probability of finding the reference system in the state specified.

Z_o is the partition function. $\sum_{i=1}^{N} h_i\left(\varsigma_i\right)$ is the non-interacting Hamiltonian H_o of the system.

In the 1 = D Hubbard Hamiltonian [3]

$$\in_k = -t \sum_i e^{ik.R_i} = -2t \; Cosk_x$$

is the kinetic energy of the electron excitations.

The purpose of this paper to solve the 1 – D Hubbard Hamiltonian. The variation of the ground state free energy with the pairing parameter is investigated. The investigation shows that the theory reproduces the results in [5] between $\left|\Delta\right| = +0.3$ through 1.9 to $\left|\Delta\right|$ = 3.0. The curve is a parabola in this range. This suggests that in this range, the free energy agrees with Landau's theory [6] in which the free energy is expanded in the order parameter with the second order term dominating.

The paper is organized as follows: In section 2, the path integral formulation is used to solve the Hubbard Hamiltonian. In section 3, the free energy is evaluated as a function of the pairing parameter. The entropy and the specific heat capacity were also determined. Section 4 is a summary of the results.

2. THE HUBBARD HAMILTONIAN IN MOMENTUM SPACE [4] IS:

$$H = \sum_k \in_{k\sigma} C^+_{k\sigma} C_{k\sigma} + \frac{U}{N_s} \sum_{k,k^1} C^+_{k\uparrow} C^+_{-k\downarrow} C_{-k\downarrow} C_{k\uparrow}$$

This can be re-written as

$$H = \sum_k \in_{k\sigma} C^+_{k\sigma} C_{k\sigma} - \frac{g_o}{V} A^+ A \cdot$$

where $A^+ = \sum_k C^+_{k\uparrow} C_{-k\downarrow}$

and $A = \sum_k C_{-k\downarrow} C_{-k\uparrow}$

$$-\frac{g_o}{V} = \frac{U}{N_s}$$

This simplified pairing Hamiltonian is the BCS Hamiltonian. The partition function is

$$Z = \int D\left[\overline{C}, C\right] e^{-s}$$

where S = $S = \int_o^\beta \sum_{k\sigma} \overline{C}_{k\sigma} \left(\partial_\tau + \in_k\right) C_{k\sigma} - g\overline{A}A$

The mean field free energy [4] is

$$F = -T \sum_{kn} \ln\left(\omega_m^2 + \varepsilon_k^2 + |\Delta|^2\right) + \frac{|\Delta|^2}{g}$$

Minimizing the free energy with respect to $|\Delta|$ leads to the gap equation:

$$\frac{1}{g_o} = \frac{1}{\beta v} \sum_{kn} \frac{1}{\omega_n^2 + E_k^2}$$

where $E_k = \sqrt{\varepsilon_k^2 + |\Delta|^2}$

Replacing $\frac{1}{V}\sum_k$ with $N(o)\int d\in$ where N(o) is the density of states per spin, the free energy becomes [7]

$$F = T|\Delta|^2 \; N(o)\,\pi \sum_{\omega_n \angle \omega_D} \frac{1}{\sqrt{\omega_n^2 + |\Delta|^2}}$$

$$-T\sum_n \ln\left(\omega_n^2 + |\Delta|^2\right) - TV\; N(o) \sum_n \frac{8t^3 B}{|\Delta|^2 + \omega_n^2}$$

In the limit of $T \to 0$, one can replace $T\sum_{\omega_n}$ with $\int_o^{\omega_\Delta} \frac{d\omega}{2\pi}$. The energy becomes

$$F = |\Delta|^2 \; N(o)\,\pi \ln 2\omega_D/|\Delta| - \frac{VN(o)\,\pi\; 2t^3 B}{|\Delta|} + \frac{2t^3 B}{\pi\,|\Delta|^2}$$

3. THE FREE ENERGY IS APPROXIMATED BY THE EXPRESSION.

$$F = 2|\Delta|^2 \ln 5/|\Delta| - \frac{3}{|\Delta|^2}\left(1 - 4|\Delta|\right)$$

This equation can be rewritten as:

$$F = 5.2\,|\Delta|^2 - 2\,|\Delta|^3 + \frac{3}{|\Delta|^2} - \frac{12}{|\Delta|}$$

Minimizing F with respect to $|\Delta|$ leads to:

$$|\Delta| = -\, a\, \frac{(T_c - T)}{12} \quad T \angle T_c$$

$$|\Delta| = 0 \qquad T > T_c$$

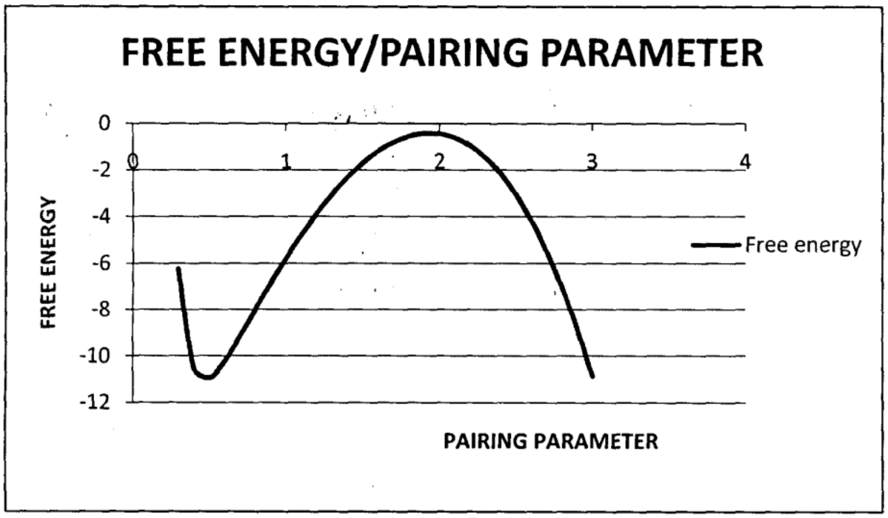
The dominant terms in F are

$$F \approx \frac{3}{|\Delta|^2} - \frac{12}{|\Delta|}$$

$$F = \frac{432}{a^2 (T_c - T)^2} + \frac{144}{a(T_c - T)} \quad T < T_c$$

$$F = 0 \qquad T > T_c$$

Fig 3.1



The entropy is

$$S = \frac{144}{a(T_c - T)^2} + \frac{432}{a^2(T_c - T)^3} \quad T \angle T_c$$

$$S = 0 \quad T > T_c$$

The specific heat capacity is

$$C_v = -\frac{T\partial^2 F}{\partial T}$$

$$= \frac{288T}{a(T_c - T)^3} + \frac{2592T}{a^2(T_c - T)^4} \quad T < T_c$$

4. THERE ARE TWO TYPES OF PHASE TRANSITIONS: First And Second Order Phase Transitions.

In the second order phase transition, there is no latent heat involved. It corresponds to divergent susceptibility, an infinite correlation length and a power law decay of correlations. Examples of second order transitions are superconductors, ferromagnetic and the super-fluid transitions. A second order phase transition occurs when a new state of reduced symmetry develops continuously from the disorder high temperature phase [8]. To describe the ordered phase a macroscopic order parameter that describes the character and strength of the broken symmetry is introduced.

The order parameter grows continuously from zero at the transition temperature.

According to Landau's [6] theory an expansion of the free energy in a Taylor expansion in the order parameter would tell us about the behaviour near the transition. The expansions contain only even powers of the order parameter. Sixth and higher order terms are not usually necessary for the important behaviour near T_c.

The feature of figure 3.1 between $|\Delta|$ = 0.3 and 3.0 shows that the dominant term in the expansion of the free energy is the second order term.

5. REFERENCES

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