Numerical Study of Fermi Surface on Cuprate Using One-Band Hubbard Model: Role of Charge Density Wave in The Antiferromagnetic Mott-Insulator and Pseudogap Region

M E I Akbar and I Santoso*
Departemen Fisika, Universitas Gadjah Mada, Sekip Utara BLS 21 Yogyakarta, INDONESIA

*Corresponding Author: iman.santoso@ugm.ac.id

Abstract - Numerical study of Fermi surface has been done using one-band Hubbard model with exact diagonalization method to study the effect of doping factor on Charge Density Wave (CDW) development in Anti ferromagnetic Mott Insulator (AFM) and pseudogap region in cuprate material. In this study the effect of CDW is characterized by Fermi Surface Nesting (FSN) vector in which it might be formed in pseudogap region. The wavelength of CDW increases when the value of disorder, which is representing the doping level in cuprate material, is increased. However, the CDW pattern will dissapear as the doping reaches the value which represented by Hubbard parameters: $t = 1 \, eV, U = 4 \, eV, \mu =2 \, eV,$ and $v_i = -6 \, eV,$ marked by the decreasing of charge density wavelength.

1. Introduction

Cuprate is a High Temperature Superconductor (HTSC) material which has superconductivity phase with $T_c$ above 30 $K$ as first studied by Berdnooz and Muller on the LBCO system [1]. Besides superconductivity phase, there are several other phases in cuprate material such as Anti Ferromagnetic Mott-Insulator (AFM), pseudogap, strange metal and Fermi liquid. The phase change is affected by the temperature and the amount of doping of charge carriers applied to the system.

One of interesting problem in cuprate is that how the competing order mentioned above evolved or played some role on mechanism of electron pairing [2] that drives the superconductivity, for example is pseudogap becomes the necessary precursor for superconductivity? Meanwhile, the interaction between electrons can also produce other phenomena such as Charge Density Wave (CDW). It has been known that CDW is broken symmetry states of metals, due to electron-lattice instability and found in some materials such as cuprate material [3-5]. It is argued that CDW is a driven force for in pseudogap phase in cuprate [6]. Thus it is important to study the role of CDW in pseudogap phase since it is believed to be the key for explaining the mechanism of HTSC in cuprates.

The behavior of electrons in a material can be characterized by Density of State (DOS), the magnitude of interaction between electrons and energy state around Fermi surface. CDW can be characterized by vector nesting on the Fermi surface.

In this work, we report the numerical study band structures and Fermi surfaces from cuprate materials in the AFM and pseudogap regions to investigate the pattern of CDW formation associated with the given disorder factor. The disorder factor in this study represents the potential energy of the given doping. The Hamiltonian used in this study is Hubbard model which can describe the phase transition from conductor to insulator or vice versa. Chemical potential ($\mu$) and disorder ($v_i$) factor were added to this Hamiltonian.

2. Method

In the Hubbard model the atomic state in the material is illustrated by 2 parameters: $t$ which describes the energy hopping and $U$ which describes the potential energy of the interaction between
electrons in the same state. The formulation of Hubbard’s Hamiltonian model can be written as follows:

\[ H = -t \sum_{<i,j>} \sigma c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + h.c \],  

with \( c_{i\sigma}^+ \) is creation operator of electron with spin \( \sigma \) on site \( i \), \( c_{i\sigma} \) is annihilation operator of electron with spin \( \sigma \) on site \( i \), \( n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \) is the number operator and \( h.c \) is Hermitian conjugate.

Hubbard’s model in real space can be transformed into reciprocal space by using Fourier transform for the second quantization as follows:

\[ c_{k\uparrow} = \frac{1}{\sqrt{N}} \sum_i e^{ik \cdot \mathbf{r}_i} c_{i\uparrow}^+ \],  

\[ c_{k\downarrow} = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k} \cdot \mathbf{r}_i} c_{i\downarrow}^+ \].  

The energy value is obtained when the Hamiltonian is converted into a diagonal matrix. The matrix is obtained by transform the Hamiltonian by the following methods:

\[ (c_{i\sigma} \ c_{j\sigma}) (H_{11} \ H_{12}) \begin{pmatrix} c_{i\sigma}^+ \\ c_{j\sigma}^+ \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \].  

The component values of a matrix \( a \) which are complex values can be converted into real values using the following methods:

\[ \begin{pmatrix} b & -c \\ c & b \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \].  

where \( b \) and \( c \) are respectively the real and imaginary parts of \( a \). \( \lambda \) is the eigenvalue related to the energy eigen of particular eigen state \( \begin{pmatrix} x \\ y \end{pmatrix} \).

The Householder transformation is used to convert symmetry matrices into tridiagonal matrices, then the Jacobi transformation is used to transform the tridiagonal matrix into a diagonal matrix. The value of each element of the transformed matrix represents the value of Eigen energy in each of the energy bands of the material.

The Hamiltonian model used in this study is one-band Hubbard model as presented in the following equations:

\[ H = \sum_{<i,j>} \sigma \varepsilon_{ij} c_{i\sigma}^+ c_{j\sigma} - (\mu + U) \sum_{i\sigma} n_{i\sigma} \],  

with \( \mu \) denotes the chemical potential.

In reciprocal space equation (6) change into:

\[ H = \sum_k \begin{pmatrix} -\varepsilon_k & \xi_k \\ \xi_k & -\varepsilon_k \end{pmatrix}, \]

with,

\[ \xi_k = \varepsilon_k - \mu - \mu^H \],  

and

\[ \varepsilon_k = -t \sum_k e^{ikr}. \]

In this study, we used a Plaquetee model of cuprate material in which one copper atom (Cu) is surrounded by four oxygen (O) atoms with distance \( r \), then equation (9) becomes:

\[ \varepsilon_k = -t \left( e^{ikx} + e^{-ikx} + e^{iy} + e^{-iy} \right) \]

with,

\[ e^{i\theta} = \cos \theta + i \sin \theta. \]

Equation (12) shows the matrix model (with complex elements) that is to be used in this study. Since the matrix in equation (7) is the Hermitian matrix, the transformation of the \( n \times n \) Hermitian matrix to the real symmetry matrix \( 2n \times 2n \) is required, using the transformation as shown in (5), the Hamiltonian model becomes:
The Hamiltonian model of equation (12) was used as a model for cuprate material with 6 × 6, 12 × 12 and 18 × 18 cluster size variations. The exact diagonalization then has been used for each k-point in first Brillouin Zone of Cuprate. The CDW wavelength was calculated based on the value of vector nesting in the antinodal region.

3. Result

![Band structure images](image)

**Figure 1.** Band structure of cuprate with Hubbard parameters (a) $t = 1 \text{ eV}; U = 0 \text{ eV}; \mu = 0 \text{ eV}; \nu_i = 0 \text{ eV}$ (b) $t = 1 \text{ eV}; U = 4 \text{ eV}; \nu_i = 0 \text{ eV} (c) t = 1 \text{ eV}; U = 4 \text{ eV}; \mu = 2\text{ eV}; \nu_i = -4 \text{ eV}$

The results of this study show that Hubbard model can describe the phase transition from a metallic phase (fig. 1(a)) to an insulator phase (fig. 1(b)) or vice versa. 3-dimensional of energy bands of the first Brilouin zone of cuprate material show in fig.1. When the parameter $U$ and $\mu$ were added, the band structure were divided into two parts as shown in fig 1(b) namely the upper Hubbard band and the lower Hubbard band, and form a gap between energy bands. This means that the phase of the material changes from a metallic state to an insulator. This phase indicates the AFM phase. The parameter disorder shifts the two energy bands, so that the $E = 0$ plane can cut one of the two bands as shown in fig 1(c). This phase may indicate the pseudogap phase.
CDW pattern formation based on the development of Nesting vector on the Fermi surface with Hubbard parameter values: $t = 1\ eV$; $U = 4\ eV$; $\mu = 2\ eV$ (a) $v_i = -1.5\ eV$ (b) $v_i = -2.5\ eV$ (c) $v_i = -3.5\ eV$ (d) $v_i = -4.5\ eV$ (e) $v_i = -5.5\ eV$ (f) $v_i = -6.0\ eV$ (g) $v_i = -6.5\ eV$ (h) $v_i = -7.5\ eV$

The formation of a nesting vector based on a variation of the given disorder value. In the Fig. 2(b), 2(c), 2(d), and 2(e) the formation of the antinodal region is seen. The length of the nesting vector in this area is used to calculate the CDW wavelength. Fig. 2(f) shows the Fermi surface of ordinary metal where gap in the antinodal regions were not formed.

Table 1 CDW wavelength

| No | t (ev) | U (ev) | $\mu$ (ev) | $v_i$ (ev) | $K_f$ | $\lambda$ (Å) |
|----|-------|-------|------------|-----------|------|---------|
| 1  | 1     | 4     | 2          | -1.5      | -    | -       |
| 2  | 1     | 4     | 2          | -2.5      | 1.2  | 2.62    |
| 3  | 1     | 4     | 2          | -3.5      | 1.1  | 2.85    |
| 4  | 1     | 4     | 2          | -4.5      | 0.6  | 5.23    |
| 5  | 1     | 4     | 2          | -5.5      | 0.4  | 7.85    |
| 6  | 1     | 4     | 2          | -6.0      | 2.1  | 1.48    |
| 7  | 1     | 4     | 2          | -6.5      | -    | -       |
| 8  | 1     | 4     | 2          | -7.5      | -    | -       |

The Fermi surface nesting shows that CDW patterns can be formed in antinodal areas. The greater the given factor of the disorder, the greater the wavelength value of the CDW is. However when the doping reaches a certain value which is represented by Hubbard parameters with the value: $t = 1\ eV$, $U = 4\ eV$, $\mu = 2\ eV$ and $v_i = -6\ eV$ The CDW pattern disappears which is marked by the returning of the wavelength value as shown in table 1.

4. Conclusion
The CDW phase might be manifested in the Pseudogap region when the material is doped with a certain concentration. When the doping factor is added the CDW wavelength also increases, up to a certain doping level ($v = -6$ eV) the wavelength of the material returns to normal and the CDW phase is no longer found.

5. References

[1] Bednorz J G, Muller K A 1986 Z. Phys. B. 64 (1) pp 189–193.
[2] Bardeen J, Cooper L N, Schriffer J R 1957 Phys. Rev. 108 (5) 1175.
[3] Pate M, Mottershead J D F, Elfmov I S, Peets D C, Liang R, Boon D A, Hardy W N, Chiuzbaian S, Falub M, Shi M, Pothway L, Damascelli A 2005 Phys. Rev. Lett. 95 077001.
[4] Robertson J A, Kivelson S A, Fradkin E, Fang A C, Kaptulnik A. 2006 Phys. Rev. B 74 134507.
[5] Shen K M, Ronning F, Lu D H, Baumberger F, Ingle N J C, Lee W S, Meevasana W, Kohnsaka, Y, Azuma M, Takano, M, Takagi H, Shen Z X 2005 Science 307 pp 901-904.
[6] Timusk T, Statt B W 1999 Rep. Prog. Phys. 62 pp 61-122.
[7] Loh Y L, Trivedi N 2012 Theoretical Studies of Superconductor-Insulator Transitions chapter 17, pp. 492-548 in Conductor-Insulator Quantum Phase Transitions (ed. V Dobrosavljevic, N Trivedi, and J M Valles Jr Oxford University Press)