

Chapter 1

Introduction

Quantum mechanics plays an important role in physics it is now widely used to explain atomic phenomena as well as the behavior of elementary particles [1, 2, 3].

The properties of materials which are predicted by using quantum mechanics are utilized in many fields. They are used in promoting electronic devices, computers and telecommunication beside sensors and solar cells. They are used also in the field of nano science and superconductivity [4, 5, 6].

The history of quantum mechanics dates from the discovery of plank that light behaves like particles [7]. Later on Debroglie proposed that particles like electrons behaves as waves [8]. This confirms the dual nature of atomic and sub atomic particles [9, 10]. This encourages Schrödinger and Heisenberg to formulate a quantum equation that describes atomic world [11]. Heisenberg representation was developed by so called matrix representation, which represents quantum systems in different space [12]. These includes energy, momentum and coordinate space. As far as the energy of atoms and electrons are important, it is there for important to study quantum Schrödinger equation in the energy space [12].

This is since the energy wave function gives the probability of electrons transition [13]. This energy representation is used by the so called Hubbard model to describe superconductivity behavior [8]. This model is complex and cannot directly explain why the resistance vanishes beyond some critical temperature [8]. How ever some attempts were model to do this [8]. But this model is mathematically complex. Thus there is a need for simple model.

1.1 Problems of Quantum Field Theory (Q.F.T):

Quantum field theory (Q.F.T) is concerned with studying the behavior of field and forces mediators [14, 15]. It is based on utilizing Heisenberg picture and commutation relations of the wave functions which are treated have as operators. The energy and physical quantities obtained by diagonalizing their matrix [16, 17].

(Q.F.T) looks promising in explaining some problems associated with quantum fields. But unfortunately its mathematical structure is very complex and suffer from sever divergences. It is also unable to describe some field's phenomena like the quantum gravitational field, beside superconductivity and Nano system [18, 19].

1.2 Literature Review:

Different attempts were made to describe the behavior new materials like superconductors (Sc)[20,21,22,23,24,25].Also many attempts were made to quantize and unify fields[26,27,28,29].Most of these attempts are based mainly on lagrangian formalism, Principle of least action, destruction and production operators beside Feynman diagrams[30,31,32].

Unfortunately these models have very complex mathematical structure and cannot explain all matter and fields phenomena properly [33, 34, 35, 36, 37, 38, 39].

1.3 Aim of the Work:

The researches which are done by some others show that the failure of (Q.F.T) may result from the mathematical and conceptant basis of quantum mechanics.

Thus one can promote these new versions of (Q.M) to construct a new modified (Q.F.T) based on Schrödinger picture and harmonic oscillator model, beside electromagnetic field and generalized special relativity.

1.4 Presentation of the thesis:

This research composed four chapters, including the introduction. The second chapter deals with the quantum field equations. The third chapter introduces literature review. Chapter four is devoted to explain the contributions.

Chapter 2

Quantum field Equations

2.1 Introduction:

The theory of quantum mechanics dealt with systems that, in the classical limit consist of material particles. This theory will be extended, so that it can be applied to the electromagnetic field and thus provide a consistent basis for the quantum theory of radiation. The quantization of a wave field imparts to it some particle properties in the case of the electromagnetic field, a theory of light quanta (photons) results. The field quantization technique can also be applied to a ψ field, such as that described by the non-relativistic Schrodinger equation or by one of the relativistic equations, it then converts a one - particle theory into a many - particle theory, in a manner equivalent to the transition. Because of this equivalence, it might seem that the quantization of ψ field merely provides another formal approach to the many -particle problem. However, the new formalism can deal as well with processes that involve the creation or destruction of material particles [40].

This chapter is intended to serve as an introduction to quantum field theory, with a discussion of the quantum equations of motion for a wave field without specifying the details nature of the field.

2.2 Quantum Equation for the Field:

In the first quantization we quantized the physical quantities like energy and momentum, but in the second quantization we quantize the fields, including matter field, electromagnetic field and all other fields. To

perform quantization, we treat field variables q_i and related quantities as operators, unlike the first quantization which treat them as numbers [40].

The field variables obeys Heisenberg equation of motion:

$$\frac{\partial \hat{F}}{\partial t} = \frac{\partial \hat{F}}{\partial t} + \frac{1}{i\hbar} [\hat{F}, \hat{H}] \quad (2.2.1)$$

Where:

$$[\hat{F}, \hat{H}] = \hat{F}\hat{H} - \hat{H}\hat{F} \quad (2.2.2)$$

To convert the field variables q_i and the momenta P_i to hermitian operators, they have to satisfy the commutation relations:

$$[\hat{q}_i, \hat{q}_j] = 0, [\hat{\Pi}_i, \hat{\Pi}_j] = 0,$$

$$[\hat{q}_i, \hat{\Pi}_j] = i\hbar\delta_{ij}$$

$$\delta_{ij} = 1 \text{ for } i = j$$

$$\delta_{ij} = 0 \text{ for } i \neq j \quad (2.2.3)$$

Or:

$$[\hat{q}(\underline{r}, t), \hat{q}(\underline{r}', t)] = 0, [\hat{\Pi}(\underline{r}, t), \hat{\Pi}(\underline{r}', t)] = 0,$$

$$[\hat{q}(\underline{r}, t), \hat{\Pi}(\underline{r}', t)] = i\hbar\delta_{\underline{r}\underline{r}'}$$

$$\delta_{\underline{r}\underline{r}'} = \begin{cases} 1, & \text{for } \underline{r} = \underline{r}' \\ 0, & \text{for } \underline{r} \neq \underline{r}' \end{cases}$$

2.3 Fields with more than one component:

If the field has more than one component, the Hamiltonian takes the Form [40]:

$$H = \sum_{s=1}^n \pi_s \dot{q}_s - L \quad (2.3.1)$$

The commutation relations becomes:

$$\begin{aligned}
[\psi_s(\underline{r}, t), \psi_{\dot{s}}(\underline{\dot{r}}, t)] &= 0 \\
[\pi_s(\underline{r}, t), \pi_{\dot{s}}(\underline{\dot{r}}, t)] &= 0 \\
[\psi_s(\underline{r}, t), \pi_{\dot{s}}(\underline{\dot{r}}, t)] &= i\hbar\delta_{s\dot{s}}\delta_{r\dot{r}}
\end{aligned} \tag{2.3.2}$$

2.4 Quantization of the Non-relativistic Schrodinger Equation:

The classical lagrangian takes the form [40]:

$$L = i\hbar\psi^*\dot{\psi} - \frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi \tag{2.4.1}$$

$$\pi = \frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial \dot{\psi}} = i\hbar\psi^* \tag{2.4.2}$$

Where we set:

$$q = \psi, \dot{q} = \dot{\psi} \tag{2.4.3}$$

The Hamiltonian density is given by:

$$H = \pi\dot{q} - L = \pi\dot{\psi} - L$$

$$H = i\hbar\psi^*\dot{\psi} - L \tag{2.4.4}$$

$$H = \frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi + V\psi^*\psi \tag{2.4.5}$$

But from (2.4.2):

$$\psi^* = \frac{\pi}{i\hbar} = \frac{i\pi}{i^2\hbar} = \frac{-i\pi}{\hbar} \tag{2.4.6}$$

Hence:

$$H = \frac{-i\hbar}{2m}\nabla\Pi\nabla\psi - \frac{i}{\hbar}V\Pi\psi \tag{2.4.7}$$

We have:

$$\frac{\partial \hat{F}}{\partial t} = \frac{1}{i\hbar}[\hat{F}, \hat{H}] + \frac{\partial \hat{F}}{\partial t} \tag{2.2.1}$$

$$\hat{H} = \frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi + V\psi^*\psi \tag{2.4.5}$$

To quantize Schrodinger equation we utilize Heisenberg equation (2.2.1) by ignoring and assuming:

$$\frac{\partial \hat{F}}{\partial t} = 0$$

To get:

$$\frac{\partial \hat{F}}{\partial t} = \frac{1}{i\hbar} [\hat{F}, \hat{H}] \quad (2.4.8)$$

With $\hat{F} = \psi = \text{operator}$

$$\hat{H} = \int \left(\frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi + V \psi^* \psi \right) d\underline{r} \quad (2.4.9)$$

Where we make use of equation (2.4.5).

Inserting equation (2.4.9) in (2.4.8), yields:

$$i\hbar \frac{\partial \psi}{\partial t} = [\psi, \hat{H}] = \psi \hat{H} - \hat{H} \psi \quad (2.4.10)$$

Where:

$$\psi = \psi(\underline{r}), \quad \dot{\psi} = \psi(\dot{\underline{r}}) \quad (2.4.11)$$

And H is integrated over $\dot{\underline{r}}$ to avoid confusion, thus:

$$\hat{H} = \int \left(\frac{\hbar^2}{2m} \dot{\nabla} \psi^* + \dot{\nabla} \dot{\psi} + \dot{V} \psi^* + \dot{\psi} \right) d\dot{\underline{r}} \quad (2.4.12)$$

The commutation relation $[\psi, \hat{H}]$ can split into two parts. i.e.:

$$\begin{aligned} [\psi, \hat{H}] &= \psi \hat{H} - \hat{H} \psi \\ &= \psi \left[\int \frac{\hbar^2}{2m} \dot{\nabla} \psi^* \cdot \dot{\nabla} \dot{\psi} d\dot{\underline{r}} + \int \dot{V} \psi^* \dot{\psi} d\dot{\underline{r}} \right] - \left[\int \frac{\hbar^2}{2m} \dot{\nabla} \psi^* \cdot \dot{\nabla} \dot{\psi} d\dot{\underline{r}} + \int \dot{V} \psi^* \dot{\psi} d\dot{\underline{r}} \right] \psi = \\ &= \frac{\hbar^2}{2m} \left\{ \int (\psi \dot{\nabla} \psi^* \cdot \dot{\nabla} \dot{\psi} - \dot{\nabla} \psi^* \cdot \dot{\nabla} \dot{\psi} \psi) d\dot{\underline{r}} \right\} + \int \dot{V} (\psi \psi^* \dot{\psi} - \psi^* \dot{\psi} \psi) d\dot{\underline{r}} \end{aligned} \quad (2.4.13)$$

The second term in (2.4.13) can be simplified by using the commutation relations (2.3.2) where:

$$[\Psi(\underline{r}), \Psi(\underline{r}')] = [\Psi, \dot{\Psi}] = 0$$

$$\Psi\dot{\Psi} - \dot{\Psi}\Psi = 0$$

$$\Psi\dot{\Psi} = \dot{\Psi}\Psi \quad (2.4.14)$$

Hence the bracket in the second term of equation (2.4.13) becomes [see equation (2.4.14)]:

$$\Psi\Psi^*\dot{\Psi} - \Psi^*\dot{\Psi}\Psi = \Psi\Psi^*\dot{\Psi} - \Psi^*\dot{\Psi}\Psi = (\Psi\Psi^*, \Psi^*\Psi)\dot{\Psi} \quad (2.4.15)$$

According to equation (2.4.2) the momentum is given by:

$$\pi = i\hbar\Psi^*$$

$$\Rightarrow \dot{\pi} = i\hbar\dot{\Psi}^* \quad (2.4.16)$$

Using equation (2.4.2):

$$[\Psi(\underline{r}), \pi(\underline{r}')] = i\hbar\delta_{r\dot{r}}$$

$$[\Psi, \dot{\pi}] = i\hbar\delta_{r\dot{r}}$$

$$\Psi\dot{\pi} - \dot{\pi}\Psi = i\hbar\delta_{r\dot{r}}$$

From (2.4.16):

$$i\hbar[\Psi\Psi^* - \Psi^*\Psi] = i\hbar\delta_{r\dot{r}}$$

$$\Psi\Psi^* - \Psi^*\Psi = \delta_{r\dot{r}} \begin{pmatrix} 1, & \text{for } r = \dot{r} \\ 0, & \text{for } r \neq \dot{r} \end{pmatrix} \quad (2.4.17)$$

Subs. (2.4.17) in (2.4.15) to get:

$$\Psi\Psi^*\dot{\Psi} - \Psi^*\dot{\Psi}\Psi = [\Psi\Psi^* - \Psi^*\Psi]\dot{\Psi} = \delta_{r\dot{r}}\dot{\Psi} \quad (2.4.18)$$

Thus the second term in equation (2.4.13) becomes:

$$\int \nabla (\Psi \Psi^* \dot{\Psi} - \Psi^* \dot{\Psi} \Psi) d\mathbf{r} = \int \nabla (\delta_{r\dot{r}}) \dot{\Psi} d\mathbf{r} = \int \nabla (\dot{\mathbf{r}}) \Psi(\dot{\mathbf{r}}) (\delta_{r\dot{r}}) d\mathbf{r} = \sum_{\dot{r}} \nabla (\dot{\mathbf{r}}) \Psi(\dot{\mathbf{r}}) \delta_{r\dot{r}} = \nabla (r) \Psi(r) \delta_{rr} = \nabla (\underline{r}) \Psi(\underline{r}) \quad (2.4.19)$$

To simplify the first term in equation (2.4.13) let us write:

$$\dot{\nabla} \Psi = u; \dot{\nabla} \Psi = \frac{\partial \Psi(\dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}}$$

Hence:

$$\dot{\nabla} (\Psi^* \cdot u) = (\dot{\nabla} \Psi^*) \cdot u + \Psi^* \cdot \dot{\nabla} u$$

$$\dot{\nabla} (\Psi^* \dot{\nabla} \Psi) = \dot{\nabla} \Psi^* \cdot \dot{\nabla} \Psi + \Psi^* \dot{\nabla}^2 \Psi$$

$$\therefore \dot{\nabla} \Psi^* \cdot \dot{\nabla} \Psi = \dot{\nabla} (\Psi^* \cdot \dot{\nabla} \Psi) - \Psi^* \dot{\nabla}^2 \Psi$$

Hence:

$$\int \dot{\nabla} \Psi^* \cdot \dot{\nabla} \Psi d\dot{\mathbf{r}} = \int \frac{d}{d\dot{\mathbf{r}}} [\Psi^* \cdot \dot{\nabla} \Psi] d\dot{\mathbf{r}} - \int \Psi^* \dot{\nabla}^2 \Psi d\dot{\mathbf{r}}$$

In one dimension:

$$\int \dot{\nabla} \Psi^* \cdot \dot{\nabla} \Psi d\dot{\mathbf{r}} = \int_0^\infty \frac{d}{d\dot{\mathbf{r}}} [\Psi^* \cdot \dot{\nabla} \Psi] d\dot{\mathbf{r}} - \int_0^\infty \Psi^* \cdot \dot{\nabla}^2 \Psi d\dot{\mathbf{r}} =$$

$$\int_0^\infty d(\Psi^* \cdot \dot{\nabla} \Psi) - \int_0^\infty \Psi^* \cdot \dot{\nabla}^2 \Psi d\dot{\mathbf{r}} = \Psi^*(\dot{\mathbf{r}}) \frac{\partial}{\partial \dot{\mathbf{r}}} \Psi(\dot{\mathbf{r}}) \Big|_0^\infty - \int_0^\infty \Psi^* \cdot \dot{\nabla}^2 \Psi d\dot{\mathbf{r}}$$

Since at $\dot{\mathbf{r}} = 0$ and $\dot{\mathbf{r}} = \infty$ no particle exists.

Hence:

$$\Psi(\dot{\mathbf{r}} = 0) = 0; \Psi^*(\dot{\mathbf{r}} = 0) = 0$$

$$\Psi(\dot{\mathbf{r}} = \infty) = 0; \Psi^*(\dot{\mathbf{r}} = \infty) = 0$$

Hence:

$$\Psi^*(\hat{r}) \frac{d}{d\hat{r}} \Psi(\hat{r}) \Big|_0^\infty = \Psi^*(\hat{r} = \infty) \frac{d\Psi(\hat{r})}{d\hat{r}} \Big|_{\hat{r}=\infty} - \Psi^*(\hat{r} = 0) \frac{d\Psi(\hat{r})}{d\hat{r}} \Big|_{\hat{r}=0}$$

Hence:

$$\int \hat{\nabla} \Psi^* \hat{\nabla} \Psi d\hat{r} = - \int \Psi^* \hat{\nabla}^2 \Psi d\hat{r} \quad (2.4.20)$$

This relation can be also found from Hermitian of:

$$\hat{p} = \frac{\hbar}{i} \hat{\nabla}, \quad \hat{p}^+ = \frac{\hbar}{-i} \hat{\nabla}$$

$$\int \overline{\hat{p} \Psi} \hat{\nabla} \Psi d\hat{r} = \int \overline{\Psi} \hat{p} \hat{\nabla} \Psi d\hat{r}$$

$$\int \hat{p}^* \Psi^* \hat{\nabla} \Psi d\hat{r} = \int \Psi^* \hat{p} \hat{\nabla} \Psi d\hat{r}$$

$$\overline{\Psi} = \Psi^*$$

Where:

$$\int \left(\frac{\hbar}{-i} \hat{\nabla} \right) \Psi^* \hat{\nabla} \Psi d\hat{r} = \int \Psi^* \frac{\hbar}{i} \hat{\nabla} (\hat{\nabla} \Psi) d\hat{r} - \frac{\hbar}{i} \int \hat{\nabla} \Psi^* \hat{\nabla} \Psi d\hat{r} = \frac{\hbar}{i} \int \Psi^* \hat{\nabla}^2 \Psi d\hat{r} -$$

$$\int \hat{\nabla} \Psi^* \hat{\nabla} \Psi d\hat{r} = \int \Psi^* \hat{\nabla}^2 \Psi d\hat{r}$$

Using the commutation relation (2.4.2):

$$[\Psi(r), \Psi(\hat{r})] = 0, \quad [\Psi, \hat{\Psi}] = 0$$

$$\Psi \hat{\Psi} - \hat{\Psi} \Psi = 0$$

Hence:

$$\Psi \hat{\Psi} = \hat{\Psi} \Psi$$

$$\hat{\nabla} (\Psi \hat{\Psi}) = \hat{\nabla} (\hat{\Psi} \Psi)$$

Since $\hat{\nabla}$ acts on $\hat{\Psi}$ only:

$$\Psi \hat{\nabla} \hat{\Psi} = (\hat{\nabla} \hat{\Psi}) \Psi$$

$$\hat{\nabla}(\Psi \cdot \hat{\nabla}\Psi) = \hat{\nabla}(\hat{\nabla}\Psi \cdot \Psi) \quad (2.4.21)$$

$$\Psi \cdot \hat{\nabla}^2\Psi = \hat{\nabla}^2\Psi \cdot \Psi$$

Where:

$$\hat{\nabla}\Psi = \frac{d\Psi(\hat{r})}{d\hat{r}}; \hat{\nabla}\Psi = \frac{d\Psi(r)}{dr} = 0$$

In view of equation (2.4.21) & (2.4.20) & (2.4.13) one gets:

$$\begin{aligned} \int [\Psi \hat{\nabla}\Psi^* \cdot \hat{\nabla}\Psi - \hat{\nabla}\Psi^* \cdot \hat{\nabla}\Psi \Psi] d\hat{r} &= - \Psi [\int \Psi^* \cdot \hat{\nabla}^2\Psi d\hat{r}] + [\int (\Psi^* \cdot \hat{\nabla}^2\Psi) d\hat{r}] \Psi \\ &= - \int \Psi \Psi^* \cdot \hat{\nabla}^2\Psi d\hat{r} + \int \Psi^* \hat{\nabla}^2\Psi \cdot \Psi d\hat{r} \end{aligned}$$

From (2.4.21):

$$\begin{aligned} &= - \int \Psi \Psi^* \cdot \hat{\nabla}^2\Psi d\hat{r} + \int \Psi^* \hat{\nabla}^2\Psi \cdot \Psi d\hat{r} = - \int \Psi \Psi^* \cdot \hat{\nabla}^2\Psi d\hat{r} + \int \Psi^* \hat{\nabla}^2\Psi \cdot \Psi d\hat{r} = \\ &= \int [\Psi \Psi^* - \Psi^* \Psi] \cdot \hat{\nabla}^2\Psi d\hat{r} = \int [\Psi^*, \Psi] \cdot \hat{\nabla}^2\Psi d\hat{r} = - \int \delta r \hat{r} \cdot \hat{\nabla}^2\Psi d\hat{r} = \\ &= - \sum_{r\hat{r}} \nabla_{r\hat{r}}^2 \Psi(\hat{r}) \delta r \hat{r} = - \nabla_r^2 \Psi(r) = - \nabla^2 \Psi \end{aligned} \quad (2.4.22)$$

Where we use the commutation relation:

$$[\Psi(r), \pi(\hat{r})] = i\hbar \delta_{r\hat{r}}$$

$$[\pi(\hat{r}), \Psi(r)] = [\hat{\pi}, \Psi] = -i\hbar \delta r \hat{r}$$

$$\text{But } \hat{\pi} = i\hbar \hat{\Psi}^*,$$

Hence:

$$i\hbar [\Psi^*, \Psi] = i\hbar \delta_{r\hat{r}}$$

Inserting (2.4.22) , (2.4.19) in equation (2.4.13) and (2.4.10) yields:

$$i\hbar \frac{\partial \Psi}{\partial t} = - \frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi \quad (2.4.23)$$

Which is the Schrödinger equation, but here Ψ is an operator not a number or a numerical function.

2.5 Quantum Equations:

The Hamiltonian is conveniently written by:

$$H = \int \left(\frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi + v \Psi^* \Psi \right) d^3 r \quad (2.5.1)$$

The quantized Hamiltonian given in equation (2.5.1) is the operator that represents the total energy of the field. The commutation relations are:

$$[\Psi(r), \Psi(\hat{r})] = [\Psi^*(r), \Psi^*(\hat{r})] = 0$$

$$[\Psi(r), \Psi^*(\hat{r})] = \delta^3(r - \hat{r}) \quad (2.5.2)$$

The omission of t from the argument of the field variables implies that both fields in a commutator bracket refer to the same time. The equation of motion for Ψ is:

$$i\hbar \dot{\Psi} = [\Psi, H] = \left[\Psi, \int \frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi d^3 \hat{r} \right] + \left[\Psi, \int v \Psi^* \Psi d^3 \hat{r} \right] \quad (2.5.3)$$

The second term on the right side is easily evaluated with the help of (2.5.2)

To give:

$$\int v \dot{\Psi} (\Psi \Psi^* \Psi - \Psi^* \Psi \Psi) d^3 \hat{r} - \int v (\Psi \Psi^* - \Psi^* \Psi) \dot{\Psi} d^3 \hat{r} - \int v \dot{\Psi} \delta^3(r - \hat{r}) d^3 \hat{r} = v \dot{\Psi} \Psi \quad (2.5.4)$$

Ψ Commutes with v , which is a numerical function. The first term on the right side of equation (2.5.3) can be written as:

$$\left[\Psi, \int \nabla \Psi^* \cdot \nabla \Psi d^3 \hat{r} \right] - \left[\Psi, \int \Psi^* \nabla^2 \Psi d^3 \hat{r} \right] = - \int [\Psi, \Psi^*] \nabla^2 \int (\nabla^2 \Psi) \delta^3(r - \hat{r}) d^3 \hat{r} = -\nabla^2 \Psi \quad (2.5.5)$$

Substitution of (2.5.4) and (2.5.5) into (2.5.3) yields:

$$i\hbar\Psi = \frac{-\hbar^2}{2m}\nabla^2\Psi + V(r,t)\Psi$$

So that the equations obtained from classical and quantum field theories agree.

If V is independent of t , H has no explicit dependence on the time, and equation (2.2.1) shows that H is a constant of the motion. Thus the energy in the field is constant. Another interesting operator is:

$$N = \int \Psi^* \Psi d^3r;$$

N is a Hermitian, its time derivative is given by:

$$i\hbar\dot{N} = [N, H] = \left[\int \Psi^* \Psi d^3r, \int \frac{\hbar^2}{2m} \nabla\Psi^* \cdot \nabla\Psi + \int V\Psi^*\Psi d^3r \right] \quad (2.5.6)$$

The commutator of N with the V part of H can be written as:

$$\iint \dot{V} (\Psi^*\Psi \Psi^*\Psi - \Psi^*\Psi \Psi^*\Psi) d^3r d^3r'$$

With the help of (2.5.2) the parenthesis in the integrand is:

$$\begin{aligned} \Psi^*\Psi \Psi^*\Psi - \Psi^*\Psi \Psi^*\Psi &= \Psi^*[\Psi^*\Psi + \delta^3(r - r')]\Psi - \Psi^*\Psi \Psi^*\Psi \\ &= \Psi^*\Psi^*\Psi \Psi + \Psi^*\Psi \delta^3(r - r') - \Psi^*\Psi^*\Psi \Psi \\ &= \Psi^*[\Psi \Psi^+ - \delta^3(r - r')]\Psi \\ &+ \Psi^*\Psi \delta^3(r - r') - \Psi^*\Psi \Psi^*\Psi^+ = 0 \end{aligned}$$

Since the δ vanishes unless $r=r'$.

The double integral of this over r and r' is zero. Thus eqn (2.5.4) shows that N is a constant of the motion. It can also be shown that the commutator

brackets in (2.5.2) are constants of the motion , so that these equations are always valid if they are at particular time.

2.6 The N Representation:

We need now a representation in which the operator N is diagonal. In this case the state vector, satisfies [47]:

$$\hat{N}|\cdots n_k \rangle = n_k |\cdots n_k \rangle$$

$$\langle i | \hat{N} | j \rangle = \langle n_i | \hat{N} | n_j \rangle$$

$$\hat{N}_{ij} = \langle i | \hat{N} | j \rangle = \langle n_i | n_j \rangle = n_j \delta_{ij} \quad (2.6.1)$$

$$\hat{N}_{ij} = \begin{pmatrix} N_{11} & N_{12} & N_{13} \\ N_{21} & N_{22} & N_{23} \\ N_{31} & N_{32} & N_{33} \end{pmatrix} = \begin{pmatrix} n_1 & 0 & 0 \\ 0 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix} \quad (2.6.2)$$

To find the functional form of N we have to expand the wavefunction $\Psi(r, t)$ in terms of the complete set of eigenfunctions $u_k(r)$, $\{u_1, u_2, \dots, u_n\}$

$$\Psi(\underline{r}, t) = \sum_k a_k(t) u_k(\underline{r}) \quad (2.6.3)$$

$$\Psi^+(\underline{r}, t) = \sum_k a_k^+(t) u_k^+(\underline{r}) \quad (2.6.4)$$

Where $u_k(r)$ is a number

Thus:

$$u_k^+(\underline{r}) = u_k^*(\underline{r}) \quad (2.6.5)$$

Multiply both sides of (2.6.3) by $u_n^*(\underline{r})$ and integrate over $d\underline{r}$ to get:

$$\int u_n^*(\underline{r}) \Psi(\underline{r}, t) d\underline{r} = \sum_k a_k(t) \int u_n^*(\underline{r}) u_k(\underline{r}) d\underline{r} = \sum_{k=1}^{\infty} a_k(t) \delta_{kn}$$

$$\int u_n^*(\underline{r})\Psi(\underline{r},t) d\underline{r} = a_n(t)\delta_{nm} = a_n(t)$$

$$\therefore a_n(t) = \int u_n^*(\underline{r})\Psi(\underline{r},t) d\underline{r} \quad (2.6.6)$$

Multiply equation (2.6.4) by $u_n(\underline{r})$ and integration over $d\underline{r}$ yields:

$$\int u_n(\underline{r})\Psi^+(\underline{r},t) d\underline{r} = \sum_k a_k^+(t) \int u_n(\underline{r}) u_k^+(\underline{r}) d\underline{r} = \sum_{K=1}^{\infty} a_k^+(t) \delta_{nk}$$

$$\int u_n(\underline{r})\Psi^+(\underline{r},t) d\underline{r} = a_n^+(t)\delta_{nm} = a_n^+(t)$$

$$\therefore a_n^+(t) = \int u_n(\underline{r})\Psi^+(\underline{r},t) d\underline{r} \quad (2.6.7)$$

The commutation relation for “a” can be found by multiplying the relation:

$$[\Psi(\underline{r}),\Psi^+(\hat{r})] = \Psi(\underline{r})\Psi^+(\hat{r}) - \Psi^+(\hat{r})\Psi(\underline{r}) = \delta_{\underline{r}\hat{r}}$$

Multiply by $u_k^*(\underline{r})u_i(\hat{r})$ and integrate over $d\underline{r} d\hat{r}$ to get:

$$\begin{aligned} \iint u_k^*(\underline{r})\Psi(\underline{r})u_i(\hat{r})\Psi^+(\hat{r})d\underline{r}d\hat{r} - \iint u_i(\hat{r})\Psi^+(\hat{r})u_k^*(\underline{r})\Psi(\underline{r})d\underline{r}d\hat{r} \\ = \iint u_k^*(\underline{r})u_i(\hat{r})\delta_{\underline{r}\hat{r}}d\underline{r}d\hat{r} \end{aligned}$$

Where the fact that u is a number requires:

$$u_k^* \hat{u}_i \Psi \Psi^\dagger = u_k^* \Psi \hat{u}_i \Psi^\dagger \cdot \hat{u}_i u_k^* \Psi^\dagger \Psi = \hat{u}_i \Psi^\dagger u_k^* \Psi$$

$$\begin{aligned} \left[\int u_k^*(\underline{r})\Psi(\underline{r}) d\underline{r} \right] \left[\int u_i(\hat{r})\Psi^+(\hat{r})d\hat{r} \right] - \left[\int u_i(\hat{r})\Psi^+(\hat{r})d\hat{r} \right] \left[\int u_k^*(\underline{r})\Psi(\underline{r})d\underline{r} \right] \\ = \int u_k^*(\underline{r}) d\underline{r} [u_i(\hat{r})\delta_{\underline{r}\hat{r}}d\hat{r}] \end{aligned}$$

$$a_k a_i^+ - a_i^+ a_k = \int u_k^*(\underline{r})d\underline{r} [u_i(\underline{r})] = \int u_k^*(\underline{r})u_i(\underline{r})d\underline{r} = \delta_{ki}$$

$$\therefore a_k a_i^+ - a_i^+ a_k = \delta_{ki} \Rightarrow [a_k, a_i^+] = \delta_{ki} \quad (2.6.8)$$

Which represents the commutation relation for “a”. It is apparent that a_k and a_i, a_k^+ and a_i^+ commute i. e. :

$$[a_k, a_i]=0, [a_k^+, a_i^+]=0 \quad (2.6.9)$$

The number operator \hat{N} for the whole system is given by:

$$\hat{N}=\sum_k N_k \quad (2.6.10)$$

Where:

$$N_k = a_k^+ a_k \quad (2.6.11)$$

2.7 Creation , distraction and number operator:

If one have a system in which the number of particles in the state 1, 2, ... k are given by: $|n_1, n_2, n_3, \dots, n_k, \dots\rangle$ =the state in which the number of particles in state 1 is n_1 and the number of particles in state 2 is n_2 ... state K is n_k (2.6.12)

In this case the destruction operator a_k which acts on the state vector decreases the number of particles in state K by one , where:

$$\hat{a}_k |n_1, n_2, n_3, \dots, n_k, \dots\rangle = \sqrt{n_k} |n_1, \dots, n_k - 1, \dots\rangle \quad (2.6.13)$$

In contrast the production operator a_k^+ increases the number of particles in state K by one:

$$\hat{a}_k^+ |n_1, n_2, \dots, n_k, \dots\rangle = \sqrt{n_k + 1} |n_1, \dots, n_k + 1, \dots\rangle \quad (2.6.14)$$

The operator N_k satisfies Heisenberg equation of motion:

$$i\hbar \dot{N}_k = i\hbar \frac{dN_k}{dt} = [N_k, \hat{H}] = [a_k^+ a_k, \hat{H}] \quad (2.6.15)$$

Where H is given by:

$$\hat{H} = \sum_{ij} a_j^\dagger a_i \int \left(\frac{\hbar^2}{2m} \nabla u_j^* \cdot \nabla u_i + v u_j^* u_i \right) d\mathbf{r} \quad (2.6.16)$$

$$= \sum_{ij} a_j^\dagger a_i \int u_j^* \left(\frac{\hbar^2}{2m} \nabla^2 + v \right) u_i d\mathbf{r} \quad (2.6.17)$$

The integral equation (2.6.16) can be obtained from the Hermiticity properties of the motion:

$$\hat{p} = \frac{\hbar}{i} \nabla, \quad \hat{p}^* = \frac{\hbar}{-i} \nabla$$

Where:

$$\int \frac{\hbar^2}{2m} \nabla u_j^* \cdot \nabla u_i d\mathbf{r} = \frac{\hbar}{2m} \left(\frac{1}{i} \right) \int \frac{\hbar}{-i} \nabla u_j^* \Psi_i d\mathbf{r}$$

$$\tilde{\Psi}_i = \nabla u_i$$

$$\begin{aligned} &= \frac{\hbar}{2mi} \int \left(\frac{\hbar}{i} \nabla u_i \right)^* \tilde{\Psi}_i d\mathbf{r} = \frac{\hbar}{2mi} (\hat{p} u_j)^* \tilde{\Psi}_i d\mathbf{r} = \frac{\hbar}{2mi} \int u_j^* \hat{p} \tilde{\Psi}_i d\mathbf{r} = \\ &\frac{\hbar}{2mi} \int u_j^* \frac{\hbar}{i} \nabla \tilde{\Psi}_i d\mathbf{r} = \frac{\hbar^2}{2mi^2} \int u_j^* \nabla^2 u_i d\mathbf{r} = \int -\frac{\hbar^2}{2m} u_j^* \nabla^2 u_i d\mathbf{r} \end{aligned} \quad (2.6.17)$$

Where the fact that \hat{P} is hermitian requires:

$$\int (p u_i)^* \Psi_i d\mathbf{r} = \int u_j^* \hat{P} \Psi_i d\mathbf{r}$$

$$\begin{aligned}
\hat{H} &= \sum_{ij} a_j^\dagger a_i \int \left(\frac{\hbar^2}{2m} \nabla u_j^* \cdot \nabla u_i + v u_j^* u_i \right) dr \\
&= \sum_{ij} a_j^\dagger a_i \int \left[-\frac{\hbar^2}{2m} u_j^* \cdot \nabla^2 u_i + v u_j^* u_i \right] dr \\
&= \sum_{ij} a_j^\dagger a_i \int u_j^* \left[-\frac{\hbar^2}{2m} \nabla^2 + v \right] u_i dr = \sum_{ij} a_j^\dagger a_i \int u_j^* \hat{H} u_i dr \\
&= \sum_{ij} a_j^\dagger a_i \int u_j^* E_i u_i dr = \sum_j a_j^\dagger \left(\sum_i a_i E_i \int u_j^* u_i dr \right) \\
&= \sum_j a_j^\dagger (a_j E_j \delta_{ij}) \sum_j a_j^\dagger (a_j E_j) = \sum_j N_j E_j
\end{aligned}$$

$$\therefore H = \sum_j N_j E_j$$

This particular N representation is the one in which H is also diagonal ;the ket $|n_1, \dots, n_k, \dots\rangle$ has the eigenvalue $\sum n_k E_k$ for the total energy operator H .It is apparent that all the N_j are constant in this case.

2.8 Harmonic oscillator:

We will illustrate the solution of the problem of the linear harmonic oscillator by using Heisenberg operators in which the operator are function of t.

Thus the Hamiltonian is given by [42]:

$$\hat{H}(t) = \frac{\{\hat{p}(t)\}^2}{2m} + \frac{1}{2} k \{\hat{x}(t)\}^2 = \frac{1}{2m} [\hat{p}^2(t) + m^2 \omega^2 \hat{x}^2(t)] \quad (2.8.1)$$

Where:

$$k=m\omega^2$$

The equation of motion for \hat{x} and \hat{p} are:

$$\frac{d\hat{x}}{dt} = \frac{\partial \hat{H}}{\partial \hat{p}} = \frac{\hat{p}}{m} \quad (2.8.2)$$

$$\frac{d\hat{p}}{dt} = -\frac{\partial \hat{H}}{\partial \hat{x}} = -m\omega^2 \hat{x}^2 \quad (2.8.3)$$

Differentiating (2.8.2) w.r.t. t once again, and substituting for $\frac{d\hat{p}}{dt}$ from (2.8.3), we get:

$$\frac{d^2\hat{x}}{dt^2} + \omega^2 \hat{x} = \hat{0} \quad (2.8.4)$$

Which is of the same form as the classical equation of motion for the harmonic oscillator.

The solution of equation (2.8.4) is:

$$\hat{x}(t) = \hat{c}_1 e^{-i\omega t} + \hat{c}_2 e^{i\omega t} = \hat{a}_1 \cos \omega t + \hat{a}_2 \sin \omega t \quad (2.8.5)$$

$$\hat{a}_1 = \hat{x}(0) \equiv \hat{x}_0$$

$$\hat{a}_2 = \frac{1}{\omega} \left. \frac{d\hat{x}}{dt} \right|_{t=0} = \frac{\hat{p}(0)}{m\omega} = \frac{\hat{p}_0}{m\omega}$$

So that:

$$\hat{x}(t) = \hat{x}_0 \cos \omega t + \left(\hat{p}_0 / m\omega \right) \sin \omega t \quad (2.8.6)$$

$$\hat{p}(t) = m \frac{d\hat{x}}{dt} = \hat{p}_0 \cos \omega t - m\omega \hat{x}_0 \sin \omega t \quad (2.8.7)$$

Substituting in (2.8.1) from (2.8.6) and (2.8.7), we get:

$$\hat{H} = \frac{1}{2m} (\hat{p}_0^2 + m^2 \omega^2 \hat{x}_0^2) \quad (2.8.8)$$

Which is independent of time.

A method due to Dirac avoid the dependence on the solutions of the differential equations of the Schrödinger picture for the evaluation of the matrix elements of operators in the Heisenberg picture. This method consists in finding suitable operator with which one can generate all the eigenvector. These eigenvectors will, then define a representation. Thus, the eigenvalue problem is automatically solved if we find the above operators. The method anticipates the technique of field, or second quantization.

The operators we seek are given by:

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega\hat{x}_0 + i\hat{p}_0) \quad (2.8.9)$$

$$\hat{a}^+ = \sqrt{\frac{1}{2m\hbar\omega}} (m\omega\hat{x}_0 - i\hat{p}_0) \quad (2.8.10)$$

From equations (2.8.9) and (2.8.10) , we get:

$$\hat{x}_0 = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+) \quad (2.8.11)$$

$$\hat{p}_0 = i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a}^+ - \hat{a}) \quad (2.8.12)$$

From the conditions:

$$[\hat{x}_0, \hat{p}_0] = i\hbar\hat{1}; [\hat{x}_0, \hat{x}_0] = \hat{0} = [\hat{p}_0, \hat{p}_0]$$

We have:

$$[\hat{a}, \hat{a}^+] = \hat{1},$$

$$[\hat{a}, \hat{a}] = \hat{0} = [\hat{a}^+, \hat{a}^+] \quad (2.8.13)$$

Substituting from equations (2.8.11), (2.8.12) and (2.8.13) in equation (2.8.1), we get:

$$\hat{H} = (\hat{N} + \frac{1}{2})\hbar\omega \quad (2.8.14)$$

Where:

$$\hat{N} = \hat{a}^+ \hat{a} \quad (2.8.15)$$

From equation (2.8.13) and equation (2.8.15), we have:

$$[\hat{N}, \hat{a}] = -\hat{a} \quad (2.8.16)$$

$$[\hat{N}, \hat{a}^+] = +\hat{a}^+ \quad (2.8.17)$$

Let ϕ_n represent a normalized eigenvector \hat{N} belonging to the eigenvalue n .

$$\hat{N}\phi_n = n\phi_n \quad (2.8.18)$$

Then, from (2.8.16), we have:

$$\hat{N}(\hat{a}\phi_n) = (n-1)(\hat{a}\phi_n) \quad (2.8.19)$$

Which shown that $(\hat{a}\phi_n)$ is an eigenvector of \hat{N} belonging to the eigenvalue $(n-1)$. Similarly, $(\hat{a}\phi_n)$ is an eigenvector of \hat{N} belonging to the eigenvalue $(n-r)$. Now,

$$n = (\phi_n, n\phi_n) = (\phi_n, \hat{N}\phi_n) = (\phi_n, \hat{a}^+ \hat{a}\phi_n) = (\hat{a}\phi_n, \hat{a}\phi_n) = \|\hat{a}\phi_n\|^2 \geq 0 \quad (2.8.20)$$

Since the norm of a vector in this case of $(\hat{a}\phi_n)$, cannot be negative.

Therefore, the series,

$$\phi_n, \hat{a}\phi_n, \hat{a}^2\phi_n \cdots, \hat{a}^r \phi_n, \cdots \quad (2.8.21)$$

A vector $\phi = (\hat{a}^-)^s \phi_n$ for which the eigenvalue $(n - s)$ is negative. Let the last term of the series (2.8.21) be denoted by ϕ_0 . Then,

$$\hat{a} \phi_0 = 0 \quad (2.8.22)$$

Thus, the series (2.8.21) correspond to the eigenvalues

$$n, (n - 1), (n - 2), \dots, 0$$

Similarly, from eqn (2.8.17), we get:

$$\hat{N}(\hat{a}^+ \phi_n) = (n + 1)(\hat{a}^+ \phi_n)$$

$$\hat{N}(\hat{a}^+)^r \phi_n = (n + r)(\hat{a}^+)^r \phi_n$$

Showing that the series,

$$\hat{a}^+ \phi_n, (\hat{a}^+)^2 \phi_n, \dots, (\hat{a}^+)^r \phi_n, \dots \quad (2.8.23)$$

Represents the eigenvalues:

$$(n + 1), (n + 2), \dots, (n + r), \dots, +\infty$$

Thus, the eigenvalue spectrum of \hat{N} is given by the non-negative integers:

$$n = 0, 1, 2, \dots, +\infty. \quad (2.8.24)$$

Any eigenvector of \hat{N} can be reached from a given eigenvector ϕ by repeated application of either \hat{a} or \hat{a}^+ . Let us denote by the ket $|n\rangle$ the normalized eigenvector of \hat{N} belonging to eigenvalue n . That is:

$$|n\rangle \equiv \phi_n \quad (2.8.25)$$

Then:

$$\langle n | n \rangle = \delta_{nn} \quad (2.8.26)$$

$$|n\rangle = c_n (\hat{a}^+)^n |0\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n |0\rangle \quad (2.8.27)$$

$$\hat{a}|0\rangle \equiv 0 \quad (2.8.28)$$

From equation (2.8.14) and $\langle n|N|n\rangle = \delta_{nn}$, we have the eigenvalue E_n of \hat{H} in the state $|n\rangle$, the expression:

$$E_n = \left(n + \frac{1}{2}\right) \varepsilon = n\varepsilon + E_0 \quad (2.8.29)$$

Where:

$$\varepsilon = \hbar\omega \quad (2.8.30)$$

Thus:

$$(E_n - E_0) = n\varepsilon, n = 0, 1, 2, \dots \quad (2.8.31)$$

This equation permits the oscillator in the state $|n\rangle$ each of energy. The different states of the oscillator merely correspond to different numbers of the particles. From the equation:

$$n \frac{1}{\sqrt{n!}} (\hat{a}^+)^{n-1} |0\rangle = \sqrt{n} |n-1\rangle$$

We see that the operator \hat{a} lowers the particle number by 1, where as \hat{a}^+ raises the particle number by 1. \hat{a}^+ Creates a particle while \hat{a} destroys, or annihilation operators. The relations, $\hat{a}|0\rangle = 0, \hat{a}^+|0\rangle = |1\rangle$, are consistent with this interpretation since a particle cannot be destroyed, when no particle is present as in $|0\rangle$, but a particle can be created even when no particle is initially present. The interpretation of $\hat{N} \equiv \hat{a}^+ \hat{a}$ as the number operator is, then, suggested by (2.8.18).

The representation defined by the basis vectors $|n\rangle$, ($n = 0, 1, 2, \dots, \infty$), is named the occupation-number representation (n is the number that the particle number 'n' is actually the quantum number characterizing the state of excitation of the oscillation for and it is only as a matter of convenience that it is called a particle-number).

The second method to the solution of the problem of the linear harmonic oscillator using Schrodinger picture, which the Hamiltonian is given by:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} k \hat{x}^2 \quad (2.8.32)$$

In the Schrodinger picture, \hat{p} and \hat{x} are independent of time. In the coordinate representation:

$$\hat{p} \equiv -i\hbar \frac{d}{dx} \quad \text{and} \quad \hat{x} \equiv x$$

So that:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \quad (2.8.33)$$

The time-dependent Schrödinger equation is:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \right) \Psi(x,t) \quad (2.8.34)$$

Since \hat{H} is independent of time, $\Psi(x,t)$ can be written, choosing $t_0 = 0$, thus:

$$\Psi(x,t) = \exp\left[-\left(\frac{i}{\hbar}\right)\hat{H}t\right]u(x) \quad (2.8.35)$$

With:

$$\hat{H}u_n(x) = E_n u_n(x) \quad (2.8.36)$$

That is:

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2\right) u_n(x) = E_n u_n(x) \quad (2.8.37)$$

Which is the time-independent Schrödinger equation for the linear harmonic oscillator. From equations (2.8.35) and (2.8.36), we get:

$$\Psi_n(x, t) = \exp\left[-\left(\frac{i}{\hbar}\right)E_n t\right] u_n(x) = x_n(t) u_n(x) \quad (2.8.38)$$

To transform equation (2.8.34) to the form (2.8.37) we need the technique of separation of variables, therefore equation (2.8.36) is an eigenvalue for the Hamiltonian, the values of E , permitted by the equation, are the energies that the harmonic oscillator can have. The state of the oscillator with energy E_n is represented by the state vector (wave function) $U_n(x)$. The problem of determining the E_n and U_n is reduced to solving the differential equation (2.8.37), by substituting:

$$\xi = \alpha x; \alpha = \left(\frac{mk}{\hbar^2}\right)^{1/4} = \sqrt{\frac{m\omega}{\hbar}}; (1 + 2n) = \frac{2E_n}{\hbar\omega} \quad (2.8.39)$$

Where:

$$\omega = \sqrt{\frac{k}{m}} \quad (2.8.40)$$

Is the classical frequency of the oscillator. Then equation (2.8.37) reduced to:

$$\frac{d^2\phi_n}{d\xi^2} + (1 + 2n - \xi^2)\phi_n = 0 \quad (2.8.41)$$

Where:

$$\phi_n(\xi) \propto u_n(x) \quad (2.8.42)$$

Thus:

$$\phi_n(\xi) = \frac{1}{(\sqrt{\pi}2^n n!)^{1/2}} \exp\left(-\xi^2/2\right) H_n(\xi) \quad (2.8.43)$$

Or:

$$u_n(x) = \frac{\sqrt{\alpha}}{[\sqrt{\pi}2^n n!]^{1/2}} \exp\left(-\frac{1}{2}\alpha^2 x^2\right) H_n(\alpha x) \quad (2.8.44)$$

Which are the eigenfunctions. The corresponding energy eigenvalues are from (2.8.39):

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega \quad n=0, 1, 2, \dots \quad (2.8.45)$$

2.9 The Hubbard model:

2.9.1 Introduction to Hubbard model and exact diagonalization:

Motivated by the success of production and annihilation in quantizing field, encourages some physicists to utilize the same framework to try to solve some long standing problems of condensed matter physics. This trial is not surprising as far as the system of fields consists of a large number of mediators carrying the field force, which is similar to condensed matter which consists of huge number of particles. The physics based on the notion of production operators utilized in solid state physics is called Hubbard model [43].

2.9.2 Non – interacting electron:

The Hamiltonian of non-interacting fermions on a lattice of L side labeled by i, j takes the form [43]:

$$H_0 = \sum_{ij} t_{ij} c_i^\dagger c_j \quad (2.9.1.1)$$

Where c_i^\dagger Produces while c_i annihilates fermions in a single – particle orbit localized at site j and described by the commutation relations:

$$\{c_i^\dagger, c_j\} = \delta_{ij} \quad (2.9.1.2)$$

The t_{ij} are coefficient defined to be:

$$t_{ij} = \langle \Phi_{ij} | \left[-\frac{\hbar^2}{2m} \nabla^2 + V_o \right] | \Phi_j \rangle = \int \Phi_i(X) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_o(X) \right] \Phi_j(x) dx \quad (2.9.1.3)$$

Where V_o stands for the crystal field interaction.

For practical considerations t_{ij} is non-zero, only when i,j are nearest neighbors, in which case it is usually denoted by - t. Thus H_0 in (2.9.1.1) can be reduced to the form:

$$\widehat{H}_0 = -t \sum_{ij} [c_i^\dagger c_j + c_j^\dagger c_i]$$

Assuming the periodic boundary conditions, one can write:

$$c_k^\dagger = \frac{1}{\sqrt{L}} \sum_j e^{ikj} c_j^\dagger \quad (2.9.1.4)$$

$$H_0 = \sum_k \epsilon_k c_k^\dagger c_k \quad (2.9.1.5)$$

Where:

$$\epsilon_k = -2t \cos k a \quad (2.9.1.6)$$

With L allowed K values in the first Brillion zone. The term here stands for the distance between two sides.

If the number of electrons N is equal to the number of sites L , i.e. $N = L$, in this situation each allowed K state can be occupied by two situation and each spins. Hence the ground state of H_0 is constructed by filling the lower half. $\epsilon_k < 0$, of the band which is denoted by continuous line. Since half of the band is filled, the situation, $N = L$ is called half filling. This state is known as a Fermi sea state, usually denoted by $|FS\rangle$, where:

$$|FS\rangle = \prod_{k < k_F} \hat{c}_{K\uparrow} \hat{c}_{K\downarrow} |0\rangle \quad (2.9.1.7)$$

With $|0\rangle$ standing for the vacuum state in which the lattice is empty. k_F is the maximum occupied K state known as Fermi wave vector.

The fact that K states are occupied by 2 electrons comes from the fact that the number of allowed values of K are L . But since the occupied states are these for which $\epsilon_k < 0$, specially the K axis], only occupied, while those for which $\frac{\pi}{2} < k < \pi$, $-\frac{\pi}{2} < k < -\frac{\pi}{2}$ are empty. Thus the occupied k states are $L/2$.

But as far as the number of electrons are $N = L = 2 \times (L/2) = 2 \times$ number of K states. Hence each K states is occupied by 2 electrons of spins up and down.

The Fermi sea states. Hence each K states is occupied by 2 electrons of spins up and down.

The Fermi sea state: is the eigenstate of the Hamiltonian, thus:

$$H_0 |FS\rangle = E_0 |FS\rangle \quad (2.1.9.8)$$

The total energy E_0 is given by:

$$E_0 = \sum_{|K| < \frac{\pi}{2}, \sigma} \varepsilon_k n_{k\sigma} = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} 2x (-2t \cos k a) \frac{dK}{2\pi} \quad (2.9.1.9)$$

The integral here is multiplied by 2 since each K state is occupied by 2 electrons, while we divide K by 2π since the system is confined the first Brillouin zone.

If this system is excited an electron from one of the states $|K| > \pi/2$ jump to a higher state $k+q$ such that $|k+q| > \frac{\pi}{2}$, leaving a hole in the state K . If the electron spin is up \uparrow this new state is denoted by $|\psi_n\rangle$, where:

$$H_0 |\psi_n\rangle = H_0 (\hat{c}_{k+q\uparrow} \hat{c}_{k\uparrow}) |FS\rangle = \varepsilon_k^{ph}(q) |\psi_n\rangle \quad (2.9.1.10)$$

The energy of state ψ_n is given by:

$$\varepsilon_k^{ph}(q) = \varepsilon_{k+q} - \varepsilon_k \quad (2.9.1.11)$$

In this half-filled band one has a metal as far as the filled valence band and the empty conduction band overlap.

The ground state of non-interacting electrons can be obtained by occupied by 2 electrons with \uparrow and \downarrow spins. But since the number of allowed states in K space one L , and since:

$L = N =$ number of electrons.

Hence only $L/2$ states are occupied, where:

2 electrons \times ($L/2$) states = $L = N$, thus we have half-filled band.

Such occupation to minimize energy in the K – space , can be performed by 4 possible ways in the real space, where we have 4 possible occupation of a single site .

The above situation represents the case when the electron – electron interaction the case when the electron – electron interaction is considered, one has to add to Hamiltonian term:

$$V = \frac{1}{2} \sum V_{\mu\nu\beta\alpha} c_{\mu}^{\dagger} c_{\nu}^{\dagger} c_{\alpha} c_{\beta} \quad (2.9.1.12)$$

Where the index $\alpha \equiv \{\sigma, i\}$ describes the site i and spin σ .The two particle interaction is described by the term:

$$V_{\mu\nu\beta\alpha} = \int \psi_{\mu}^*(x) \psi_{\nu}^*(x) V(|x - \hat{x}|) \psi_{\beta}(x) \psi_{\alpha}(x) dx d\hat{x} \quad (2.9.1.13)$$

In metals the coulomb potential is screened and takes the form:

$$V(r) = \frac{e^{k_0 r}}{r}, k_0 = k_f \quad (2.9.1.14)$$

When all indices correspond the same site j , Pauli principle forces [43]:

$$\mu = \alpha = \uparrow, \quad \beta = \nu = \downarrow$$

The diagonalization process aims to find the space which constitutes eigenvectors of the Hamiltonian. This comes from the fact that the Hamiltonian matrix is diagonal in the Hamiltonian eigenvectors space.

In this case the eigenvector is the energy eigenvalue while the corresponding coefficient is the energy of the corresponding coefficient is the energy of the state.

This toy model consists of two written explicitly (in unit,

Which $t = 1$) as:

$$H = H_{\uparrow} + H_U = -(c_{0\uparrow}^{\dagger}c_{1\uparrow} + c_{1\uparrow}^{\dagger}c_{0\uparrow} + c_{0\downarrow}^{\dagger}c_{1\downarrow} + c_{1\downarrow}^{\dagger}c_{0\downarrow} + (n_{0\uparrow}n_{0\downarrow} + n_{1\uparrow}n_{1\downarrow}))$$

The first term stands for the kinetic hopping process while second one represents the field contribution [43].

2.9.3 Strong correlation and spin physics:

As one already sees in previous section, the ground state of the two site Hubbard model is a singlet with energy:

$$E_s^- = \frac{U}{2} - \sqrt{\frac{U^2}{4} + 4t^2}$$

The ground state wave function:

$$|E_s^-\rangle = 4|\psi_2\rangle + (U + \sqrt{U^2 + 16})|\psi_3\rangle \quad (2.9.3.1)$$

In large U limit is dominated by $|\psi_3\rangle \sim |\emptyset_3\rangle + |\emptyset_4\rangle$ in which there is no doubly occupied configuration, and hence charge fluctuations are suppressed.

Since the first excited state is at $E = 0$. The splitting between these two states for large $U \gg t$ is:

$$-J = E_s - E_t = \frac{U}{2} - \sqrt{\frac{U^2}{4} + 4t^2} \approx \frac{4t^2}{U} \quad (2.9.3.2)$$

Therefore the singlet state is slightly below $(-4t^2 / U)$ the triplet state. This indicates that in large U limit, the low-energy physics of Hubbard model is given by spin fluctuations which are anti-ferromagnetic (AF) (singlet has lower energy). This observation in a two site Hubbard model is indeed very general and it can be shown using a unitary transformation that the Hubbard

model at large U limit can be mapped into the so called t - J model, where there are AF fluctuations along with hopping restricted to subspace with no double occupancy [43].

2.9.4 Hubbard model for superconductivity and Mott insulator:

One of the most widely used models to describe HTSC is the Hubbard model. The electric conduction in this model is performed by hopping of valence electrons from site to site. Moreover this model is used in most applications of condensed matter and many body systems. The Hubbard model is particularly applied to strongly correlated systems, including electronic within it are not free. In the free electron model Fermi gas, which obeys Pauli Exclusion Principle.

The electron state can be described by using the $\Phi_n(\mathbf{r} - \mathbf{R}_i)$ functions (basis) which describe electrons localized at \mathbf{r} on the atom at the position \mathbf{R}_i . The standard production $C_{ni\sigma}^+$ and annihilation $C_{ni\sigma}$ operators on the n th localized wannier state spin σ on the atom at the position \mathbf{R}_i . The electrons can be assumed, for aimplicity, to be affected by the coulomb repulsion between electrons on the same site, beside the kinetic hopping term which describes the quantum probability that an electron may hop from site to \mathbf{R}_i to \mathbf{R}_j or from \mathbf{R}_j to \mathbf{R}_i .

In the standard Hubbard model each atom has one electron non-degenerate orbital state. The actual atom, however, can have more than one orbital more than two electrons in the corresponding state. This assumption stems from the fact that the electrons in other states do not play significant role at low temperature, hence the Hamiltonian of the system takes the form [43]:

$$H = \sum_{ijk} t_{ij} c_{ik}^{\dagger} c_{jk} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (2.9.4.1)$$

Where:

$$n_{ik} = c_{ik}^{\dagger} c_{ik} \quad (2.9.4.2)$$

Stands for the electron number operator. To simplify treatment one can use U to describe coulomb repulsion, and t to represent kinetic hopping. Hence the quantity U/t determines whether coulomb repulsion or hopping dominates. However, it is not possible to determine the relative importance of the two in relation to the Pauli Exclusion Principle, which depends on the probability of finding two electrons on the same site. This quantity can somewhat be accounted for by electron density per spin.

$$n = \frac{1}{2N} \sum_{ik} c_{ik}^{\dagger} c_{jk} \quad (2.9.4.3)$$

Each atom has space for at most two electrons, n can be in the range from 0 to 1, Hubbard model is affected by three factors, one – site repulsions hopping and Pauli Exclusion Principle.

When each atom has one electron, one has a perfect half-filled band, to put an extra electron on that system this needs to overcome coulomb repulsion. When U is big the band will split into two sub bands with a gap in the middle, for half-filled band, i.e. n=0.5 the Fermi energy will cross the energy gap. Thus the lower band is filled and stands for the valence band while the upper band is empty and behaves as a conduction band. Therefore the electron to become free needs very large energy to cross the energy gap E_g to be free where:

$$E_g \propto AE \propto U \rightarrow \infty$$

In this case, the material become an insulator called Mott- insulator. If n is not perfectly equal to 0.5 the Fermi energy will cross either the upper or the lower Hubbard band. This can be understood in terms of Fermi Dirac statistics where:

$$n = \frac{1}{[e^{\beta(E-E_F)} + 1]} \quad (2.9.4.4)$$

$$e^{\beta(E-E_F)} = \frac{1}{n} - 1$$

$$E - E_F = \text{Ln} \left(\frac{1-n}{n} \right) \quad (2.9.4.5)$$

$$E_F = E + \text{Ln} \left(\frac{n}{1-n} \right)$$

For zero filling $n = 0$

$$E_F = E + \text{Ln} 0 = E + \text{Ln} e^{-\infty}$$

$$E_F = E - \infty \rightarrow -\infty \quad (2.9.4.6)$$

Since the zero energy is at the interface of upper and lower band. Thus E_F becomes far below the interface. Therefore E_F crosses the lower band. Hence there is no gap between conduction and valence band, as for as E_F separates conduction and valence band. As a result the material is converted into metal.

For complete filling $n = 1$

$$E_F = E + \text{Ln} \infty = E + \text{Ln} e^{\infty} = E + \infty \rightarrow \infty \quad (2.9.4.7)$$

Hence E_F crosses the upper band, again the material becomes a conductor as far as E_F , does not cross an energy gap. Thus electrons can easily become conduction electrons [43].

Chapter 3

Literature Review

3.1 Introduction:

Many attempts were made to construct new quantum models that can describe new materials properties [44,45,46,47] or to unify fundamental forces [48,49,50,51]. Some of them are based on changing energy expressions, while others are based on modifying the wave function itself [52,53,54,55]. In this chapter some attempts, especially those which are concerned with bulk matter, are exhibited.

3.2 On the Heisenberg and Schrödinger pictures:

Both Heisenberg (HP) and Schrödinger pictures (SP) are used in quantum theory. Schrödinger solved Schrödinger eigenvalue equation for a hydrogen atom, and obtained the atomic energy levels. Heisenberg discussed the uncertainty principle based on the fundamental commutation relations. Both pictures are equivalent in dealing with a one-electron system. In dealing with many electrons or many photons a theory must be developed in the HP, incorporating the indistinguishability and Pauli's exclusion principle. A quantum theory must give a classical result in some limit. We will see that this limit is represented by $\hbar \rightarrow 0$. The HP, and not the SP, give the correct results for a many-particle system. The quantum field equation is nonlinear if a pair interaction exists [56].

representation:

$$r = (x, y, z) \equiv (q_1, q_2, q_3). \quad (3.2.1)$$

The canonical momentum p is:

$$p = (p_x, p_y, p_z) \equiv (p_1, p_2, p_3) \quad (3.2.2)$$

The Hamiltonian H of the system is:

$$H = \frac{p^2}{2m} + V(r) \quad (3.2.3)$$

In the HP the coordinates and momenta (q, p) are regarded as Hermitean operators satisfying the fundamental commutation relation (quantum conditions):

$$[q_j, p_k] \equiv q_j p_k - p_k q_j = i\hbar \delta_{jk}, [q_j, p_k] = [q_j, p_k] = 0, \quad (3.2.4)$$

Where δ_{jk} is Kronecker's delta:

$$\delta_{jk} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases} \quad (3.2.5)$$

And $\hbar \equiv h/(2\pi)$, $h \equiv$ Planck constant.

The equations of motion for q_j and p_j are:

$$\frac{dq_j}{dt} = \frac{1}{i\hbar} [q_j, H], \frac{dp_j}{dt} = [p_j, H], j = 1, 2, 3. \quad (3.2.6)$$

The two equations can be included in a single equation:

$$\frac{d\xi}{dt} = \frac{1}{i\hbar} [\xi, H], \quad (3.2.7)$$

Where ξ represent any physical observable made out of the components of the position $r = (x, y, z)$ and momentum $p = (p_x, p_y, p_z)$. The angular

momentum $I = r \times p = (I_x, I_y, I_z)$ can be included also. Dirac has shown that in the small \hbar limit:

$$\frac{1}{i\hbar} [q_j, p_k] \rightarrow \{q_j, p_k\} \text{ as } \hbar \rightarrow 0, \quad (3.2.8)$$

Where:

$$\{A, B\} \equiv \sum_J \left\{ \frac{\partial A}{\partial q_j} \frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j} \frac{\partial B}{\partial q_j} \right\} \quad (3.2.9)$$

Is the classical Poisson brackets.

In the SP we use the equivalence relations:

$$p = -i\hbar \frac{\partial}{\partial q_j} \quad (3.2.10)$$

And write down the Schrödinger wave equation as:

$$i\hbar \frac{\partial \Psi(r, t)}{\partial t} = H\Psi(r, t) = \left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z) \right] \Psi(x, y, z, t) \quad (3.2.11)$$

The function Ψ is called the wave function. Normally, it is normalized such that:

$$\int_{\Omega} d^3r \Psi^*(r, t) \Psi(r, t) = 1 \quad (3.2.12)$$

Where Ω is a normalization Volume. The quantum average of an observable $\xi(r, p)$ is defined by:

$$\langle \xi \rangle = \int d^3r \Psi^+(r, t) \xi(r, -i\hbar \nabla) \Psi(r, t) \quad (3.2.13)$$

If we use Dirac's ket and bra notations, then we can see the theoretical structures more compactly. The quantum state Ψ is represented by the Ket

vector $|\Psi, t \rangle$ or the bra vector $\langle \Psi, t | \equiv (|\Psi, t \rangle)^*$. The Schrödinger equation of motion is:

$$i\hbar \frac{d}{dt} |\Psi, t \rangle = H |\Psi, t \rangle \quad (3.2.14)$$

Whose Hermitean conjugate is:

$$-i\hbar \frac{d}{dt} \langle \Psi, t | = \langle \Psi, t | H \quad (3.2.15)$$

If we use the position representation and write:

$$\langle r | \Psi, t \rangle = \Psi(r, t) \quad (3.2.16)$$

Then we obtain equation (3.2.11) from Equation (3.2.14). We introduce the density operator ρ defined by:

$$\rho(t) \equiv |\Psi, t \rangle \langle \Psi, t | \quad (3.2.17)$$

Using Equation (3.2.14) and (2.3.15), we obtain:

$$i\hbar \frac{d\rho}{dt} = -[\rho, H] \quad (3.2.18)$$

This equation, called the quantum Liouville equation, has a reversed sign compared with the equation of motion for, see Equation (3.2.7). We can express the quantum average $\langle \xi \rangle$ of an observable ξ as:

$$\langle \xi \rangle = tr\{\xi\rho\} = tr\{\rho\xi\}, \quad (3.2.19)$$

Where tr denotes a one-particle trace. Operators under a trace commute.

We assume that the Hamiltonian H in equation (3.2.11) is a constant of motion. Then, equation (3.2.14) can be reduced to the energy (E) eigenvalue equation:

$$H\Psi_E(r) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \Psi_E(r) = E\Psi_E(r) \quad (3.2.20)$$

After using a separation of variable method for solving equation (3.2.11). Equation (3.2.20) is known as the Schrödinger energy-eigenvalue equation. The hydrogen atom energy-levels can be obtained from equation (3.2.20) with $v(r) = -e^2/4\pi\epsilon_0 r$, $\epsilon_0 =$ permittivity.

Except for simple system such as free electrons and simple harmonic oscillators, the Heisenberg equation of motion (3.2.7) or the quantum Liouville equation (3.2.18) are hard to solve. This is so because the number of unknowns in the $n \times n$ matrix are more numerous than in the $1 \times n$ vector.

The follow items difficulties in the SP . They cannot be addressed properly.

(a) The Classical Mechanical Limit ($\hbar \rightarrow 0$):

Dirac showed that the fundamental commutation relations (3.2.8) can also be applied to a many particle system only if the Cartesian coordinates and momenta are used. The equation of motion (3.2.7) in the HP can be reduced to the classical equation of motion:

$$\frac{d\xi}{dt} = \{\xi, H\} \quad (\text{classical}) \quad (3.2.21)$$

In the classical limit:

$$\hbar \rightarrow 0. \quad (3.2.22)$$

The Schrödinger equation of motion (3.2.11) does not have such a simple limit.

(b) Indistinguishability:

All electrons are identical (indistinguishable) to each other. This is known as the Indistinguishability. This property can be stated as follow:

Consider a system of N electrons interacting with each other characterized by the Hamiltonian:

$$H = \sum_{j=1}^N \varepsilon^{(j)} + \frac{1}{2} \sum \sum_{j \neq k} \phi^{(jk)}, \quad (3.2.23)$$

Where $\varepsilon^{(j)}$ is the kinetic energy and $\phi^{(jk)} \equiv \phi(|r_j - r_k|)$ is the pair interaction energy. Here the upper indices j and k denote the electrons.

The indistinguishability requires that:

$$[p, H] = 0 \text{ for all } p \quad (3.2.24)$$

Where p are the permutation operators. For a three particle system the permutation operators are:

$$\begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} \quad (3.2.25)$$

The order of the permutation group for an N -particle system is $N!$. The total momentum, the total angular momentum, and the total mass satisfy the same equation (3.2.24). One may express this by:

$$[p, X] = 0 \text{ for all } p, X = \sum_{j=1}^N \xi^{(j)} \quad (3.2.26)$$

Photons are bosons with full spin. They can be created and annihilated spontaneously. These processes can only be described by using creation and annihilation operators (a, a^+) both of which move, following the Heisenberg equations of motion. One can no more limit the number of bosons in the system.

Bosons can be treated using second –quantization operators (a, a^+) satisfying the Bose commutation rules:

$$[a_\mu, a_\nu^+] \equiv a_\mu a_\nu^+ - a_\nu^+ a_\mu = \delta_{\mu,\nu}$$

$$[a_\mu, a_\nu] = [a_\mu^+, a_\nu^+] = 0 \quad (3.3.27)$$

Where (μ, ν) indicates particle states. Both operators a and a^+ move, following the Heisenberg equations of motion, e.g.:

$$i\hbar \frac{da_\mu}{dt} = [a_\mu, H] \quad (3.2.28)$$

Where H is a many-boson Hamiltonian. The Hamiltonian for free photons is given by:

$$H = \sum_p \sum_\sigma \left(\frac{1}{2} + a_{p\sigma}^+ a_{p\sigma} \right) \hbar\omega_{p,\sigma} \quad (3.2.29)$$

Where $\omega_{p,\sigma}$ is angular frequency and σ ($=1$ or 2) denotes the polarization indices. Many fermions can be treated by using the complex dynamical operators (c, c^+) satisfying the Fermi anticommutation rules:

$$[c_\mu, c_\nu^+] \equiv c_\mu c_\nu^+ + c_\nu^+ c_\mu = \delta_{\mu,\nu},$$

$$[c_\mu, c_\nu] = [c_\mu^+, c_\nu^+] = 0 \quad (3.2.30)$$

Both operators c and c^+ move following the Heisenberg equations of motion. If the system contains many electrons, one consider Pauli's exclusion principle that no more than one fermions can occupy the same particle state. This is a restriction which cannot be describe without considering permutation symmetry [56].

3.3 The simplified Hubbard model in one and two dimensions:

Hubbard model has been used for studying the basic properties of strongly interacting fermions systems. Despite its apparent simplicity the model has resisted an exact treatment except in the one- dimensional (1D)

case. Only a limited number of rigorous statements are available for higher dimensions [57].

In a wide variety of applications, approximate theoretical studies and numerical work on finite crystals was made. A recent approach has been to study the simplifying limit $d \rightarrow \infty$, which allows a more thorough analysis of the many-body model.

Phenomena resulting from strong correlation effects that are of interest are, e.g., superconductivity, the occurrence of magnetic long-range order (LRO) and a metal-insulator (MI) transition as the (on-site) Coulomb interaction constant U is varied. Related to the latter, it is also of interest to study the properties of the single particle density of states (DOS) as a function of U , temperature and band filling. The manner in which spectral weight may appear in an insulating gap can be relevant for the proper description of the MI transition and may elucidate the various approaches for understanding the high-temperature superconducting oxides. For the two-dimensional (2D) Hubbard model the behavior of gaps and pseudo gaps in the DOS has recently been investigated numerically.

A simplified Hubbard (SH) model, which was already used by Hubbard, is presented here. The SH model is obtained from the latter by immobilizing one species of electrons ($\sigma = \uparrow$ or $\sigma = \downarrow$). Some rigorous results exist for this model on bipartite lattices and at half filling. In the limit of infinite dimensionality ($d \rightarrow \infty$) the half-filled SH model has recently been solved exactly. The SH is formally equivalent to the Symmetric version of the spinless Falicov-Kimball (FK) model. Many studies have employed the general asymmetric, version of this model, see e.g. The FK model is exactly solvable for here we present results obtained using exact diagonalization and

Quantum Monte Carlo methods for the 1D and 2D SH model on bipartite lattices. Ground-state as well as finite-temperature properties are studied as a function of U . Static and dynamic quantities are investigated for variable band fillings. The DOS, the occurrence of a MI transition and of magnetic LRO are of particular interest.

The Hamiltonian for the SH model is given by:

$$H = -t \sum_{\langle i,j \rangle} (c_{i\uparrow}^\dagger c_{j\uparrow} + c_{j\uparrow}^\dagger c_{i\uparrow}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} \quad (3.3.1)$$

Where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are creation and annihilation operators, respectively, for an electron with spin $\sigma = \uparrow, \downarrow$ at site i , and $n_{i\sigma}$ is the corresponding number operator, $\sum_{\langle i,j \rangle}$ denotes a sum over nearest-neighbor pairs, t is the hopping amplitude, U is the on-site Coulomb interaction constant and the chemical potential. At half filling, the electron density $\rho \equiv \sum_{i\sigma} \langle n_{i\sigma} \rangle / N = 1$ (N denotes the number of lattice sites) and $\mu = U/2$.

The above Hamiltonian can be interpreted in different ways. Besides studying the model on its own merits, it can be viewed as an approximation to the Hubbard model where the $\sigma = \downarrow$ electrons are not allowed to move. It can also be interpreted as a model for crystallization, where the $\sigma = \uparrow$ and $\sigma = \downarrow$ fermions represent electrons and classical ions, respectively, or as an alloy model in which the impurities (ions) are thermodynamically correlated by annealed averaging. As already mentioned above, the SH model is equivalent to the symmetric version of the spinless FK model, which was used to study correlations of d and localized f electrons of transition metal oxides. In the general version of the FK model the two electron species are given different chemical potentials or potential-energy levels in order to regulate the electron densities with respect to one another. In the SH model ρ_\uparrow and ρ_\downarrow are interdependent.

Another interesting interpretation concerns the Standard Hubbard model in which spin-flip hopping processes have been included:

$$\hat{H} = -\frac{1}{2} \sum_{\langle ij \rangle} \sum_{\sigma, \sigma'} (C_{i\sigma}^+ C_{j\sigma'} + C_{j\sigma'} C_{i\sigma} + U \sum_i N_{i\uparrow} N_{i\downarrow} - \mu \sum_{i, \sigma} N_{i\sigma}) \quad (3.3.2)$$

Where $C_{i\sigma}^+$, $C_{i\sigma}$ and $N_{i\sigma}$ are standard fermion operators, and where spin-orbit coupling may account for the spin-flip hopping terms. Invoking the transformation $A_i \equiv (C_{i\uparrow} + C_{i\downarrow}) / \sqrt{2}$, $B_i \equiv (C_{i\uparrow} - C_{i\downarrow}) / \sqrt{2}$, Hamiltonian can be mapped exactly onto the SH model with $n_{i\downarrow}$ and C_{\uparrow}^+ replaced by $B_i^+ B_i$ and A_i^+ , respectively. Many physical quantities expressed in $\{C_{i\sigma}^+, C_{i\sigma}\}$ are equivalent with the corresponding ones expressed in $\{C_{i\sigma}^+, C_{i\sigma}\}$. Of the quantities considered below, those written in terms the magnetization operators:

$$M_x(q) = \frac{1}{\sqrt{N}} \sum_j e^{iq \cdot r_j} (C_{j\uparrow}^+ C_{j\downarrow} + C_{j\downarrow}^+ C_{j\uparrow}),$$

$$M_x(q) = \frac{1}{\sqrt{N}} \sum_j e^{iq \cdot r_j} (n_{j\uparrow} - n_{j\downarrow}), \quad (3.3.3)$$

have another meaning for Hamiltonian \hat{H} . In particular, $M_x \rightarrow M_z, M_z \rightarrow M_x$. In addition, dynamical single-particle correlation function $\{\sum_{\sigma, \sigma'} \langle C_{k\sigma}(t), C_{i\sigma'}^+ \rangle\}$ are equivalent with $\{\langle C_{k\uparrow}(t), C_{i\uparrow} \rangle\}$.

Adding bond-charge interactions terms, i.e. hopping terms that depend on site occupations, to the above model one gets a generalized Hubbard model which was proposed by Montorsi and Rasetti. Recently, it was shown that for $d = 1, 2, 3$ this generalized model exhibits a MI transition at $[U_c] = 4 dt$, while for $d = 1, 2$ the model does not. Bond-charge interaction terms therefore seem essential for the occurrence of a MI transition driven by U .

For the half-filled SH model, Kennedy and Lieb and Brandt and Schmidt have rigorously shown that for bipartite lattices the ground state exhibits antiferromagnetic (AF) LRO for all dimensions. The immobile $\sigma = \downarrow$

electrons fully occupy one sublattice in the ground state. For $U \neq 0$ and $\rho = 1$ the SH model is an insulator. In addition, for $d \geq 2$ the LRO was shown to persist up to some (unknown) finite temperature, for other p not much is known except for $d \rightarrow \infty$. The FK model, on the other hand, has been studied for variable ρ_{\uparrow} and (usually fixed) ρ_{\downarrow} .

The SH Hamiltonian is diagonal in the occupation-number representation of the $\sigma = \downarrow$ electrons, since $[H, n_{i\downarrow}] = 0$. Introducing local eigenstates $n_{i\downarrow} |s_i\rangle = s_i |s_i\rangle, S_i = 0, 1$, the partition function for the SH model can be written exactly as:

$$Z = \sum_{\{s_i=0,1\}} \det(1 + \exp[-\beta M(\{s_i\})] \exp(\beta \mu \sum_i s_i)) \quad (3.3.4)$$

Where β is the inverse temperature, $M_{ii}(\{s_i\}) = U s_i - \mu$, $M_{ij}(\{s_i\}) = -t$ for nearest neighbors, and $M_{ii}(\{s_i\}) = 0$ otherwise. The determinant in (3.3.4) is strictly positive and follows from performing the trace over the $\sigma = \uparrow$ fermion degrees of freedom analytically. Contrary to the case of the Hubbard model, no path-integral representation are required, and consequently, no minus -sign or instability problems characteristic of Quantum Monte Carlo simulations of fermion models are encountered. Our computational approach is to diagonalize the $(N \times N)$ matrix M for a particular configuration of $\{s_i\}$, then to calculate the contributions to (3.3.4) and the desired thermodynamic quantities. The sum over all configuration can be performed exactly for small lattices. For large lattices a classical Monte Carlo method can be employed. In the present formulation dynamical single-particle correlation functions for the itinerant electrons can readily be expressed as:

$$\begin{aligned} \langle \{c_{k\uparrow}(t), c_{l\uparrow}^+\} \rangle &= \langle \langle e^{-itM} \rangle \rangle \\ &\equiv z^{-1} \sum_{\{s_i=0,1\}} \det(1 + e^{-\beta M(\{s_i\})})^{-1} e^{\beta \mu \sum_i s_i} (e^{itM(\{s_i\})})_{kl} \end{aligned} \quad (3.3.5)$$

Note that these functions can be evaluated directly during the course of the computations without employing any additional approximation or analytical continuation procedure. From the knowledge of spectral functions and DOS follow straightforwardly.

To appreciate that the 2 D SH model, contrary to the Hubbard model, exhibits a phase transition at nonzero temperatures, one can consider the partition function (3.3.4).

Expressed as $Z = \sum_{(w_i=-1,1)} \exp[-\beta E(\{w_i\})]$, where:

$S_i = \frac{w_i+1}{2}$, in the large $-U$ limit. The spin energy E resembles a “classical” spin Hamiltonian with complicated couplings and to lowest order in $1/U$, reduces to:

$$E(\{w_i\}) \approx \frac{1^2}{2|U|} \sum_{\langle i,j \rangle} w_i w_j, \quad (3.3.6)$$

Yielding a finite T_c for $d \geq 2$.

Consideration is made here for the half-filled case and discuss the ground-state and thermodynamic properties. Results for dynamical quantities are also presented. The case away from half filling is studied for low temperature also. Results presented below is for lattices with 16 sites are from exact diagonalizations and exact summations. For larger lattice sizes (N up to 100) the summations were performed using the metropolis Monte Carlo method. Periodic boundary conditions have been used. All energies are measured in units of t .

For the half-filled ($\mu = U/2$) case, it is appropriate to study model (1) only for $U > 0$. The properties of the attractive half-filled SH model can be obtained invoking the particle-hole transformation (3.4.1.1)

$$C_{i\uparrow} = a_i\uparrow; C_{i\downarrow} = (-1)^i a_{i\downarrow} \quad (3.3.7)$$

Which maps $H(U)$ onto $H(-U) - UN/2$. At half filling the densities of the spin-up and spin-down electrons are equal and independent of the temperature and U .

We first focus our attention on static properties. The double occupancy per site, $D \equiv \langle n_{i\uparrow} n_{i\downarrow} \rangle$, is a measure for the localization of the itinerant electrons and / or the formation of a local magnetic moment as depends on D through $\langle (n_{i\uparrow} - n_{i\downarrow})^2 \rangle = p - 2D$. The double occupancy per site as a function of temperature T on a 4×4 lattice. For various values of U . For fixed temperature decreases as a function of U as expected. For low temperature, we found that $D \rightarrow 0$ for $U \rightarrow \infty$. Different temperature dependencies are clearly observed for small and large coupling values. For temperatures, D decreases as a function of U . For fixed temperature below $T_1 = T_1(U)$, D is approximately constant for all U . At $T = T_1$, there is a rapid increase for $U < 4$ and a (slow) decrease for $U > 4$. Anticipating a magnetic transition in the thermodynamic limit a discontinuity at $T = T_1$ may develop. Such a discontinuity could also signal the presence of a MI transition. For $U > 4$, D begins to grow at $T_2 = T_2(U)$ which increase with larger couplings. For these U values the local magnetic moment is maximal at some nonzero temperature $T > T_1$.

More insight into this behavior is obtained by considering the kinetic, Potential and internal energy as a function of T for $U=2$ and 7.5 . Note that the internal energies exhibit qualitatively the same behavior, while the kinetic and potential energies do not.

The potential energies are proportional to D . The kinetic energy for $U = 2$ does not exhibit any particular feature at the temperature where the potential energy displays a rapid increase. In the thermodynamic limit and for $U < 4$ the kinetic energy may be expected to remain an analytical function. As the temperature is lowered the kinetic energy for $U = 7.5$ exhibits a rapid

decrease to an approximately constant value at $T = T_1 > 0$, for $U > 4$ and $T \leq T_1$, the itinerant $\sigma = \uparrow$ electrons tend to become more delocalized relative to the case at slightly higher temperature, hence, in the latter regime the local magnetic moment reaches its maximum and, correspondingly, D reaches its minimum. When AF order, see below, sets in at $T \approx T_1$ the increase for large U of the (virtual) hopping of the $\sigma = \downarrow$ and $\sigma = \uparrow$ electrons becomes strongly exhibited.

The specific heat C/N for half-filled square lattices for $U = 1$ and 7.5 since we are working in the grand –canonical ensemble, C/N for fixed particle density p is calculated using:

$$C/N = \beta^2 (\langle H^2 \rangle - \langle H \rangle^2) N - T [(\partial p / \partial T)_\mu]^2 / (\partial p / \partial \mu)_T \quad (3.3.8)$$

System size, suggesting the presence of a phase transition. The position of this maximum coincides with the temperature T_1 discussed above. For the 1D case values of the sharp maxima are approximately constant as a function of N . Estimates for the positions of the maxima are the same for the lattice sizes considered.

In accordance with rigorous results for $d \geq 2$, the $\sigma = \downarrow$ electrons are found to fully occupy one sub-lattice at very low temperatures and this LRO is observed to vanish at $T \approx T_c > 0$, where T_2 corresponds with the position of the sharp maximum of C/N . The 1 D SH model exhibits LRO only in ground state. In the regimes of LRO the static magnetic –structure factor, $S_{zz}(q) \equiv \langle |M_z(q)|^2 \rangle - \langle M_z(q) \rangle^2$. Scales linearly with the size for $q = (\pi)$ and (π, π) , for $d=1$ and 2 , respectively, it must be noted that. Because Hamiltonian (1) does not have off-diagonal terms for the $\sigma = \downarrow$ electrons, no transverse AF LRO is possible : $\langle M_\alpha(q) \rangle = 0$ and $S_{\alpha\alpha}(q) = \delta_{q,0} S_{\alpha\alpha}(0)$ ($\alpha = x, y$) the checker-board distribution of the non-itinerant $\sigma = \downarrow$ electrons for

$T < T_c$ also leads to charge-density LRO. The static charge-density structure factor.

$$C(q) \equiv N^{-1} \sum_{i,j} \exp[iq \cdot (r_i - r_j)] \{ \langle (n_{i\uparrow} - n_{i\downarrow}) (n_{j\uparrow} - n_{j\downarrow}) \rangle - \langle n_{i\uparrow} + n_{i\downarrow} \rangle \langle n_{j\uparrow} + n_{j\downarrow} \rangle \},$$

As a function of U for momentum $q = (\pi)$ for rings for $T = 0.001$. For the U values considered $c(\pi)$ scales linearly with N . For increasing U , $C(\pi) / N$ decreases, while the mean-squared staggered magnetization, $\langle (M_z^S)^2 \rangle \equiv S_{zz}(\pi) / N$ ($\langle M_z^S \rangle = 0$), increase, the temperature at which magnetic and charge – density LRO vanish are the same. Critical temperature T_c for LRO as a function of U for the 2D SH model. The observed transition is not exactly ising-like, since $S_{zz}(\pi) \propto N$ for $T < T_c$. The values of T_c are not of the order of t or U . Qualitatively similar results were obtained for the half-filled $d = \infty$ SH model.

The above results imply that also the $U < 0$ SH model simultaneously exhibits charge –density and AF LRO.

Employing the particle –hole transformation the absence of transverse AF LRO for positive U indicates that there is no on-site s –wave superconductivity for the attractive SH model. The latter result can also be derived analytically: the s –wave pairing correlation function

$$P_s = \langle \Delta^+ \Delta + \Delta \Delta^+ \rangle, \text{ where } \Delta^+ = \sum_i C_{i\uparrow}^+ C_{i\downarrow}^+ / \sqrt{N}, \text{ simply reduces to } P_s = 1 - \rho + 2D \text{ due to the structure of Hamiltonian (1). } P_s \text{ is of the order of unity for all } U, \mu, T \text{ and } N. \text{ which excludes off – diagonal LRO.}$$

We now turn to discuss dynamic properties. Single –particle DOS, Drude coefficients and optical conductivities have been calculated in order to investigate the possibility of a MI transition. Concerning the DOS, one of

the interesting questions is the amount of spectral weight at the chemical potential for particular U and T.

The single-particle DOS $N(\omega)$ gives the probability for removing or adding one (itinerant) $\sigma = \downarrow$ electron from or to the lattice. Spectra (not shown) corresponding to the $\sigma = \downarrow$ electrons are given by the Fourier transform of:

$$\frac{1}{N} \sum_{\mathbf{k}} \langle \{c_{\mathbf{k}\downarrow}(t), c_{\mathbf{k}\downarrow}^{\dagger}\} \rangle = \frac{1}{N} \sum_{\mathbf{k}} \sum_{[s_i=0,1]} e^{\beta \mu \sum_i s_i} \det[1 + e^{-\beta M} \times e^{it(M - Q_1^{(\mathbf{k})})} e^{-it(M + Q_0^{(\mathbf{k})})}] / Z \quad (3.3.9)$$

Where $(Q_v^{(\mathbf{k})})_{ij} = U \delta_{i,k} \delta_{j,k} \delta_{s_k,v}$. This expression demonstrates that the immobile electrons display nontrivial dynamics. Which is mediated by the interaction with the itinerant $\sigma = \uparrow$ electrons. The DOS of $\sigma = \downarrow$ electrons has been calculated in for the $d \rightarrow \infty$ SH model.

Single-particle DOS for the 1 D and 2 D half-filled SH model are shown for various couplings U and temperature T. In agreement with rigorous results for the ground state we found for very low temperatures that the chemical potential lies in a gap of the DOS : At $T = 0$ the half-filled SH model in an (AF) insulator and exhibits no MI transition as a function of U. In the ground state, no spectral weight is present for energies $0 < \omega < U$ for all $U \neq 0$: The size of the gap is U. For small and intermediate ($U < 4d$). The band widths of the upper and lower Hubbard bands decrease with increasing U. For $U > 4d$ the band width approaches a nonzero value as $U \rightarrow \infty$. Upon increasing T the widths of lower and upper bands increase. For $0 < U < W \equiv 4d$ the gap closes as the temperature is raised. At the chemical potential no specific feature are observed as the gap disappears. Note that W equals the free-particle band width.

Substantial spectral weight is found at $\omega = \mu$ for $0 < U < W/2$ for sufficiently large T. Then the system exhibits metallic behavior as demonstrated. The

temperature T_0 at which gaps in the DOS close, increases very strongly for $\frac{1}{2} < U/W < 1$: E.G. for $d=2$ one finds $T_0 \approx 0.15$ for $U = 5$ and $T_0 \approx 15$ for $U = 7.5$. For fixed large temperature the weight at the chemical potential decrease with increasing U . For $\frac{1}{2} < U/W < 1$ a pseudo gap is observed for large temperature: $N(\omega = \mu)$ remain relatively small. The size dependence of the spectral weight $N(\omega = \mu)$ was small for all U employing lattices with up to 64 sites. For $U > W$ and increasing T spectral weight also appears in the energy range $0 < \omega < U$, but a finite gap remains for all temperature, indicating insulating or semiconducting behavior. Note that for nonzero temperature and all U the DOS displays local minima at $\omega = \varepsilon$ and $\omega = U - \varepsilon$, where ε is a positive small number. These are due to AF spin correlations. The temperatures T_0 as a function of U for $d= 1$ and 2 . The dashed and dotted curves can be considered as metal insulator phase boundaries. Although the insulator phases are exactly non-conducting only at $T = 0$. The co-existence in two dimensions of metallic behavior and AF (and charge – density) LRO is apparent. The metallic behavior reflects the motion of the $\sigma = \uparrow$ electrons. While the AF properties are mainly displayed by the $\sigma = \downarrow$ electrons. Due to the asymmetry in the SH model (1) of the $\sigma = \uparrow$ and $\sigma = \downarrow$ electrons the closing of the gap in the DOS at T_0 is not related to the disappearance of AF LRO at T_c . It is interesting to compare these results with those known for the Hubbard model. In $d = 1$ both the SH and Hubbard model (2) exhibits temperature (s) for which a gap in the DOS occurs. While LRO is absent.

The “phase diagram” of the 2 D SH model is qualitatively the same as the one obtained for the $d \geq$ Hubbard model. Employing a random one-body approximation and for which also a regime exists where $0 < T_0 < T_0$. Since the 2 D Hubbard model has $T_c = 0$ and a gap in the DOS at $T = 0$. One cloud

therefore expect that for not too large U the gap closes for nonzero temperature. This behavior has recently been demonstrated for $U = 4$. The temperature behavior of the gap for $U > W$ has not been studied yet.

The Drude coefficient D and the optical conductivity $\sigma(\omega)$ have been computed for very low temperatures. D is determined employing a sum rule involving $\sigma(\omega)$ and the kinetic energy, $\sigma(\omega)$ is calculated using a current-current correlation function only the itinerant electrons contribute to both quantities. We find that for small lattice sizes $D \rightarrow 0$ as U increases. $D \rightarrow 0$ is also obtained for fixed U as N increases. For $d = 1$ and $U = 1$ the Drude coefficient was already of the order of 10^{-3} for $N > 16$.

The optical conductivity $\sigma(\omega)$ is presented for rings of 100 sites for $T = 0.01$ and $U = 1$ and 8. For this lattice size $\sigma(\omega)$ is calculated by making use of the fact that for $T \rightarrow 0$ the dominant contribution to the partition function comes from checker-board configurations of the spin-down electrons. An optical gap of size U is clearly observed. These results are in accordance with those discussed above for the DOS.

When no half filling was consider, one can study doped lattices are considered for very low temperatures. Due to the asymmetry in mobility of the $\sigma = \uparrow$ and $\sigma = \downarrow$ electrons the respective electron densities $\rho \uparrow$ and $\rho \downarrow$ can exhibits different behaviors as a function of the chemical potential. The distribution and density of $\sigma = \downarrow$ electrons for the ground state of the FK model have been identified for almost the entire results for $\rho \downarrow$ also displayed for $U = 4$. The small step-like structure is a finite-size effect. For $U > 0$, $\rho < 1$ and low temperature one may have $\rho \uparrow > \rho \downarrow$. So that upon doping the SH can become ferromagnetic. i.e. a finite magnetic moment appears. For increasing temperatures $(\rho \uparrow - \rho \downarrow) \rightarrow 0$. The “plateaus” at half filling are consistent with the fact that in this case the system is an insulator.

For $U < -W$ the length of the “plateaus” becomes smaller as U is lowered. For $U \rightarrow \infty$ the length approaches $U - W$ from above. Note that the length are not equal to the size U of the gaps in the DOS. All “plateaus” eventually disappear for large enough temperature follows that for $U > \tilde{U}$ the SH model simply reduces to the free-particle system with $\rho \downarrow = 0$ for $\rho < \rho^*(U)$. Where $\rho^*(U) \rightarrow 1$ and $\mu^*(U) \rightarrow W/2$ as $U \rightarrow \infty$. In this case the lattice is fully spin polarized. The range of μ for which $0 < \rho \downarrow < 1/2$ depends sensitively on temperature. Upon lowering T this range decrease and the behavior of ρ becomes more step-like. This “pinning” of μ for a range the electron density has already been observed in the $d \rightarrow \infty$ SH model. The 2D case displays similar behavior as above.

In both 1 and 2 dimensions we observed no LRO for $U < 0$ for the model off half filling. On the other hand, Large charge – density short-range correlations for momentum q close to. But not exactly. Π are present for not too small ρ . For the doped repulsive SH model both long and short-range correlations are found for densities close to half filling. The charge – density (C) and magnetic (S_{zz}) structure factors as a function of the wave vector for a ring of 64 sites for $U = 1$, $\rho = 0.87$ and $T = 0.01$. The contributions for $q = \pi$ for both structure factors increase as a function of the lattice size and are indicative of the presence of LRO. Note that the doped repulsive Hubbard model does not display any LRO. The peaks at $q = 0$, which do not change for increasing N , reflect short-range ferromagnetic correlations. Hence, the doped SH model may exhibit ferromagnetism without *LRO for $U > \tilde{U}$* . for smaller ρ the (AF) LRO disappears. When the doping is such that the lattice becomes completely spin polarized, also all short-range correlations vanish.

Typical DOS for $0 < |U| < \frac{W}{2}$ and $U \geq \frac{W}{2}$.

$U=1$ and $U=15$, respectively, the corresponding half-filled cases. The DOS for $0 < |U| < \frac{w}{2}$ describes a one-band metal, where for increasing density a pseudo gap develops at the chemical potential. For $\rho=1$ the pseudogap becomes a true gap of size U . The pseudogap is the result of AF LRO. In the other case there are only weak short-range correlations present. For $\rho \geq \frac{w}{2}$, as e.g. the DOS consists of two well-separated bands, i.e. there is a gap just as for $\rho=1$, with μ lying in the lower band, and signals metallic behavior. This behavior of the DOS is also found for the Hubbard model for $U < w$. The DOS has a local minimum or pseudogap at $\omega = \mu$. The doped Hubbard model, however, exhibits a pseudogap at $\omega \neq \mu$. Calculations (not shown) for $U \leq \tilde{U}$ ($d = 1$: $\tilde{U} \approx -3.7$) show that the SH model off half filling also has two well-separated bands. In this case, however, the chemical potential lies in the gap, so that the system is now an insulator. The above results indicate that the doped SH model exhibits a MI transition as a function of U with $\tilde{U} < U_c(\rho) < -W/2$. For the SH model we have observed that for $U > 0$ spectral weight appears in the energy range $0 < \omega < W/2$ as soon as the system is doped away from $\rho = 1$. For $-W/2 < U < 0$ the gap in the DOS vanishes for $\rho \neq 1$. For $\tilde{U} < U < -W/2$ the appearance of spectral weight in the range $-\frac{W}{2} < \omega < 0$ seems to depend on the amount of doping. For the lattice sizes considered a finite weight at $\omega \approx -W/2$ was observed for describing ρ as U is lowered in the range $\tilde{U} < U < -W/2$. In this range the DOS consists of two separate bands, unless the system has become fully spin polarized. Depending on the position of μ one then either has a metal or an insulator. For $\rho \approx 0$ and 1 a MI insulator transition occurs at $U_c(\rho) \approx \tilde{U}$ and $-W/2$, respectively [57].

3.4 On the particle – hole symmetry of the fermionic spin less Hubbard model in D=1:

The one-band Hubbard model partially describes quantum magnetic phenomena. These are missing terms which should be included in the fermionic Hamiltonian to account for the diversity of phenomena in a strongly correlated electron system [58].

The development of optical lattice over the last two decades has made the experimental simulation of chain models possible. The three-dimensional Hubbard model at low temperature has been simulated by a fermionic quantum gas trapped in an optical lattice. The simplest one-dimensional fermionic model is the fermionic spin less Hubbard model .The generalization of which have been applied to the description of verwey metal-insulator transitions and charge- ordering phenomena of the $Fe_3O_4, Ti_4O_7, LiV_2O_4$ and other d-metal compounds.

In this work the study is concerned with consequences of the particle- hole symmetry on the thermodynamics of the one- dimensional fermionic spin less Hubbard model in the whole range of temperatures. By mapping it into the exactly solvable D=1 spin -1/2 XXZ Heisenberg model.

The spin less fermionic Hubbard model in $D = 1$ is a very simple anti – commutative model the Hamiltonian of which is:

$$H(t, V, \mu) = t \sum_{i=1}^N (c_i^+ c_{i+1} + c_{i+1}^+ c_i) + V \sum_{i=1}^N n_i n_{i+1} - \mu \sum_{i=1}^N n_i \quad (3.4.1)$$

In which (c_i, c_i^+) , with $i \in [1, 2, \dots, N]$, are fermionic annihilation and creation operators, respectively, and N is the number of sites in the chain. These operators satisfy anti commutation relations. $(c_i, c_j^+) = \delta_{ij}$ and $(c_i, c_j) = 0$, in which t is the hopping integral, V is the strength of the repulsion ($V > 0$) or attraction ($V < 0$) between first –neighbor fermions. μ is the

chemical potential and $n_i = c_i^\dagger c_i$ is the operator number of fermions at the i^{th} site of the chain.

Sznajd and Becker [58] have shown that the Hamiltonian (3.4.1) has particle – hole symmetry; consequently. The HFE of this model, $W(t, v, \mu; \beta)$, Satisfies the relation:

$$W(t, v, \mu; \beta) = W(t, V, -\mu + 2V; \beta) - (\mu - V) \quad (3.4.2)$$

In which $\beta = \frac{1}{kT}$, k is the Boltzmann's constant and T is the absolute temperature in Kelvin, the relation (3.4.2) is valid for any values (positive, null or negative) of V and μ . Equation (3.4.2) provides the condition for having the same number of particles and holes at the same potential V but at distinct chemical potentials.

$$\langle n_i \rangle(t, V, \mu; T) = 1 - \langle n_j \rangle(t, V - \mu + 2V; T) \quad (3.4.3)$$

In which $\langle n_i \rangle$ is the average number of fermionic particles at each site of the chain at temperature T . There is an equivalence of the model (1) and the spin $-\frac{1}{2}$ XXZ Heisenberg model in $D = 1$. One used the inverse Wigner –jordan transformation to Heisenberg model with transformation to show that the Hamiltonian (3.4.1) is mapped onto the Hamiltonian of the one-dimensional spin $-\frac{1}{2}$ XXZ Heisenberg model with a longitudinal magnetic field.

$$H_s = \frac{1}{2} (J, \Delta, h) = \sum_{i=1}^N [j(s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + \Delta s_i^z s_{i+1}^z) - h s_i^z] \quad (3.4.4)$$

In which $S^1 = \sigma^1 / 2$, $1 \in \{x, y, z\}$ and σ^1 are the Pauli matrices. The norm of the spin is operators \vec{S} is $\|\vec{S}\| = \frac{\sqrt{3}}{2}$.

The Hamiltonians (3.4.1) and (3.4.4) are related by:

$$H(t, V, \mu) = H_s = \frac{1}{2} (j=2t, \Delta = V/(2t), h = \mu - V) - N \left(\frac{j\Delta}{4} + \frac{h}{2} \right) I \quad (3.4.5)$$

And 1 is the identity operator of the chain. This relation shows a constant shift between the energy spectrums of these two models.

Let $W_s = \frac{1}{2} (1, \Delta, h, \beta)$ be the HFE associated to the Hamiltonian (3.4.4) of the $D = 1$ spin $-1/2$ XXZ Heisenberg model. A direct consequence of (3.4.4)

$$W(t, V, \mu; \beta) = \frac{1}{2} (J = 2t, \Delta = V / (2t), h = \mu - V; \beta) + (V/4 - \mu/2) \quad (3.4.6)$$

At finite temperature ($T \neq 0$), the HFE of the one-dimensional $S = 1/2$ XXZ Heisenberg model is an even function of the longitudinal magnetic field h :

$$W_s = \frac{1}{2} (J, \Delta - h; T) = W_s = \frac{1}{2} (J, \Delta, h; T) \quad (3.4.7)$$

Such invariance of $W_s = \frac{1}{2}$ comes from the symmetry of the Hamiltonian (3.4.4) upon reversal of the external magnetic field, $h \rightarrow -h$, and of the spin operators. $\vec{S}_i \rightarrow -\vec{S}_i$. In which $i \in \{1, 2, \dots, N\}$.

For a given magnetic field h and a fixed value (positive, null or negative) of V , the chemical potential μ so that $h = \mu - V$. For a reversed magnetic field, the corresponding chemical potential μ_2 for which $-h = \mu_2 - V$ is:

$$\mu_2 = -\mu + 2V \quad (3.4.8)$$

The identity (3.4.7) and the condition (3.4.8) recover the result (3.4.2) satisfied by the HFE of the spin less Hubbard model for any values of V and μ . Notice that in the half-filling condition ($\mu = V$), we have $\mu_2 = \mu$, and there is no visible consequence of the symmetry (3.4.7).

one point out of that the quantity $-\mu + 2V$, which appears on the r.h.s. of (3.4.8) also appears as an argument of W (the HFE of $D = 1$ spin less fermionic Hubbard model) in the r.h.s. of (3.4.2) which in its turn comes from the particle – hole symmetry of the Hamiltonian (3.4.1) on the other hand (3.4.7) comes from the fact that the HFE of the $D = 1$ spin $- 1/2$ x x z

Heisenberg model is insensitive to a reversal of the longitudinal magnetic field.

Equation (3.4.3) can be interpreted as follows: the number of particles in the chain a potential V and a chemical potential μ_2 given by (3.4.8) those configurations correspond to distinct distributions of the fermionic particles in the chain. And certainly have some different thermodynamic functions at temperature T . In what follows, we explore the consequences of the equality (3.4.7) in the thermodynamic functions of those two configurations.

The specific heat C and the entropy S , both per site, are related to the HFE of the model (3. 4.1) by $C(t, V, \mu; \beta) = -\beta^2 \partial^2 / \partial \beta^2 [\beta W(t, V, \mu; \beta)]$ and $s/k = \beta^2 \frac{\partial}{\partial \beta} [W(t, V, \mu; \beta)]$ respectively. Due to equation (3.4.6) we obtain:

$$C(t, V, \mu; T) = C(t, V, -\mu + 2V; T) \quad (3.4.9a)$$

And:

$$S(t, V, \mu; T) = S(t, V, -\mu + 2V; T) \quad (3.4.9b)$$

Both (3.4.9 a) (3.4.9a) are valid in the whole range of temperatures $T > 0$. This can be verified at each order of the β –expansion of the thermodynamic function (3.4.1) of the HFE of the model.

However, not all thermodynamic functions of the model (3.4.1) are identical for the chemical potentials μ and μ_2 . At the same potential V . The internal energy per site $\varepsilon(t, V, \mu; \beta) = \partial / \partial \beta [\beta W(t, V, \mu; \beta)]$ distinguishes the distributions of the fermionic particles in the chain:

$$\varepsilon(t, V, \mu; \beta) = -V + \mu + \varepsilon(t, V, \mu; \beta) \quad (3.4.9.10)$$

Notice that the different of internal energies per site does not depend on the temperature. This equality is valid for any temperature $T > 0$ and it is verified at each order of the expansion in β for this thermodynamic function.

In the spin $- 1/2$ Heisenberg model (3.4.4), the parallel and anti-parallel configuration of spin with respect to the external magnetic field can be distinguished. For instance by the average value of the z – component of the spin operator S_i^z at a site and the correlation function of odd powers of such operators. In terms of fermionic operators, we have $S_i^z = n_j - 1/2 1_i$, in which 1_i , is the identify operator at the i -th site.

For the spin less fermionic Hubbard model, the first –neighbor correlation function $G_{i,i+1}(t, V, \mu ; T) \equiv \langle n_i n_{i+1} \rangle$ also relates configurations in which the number of particles in one equals the number of holes in the other. For two values of the chemical potential, μ and μ_2 .

The two – point correlation function $G_{i,i+1}$ is related to the HFE by:

$$G_{i,i+1} (t, V, \mu ; T) = \frac{\partial W(t, V, \mu ; T)}{\partial V} \quad (3.4.11)$$

From relation (3.4.6) the symmetry condition (3.4.7) and the definition of the z - component of the magnetic of the $D=1$ spin- $1/2$ XXZ Heisenberg model:

$$M_z^{s=1/2} (J, \Delta, h; T) = - \partial W_{s=1/2}(j, \Delta, h; T) / \partial h = \langle s_i^z \rangle (j, \Delta, h; T) \quad (3.4.12)$$

In which $i \in \{1, 2 \dots N\}$ and $\langle s_i^z \rangle (J, \Delta, h; T)$ is the mean value of the z -component of the spin $-1/2$ operator at the i^{th} site of the chain and at temperature T , we obtain:

$$G_{i, i+1} (t, V, \mu_2; T) - G_{i, i+1}(t, V, \mu; T) = - 2M_z^{s=1/2}(J, \Delta, h; T) \quad (3.4.13)$$

Where on its r.h.s we have the z -component of the magnetization $M_z^{s=1/2}$ in the presence of a longitudinal magnetic field. (Notice that M_z a one –point function of the model, whereas $G_{i,i+1}$ is a two-point function.) Equation (3.4.13) is valid for each order of the β -expansion of the function $G_{i,i+1}(t, V, \mu; \beta)$.

As a consequence of the symmetry in equation (3.4.7) the magnetization $M_z^{s=1/2}$ is an odd function of the magnetic field h ,

$$M_z^{s=1/2}(J, \Delta, -h; T) = -M_z^{s=1/2}(J, \Delta, h; T) \quad (3.4.14)$$

By writing equation (3.5.14) in terms of fermionic operators $s_i^z = n_i - 1/2$.

One obtains

$$\langle n_i \rangle(t, V, \mu; T) = 1 - \langle n_i \rangle(t, V, -\mu + 2V; T) \quad (3.4.15)$$

thus, recovering equation (3.4.3).

In summary. One verified that the particle-hole of the one-dimensional spinless fermionic Hubbard model (3.4.1) is associated to the invariance of the HFE of the $D = 1$ spin $-1/2$ XXZ Heisenberg model (3.4.4) with respect to a reversal of the longitudinal external magnetic field.

The thermodynamic of the chain off the half-filling condition ($\mu \neq V$) with chemical potentials μ and μ_2 . Under the same potential V , are not identical; rather. Some thermodynamic functions permit their distinction. Although the number of fermionic particles in the chain differ for μ and μ_2 , we obtain unexpected results. expressed in (3.4.9 a) and (3.4.9 b) where both configurations exhibit the same specific heat and entropy per site at any finite temperature T and at any value of V . Distinction arises from other thermodynamic functions of the chain. Though; the values of the internal energy per site of these two distributions of particles in the chain differ by a constant that is independent of the temperature; and the difference of their first-neighbor correlation functions is a one-point function proportional to the z -component of magnetization per site of the spin $-1/2$ model (3.4.4).

The equality of the number of particles in the chain for the chemical potential μ and the number of holes in the chain for the chemical potential

μ_2 is a consequence of the odd parity of magnetization $M_z^{s=1/2}(J, \Delta, h; \beta)$ under reversal of the magnetic field $h \rightarrow -h$, for any temperature.

The results presented here are valid for any value of V (negative, null or positive) and any value of temperature $T > 0$, verified at each order of the β -expansion of the respective thermodynamic function.

These results are also valid at very low temperatures and could be checked in an optical lattice simulation of the one – dimensional fermionic spin less Hubbard model [58].

3.5 On the Quantization of One –Dimensional Conservative System with Variable Mass:

The harmonic oscillator with $m_1 = 0$ in the Weyl algebra basis $\{I, a, a^+\}$ has the following characteristics [59].

$$\hat{K}_0 = \hat{H}_0 = \hbar\omega a^+ a, E_n^{(0)} = \hbar\omega(n + 1/2), \Phi_n^{(0)} = |n\rangle, \quad (3.5.1)$$

With the following identifications

$$x = \sqrt{\frac{\hbar}{2M_0\omega}}(a + a^+), \hat{p} = -i\sqrt{\frac{m_0\hbar\omega}{2}}(a - a^+), \text{ and } \hat{v} = -i\sqrt{\frac{\hbar\omega}{2m_0}}(a - a^+),$$

and having the well-known properties

$$\langle n|m\rangle = \delta_{nm}, a^+|n\rangle = \sqrt{n+1}|n+1\rangle, a|n\rangle = \sqrt{n}|n-1\rangle, \text{ and } [a, a^+] = I. \quad (3.5.2)$$

Note that all the expectation value of monomial terms of odd power have zero values. The expression for \widetilde{W} up to fourth order in "x" is given by:

$$\widetilde{W} = \frac{km_1}{2m_0x_1}x^3 - \frac{km_1}{8m_0x_1^2}x^4 \quad (3.5.3)$$

Thus, the expectation value of the terms appearing in Equations can be calculated, resulting the following eigenvalues at first order:

$$E_k^{(1)} = E_n^{(0)} - \frac{km_1}{8m_0x_1^2} \left(\frac{\hbar}{2M_0\omega} \right)^2 (6n^2 + 6n + 2) - i \frac{m_1\hbar}{3m_0x_1^2} (\langle D(x, f\hat{v}) \rangle_n + \langle f\hat{v} \rangle_n) + \frac{m_0}{2x_1^2} \left(\frac{m_1^2}{m_0^2} - \frac{m_1}{m_0} \right) \quad (3.5.4)$$

And:

$$E_k^{(1)} = E_n^{(0)} - \frac{km_1}{8m_0x_1^2} \left(\frac{\hbar}{2M_0\omega} \right)^2 (6n^2 + 6n + 2) - i \frac{m_1\hbar}{3m_0x_1^2} (\langle D(x, f\hat{v}) \rangle_n + \langle f\hat{v} \rangle_n) + \frac{m_0}{2x_1^2} \left(\frac{m_1^2}{m_0^2} - \frac{m_1}{m_0} \right) \times \left[\langle x^2\hat{v}^2 \rangle_n - \frac{i\hbar}{6m_0} (2\langle xf\hat{v} \rangle_n + \langle g\hat{v} \rangle_n) + \frac{\hbar^2}{6m_0^2} \langle h(x) \rangle_n - \frac{i\hbar}{m_0} \langle xf\hat{v} \rangle_n - \frac{i\hbar}{6m_0} \langle xD \rangle_n - \frac{\hbar^2}{6m_0^2} \langle xg \rangle_n \right] \quad (3.5.5)$$

Where one has used the definition $\langle \xi \rangle_n = \langle n | \xi | n \rangle$. Let us define the following parameter j as:

$$E_H^{(1)} = E_n^{(0)} - \frac{km_1}{8m_0x_1^2} \left(\frac{\hbar}{2m_0\omega} \right)^2 (6n^2 + 6n + 2) + \frac{\hbar^2}{8m_0x_1^2} \left(\frac{m_1}{m_0} + \frac{3m_1^2}{2m_0^2} \right) (2n^2 - 1), \quad (3.5.6)$$

This parameter represents the relative variation of the eigenvalues of the constant of motion quantization and the Hamiltonian approaches [59].

3.6 One-dimensional Hubbard model of quarter filling on periodic potential:

The Peierls model is the prototypical model to study the coupling of noninteracting electrons to the lattice. The Hamiltonian is given by [60]:

$$H_{\text{peierls}} = - \sum_{i,\sigma}^N t_i (C_{i,\sigma}^+ C_{i+1,\sigma} + \text{H. c.}) \quad (3.6.1)$$

Where we consider a modulated hopping term with $t_i = t [1 + u \cos(Qa \cdot i)]$. N

denotes the number of lattice sites and the lattice constant. In addition, N_e is the number of electrons on the chain and Q the wave vector of the periodic distortion. In the case of a commensurate distortion we have $Q=2mk_F$, $m=1, 2 \dots$. The dimerized chain $Q=\pi/a$ at half filling $n=N_e/N=1$ was investigated by Su, Schrieffer, and Heeger (SSH). Due to the periodic distortion a band gap $\Delta=4ut$ opens at $k_\Delta=Q/2$. Since at half filling we have $k_\Delta=k_F$, the system is insulating. As is characteristic for a band insulator, the gaps for charge and spin excitations are identical. In the following, we concentrate on the quarter-filled band and 4a-periodic distortions, because in case of the 2a-periodic distortion the quarter-filled system is metallic, since $k_\Delta \neq k_f$.

One determine the energy bands and the energy gain due to a periodic modulation of the hopping parameter with $Q= \pi/2a$. For quarter filling, $k_f= \pi/4a$, this system shows the peierls transition, since $Q = \pi/2a = 2k_f$. The Fourier transformation of the hopping term yields in analogy with the SSH model, the expression:

$$H_{\text{peierls}} = \sum_k (c_k^\dagger c_{k+Q}^\dagger c_{k+2Q}^\dagger c_{k+3Q}^\dagger) t \widehat{h}_{\alpha\beta} \begin{pmatrix} c_k \\ c_{k+Q} \\ c_{k+2Q} \\ c_{k+3Q} \end{pmatrix} \quad (3.6.2)$$

Where the matrix $\widehat{h}_{\alpha\beta}$ is given by:

$$\widehat{h}_{\alpha\beta} = \begin{pmatrix} -2\coska & -u(e^{ika+ie^{-ika}}) & -u(e^{-ika} + ie^{ika}) & u(e^{ika-ie^{-ika}}) \\ u(ie^{ika} - e^{-ika}) & -2\sinka & u(e^{-ika} - ie^{ika}) & u(e^{ika} + ie^{-ika}) \\ u(e^{-ika} + ie^{ika}) & u(ie^{-ika} - e^{ika}) & 2\coska & 2\sinka \\ & & u(e^{-ika} - ie^{ika}) & \end{pmatrix} \quad (3.6.3)$$

$$\varepsilon(k) = \pm t \sqrt{2[1 + 2u^2 \pm \sqrt{\cos^2 2ka + 4u^2(1 + \sin^2 2k)}]} \quad (3.6.4)$$

$$\Delta_1 = 4ut, \Delta_2 = 2u^2t, \text{ and } \Delta_3 = \Delta_1 \quad (3.6.5)$$

Where $\Delta_1 = \varepsilon_2(k=k_f) - \varepsilon_1(k=k_f)$ and $\Delta_2 = \varepsilon_3(k=2k_f) - \varepsilon_2(k=2k_f)$. The energy gain of the fermions, for the quarter-filled case, obtained by summing up the contributions of all occupied states, is found to be $\alpha u^2 t$ in u , as for half filling.

Another type of periodic distortion is given by local potentials, resulting in the so-called ionic model.

$$H_{ionic} = -t \sum_{i,\sigma}^N (c_{i,\sigma}^+ c_{i+1,\sigma} + H.c.) + \sum_i^N W_i n_i - \sum_i^N h_i S_i^z \quad (3.6.6)$$

Again, for the half-filled band the same calculation as before. can be performed for a periodic potential, with $\Delta_c = \Delta_s = 2W$, in case of the ionic model for a quarter-filled system we compare several potentials, which correspond to different charge and spin patterns.

- (a) First, we study a simple potential with $2k_f$. (4a) period given by $W_i = W \cos(\pi i/2)$. Here, the charge order for zero hopping is given by 1/0.5/0/0.5 electrons per site, periodically continued. Spin order is not established.
- (b) A modification of (a) given by $W_i = W \cos(\pi i/2) + W \cos[\pi(i+1)/2]$, which leads to two occupied and two unoccupied sites ("cluster"), i.e. 1/1/0/0 charge order.

(c) A charge order with a I/0/1/0 pattern, i.e., a $4k_f$ ($2a$) -periodic order, is forced by a potential $W_i = W \cos(\pi i)$ interaction we likewise expect magnetic ordering.

(d) In addition, a local magnetic field with $h_i = W \cos(\pi i/2)$ ($\mathbf{n}_{i\uparrow} - \mathbf{n}_{i\downarrow}$) enforces a $\uparrow/0/\downarrow/0$ pattern. As in (c), we expect a $2k_f$ ($2a$) period for the spin and correspondingly a $4k_f$ ($2a$) period for the charge.

Diagonalizing the resulting Hamilton matrix, as described above, yield the dispersions.

$$(a), (d) \ \varepsilon(\mathbf{k}) = \pm t \sqrt{2 + \frac{w^2}{2} \pm \sqrt{4\cos^2(2\mathbf{k}) + 2w^2 + w^4/4}},$$

$$(b) \ \varepsilon(\mathbf{k}) = \pm t \sqrt{2 + \frac{w^2}{2} \pm \sqrt{4\cos^2(2\mathbf{k}) + 4w^2}}$$

$$(c) \ \varepsilon(\mathbf{k}) = \pm t \sqrt{w^2 + 4\cos^2 \mathbf{k}}$$

In comparison to the Peierl model not only a gap opens at $k=Q/2$ but the lower and upper bands are shifted down and up, respectively. In case of a small perturbation, the dispersion is similar for the Peierls and the ionic model, as well as for potentials (a) and (b). Potentials (a) and (d) are equivalent in the non-interacting case.

The energy gain in the quarter-filled band is found to be about $-W$ ^{1.65} in cases (a), (b), and (d). For small W . the energy gain is nearly the same in cases (a) and (b). Whereas it becomes weaker in case (b) than in case (a) at $W \approx 0.5t$. In case (c), the energy gain is quadratic. $E(W) - E(0) = 8/3 W^2$. It mainly traces back to the Band shift. Accordingly, the gaps are given by:

$$(a),(d) \ \Delta_1 = W, \Delta_2 = \sqrt{2}W, \Delta_3 = W$$

(b) $\Delta_1 \sim \mathbf{W}$ for small $W, \Delta_1 \rightarrow \Delta_1^\infty$ for strong $W, \Delta_1 = \sqrt{2} - \frac{W}{2}, \Delta_2 = \Delta_1;$

(c) $\Delta_1 = \mathbf{0}, \Delta_2 = \mathbf{W}, \Delta_3 = \mathbf{0}$

The Hubbard model is known to capture the interplay between kinetic energy (delocalization) and interaction (localization) in electronic systems. The Hamiltonian is given by:

$$H_{Hubb} = - \sum_{i,\sigma}^N t_i (c_{i,\sigma}^\dagger c_{i+1,\sigma} + H.c.) + U \sum_i^N n_{i,\uparrow} n_{i,\downarrow} \quad (3.6.7)$$

The Hubbard model in one dimension is exactly solvable by means of the Bethe Ansatz. Note that in one dimension another useful formulation of the Hubbard model is available on the basis of the bosonization technique. The low lying excitations of the noninteracting as well as the interacting fermions system are sound waves, i.e., the Fermi system can be described as a non-interacting Bose system, called a Luttinger liquid, showing spin-charge separation. In the clean case, the Hubbard model has three phases. For $U < 0$, the spin excitation spectrum has a gap and the low-lying charge excitations are those of a Luttinger liquid. The last phase occurs for $U > 0$ and half filling, where the charge excitations have a gap and the spin excitations are of Luttinger type, a relevant $4k_f$ -Umklapp scattering term, only present for half filling, is responsible for the Mott gap in the latter phase. The bosonization technique is adequate for metallic systems or in the weak coupling regime. It is useful to determine the phase boundary between metals and insulators but it is not suitable for distinguishing different insulating phases for intermediate or strong perturbations.

A commensurate periodic distortion-i.e., commensurate to the band

filling—introduces an additional nonlinear term in the bosonized Hamiltonian, which couples spin and charge degrees of freedom and destroys the integrability of the clean Hubbard model. In the half-filled case we therefore find a transition between two possible insulating phases, i.e., the band (Peierls) insulator ($W, ut \gg U$) with charge and spin gap of the same order and the Mott insulator ($W, ut \gg U$) with a charge proportional to the interaction, but vanishing spin gap, where periodic distortion and interaction oppose each other. However, the transition is fundamentally different for the Peierls and the ionic Hubbard model. In the Peierls is smooth and continuous, whereas a third phase – a spontaneous dimerized insulating phase—is found in the ionic Hubbard model. Within this phase, charge and spin gap are non-zero, and the dimerization operator has a nonzero expectation value. In fact, the extension of this phase is discussed controversially.

The situation in the quarter filled band is completely different. With interaction, no insulating phase is established, except for very strong interaction, where higher order terms of the Umklapp scattering can cause a Mott insulator on its own. In the quarter-filled Case with $2k_f$ -periodic potential we expect from bosonization a transition from the Luttinger liquid to the band insulator in the noninteracting as well as in the interacting system. The interaction modifies the exponents of the gaps and the energy gain. Since they become smaller with increasing interaction, interaction stabilizes the band insulator. Here, the interplay between periodic distortion and interaction is weak, since the quarter filled model with interaction is still a metal. A similar situation is found for half-filled spin less fermions for weak interaction, where the Umklapp scattering induces the insulator at finite interaction strength. In case of $4k_f$ -periodic potential Umklapp

scattering becomes relevant, due to the doubling of the unit cell or, equivalently, due to the reduction of the Brillouin zone. In this case, the system undergoes a transition from the Luttinger liquid to a Mott insulating phase when the potential and the interaction are present. Potential and interaction hence cooperate rather than oppose each other as in the half filled ionic model.

An analysis of the ionic Hubbard model with another $2k_f$ -periodic potential one find the band insulator for weak interaction but strong potential. Our $4k_f$ -periodic pattern, hence the Mott insulator, is obtained in their model in the limit of strong interaction. Both phases arc separated by a bond ordered phase. Reveals the features of the analysis, however, concentrates on large $[U - W]$.In our case, the $4 k_f -$ periodic pattern is not a limit of the $2 k_f$ - periodic patterns.

In the following, we concentrate on the ionic Hubbard model at weak to intermediate potential strength and intermediate to strong interaction. In addition, we study the region of stability for each potential.

In the following, we discuss the numerical data for the ground state energy, the charge and spin gap, and the spin- spin correlation function. The numerical results arc obtained by the density matrix renormalization group method (DMRG), as implemented by Brune. The DMRG is a quasiexact numerical method to determine the ground state properties, i.e., the ground state and the ground state energy, of long one-dimensional (non-integrable) systems will, reasonable accuracy. Regarding different boundary conditions, it is useful to lake into account the equivalence of fermion and spin models and 10 implement the spinless. Fermion model in terms of an equivalent spin chain, and the Hubbard model its two coupled spin chains without

perpendicular XY coupling. Using the DMRG, it is possible to extend the tractable system length is for the Hubbard chain to $N = 60, \dots 100$ sites. In our simulations we perform live lattice sweeps and keep 300 to 500 states per block. Correlation functions can be obtained within an error of 10^{-6} in the Hubbard model when using open boundary conditions. A memory of about 700 MB is required.

One can determine the ground state energy as a function of W and U . The energy gain depends almost quadratically on the potential strength for all potential types, and is dominated by the band shift. In case of a coupling to the charge density W_{in_i} , the $2k_f$ -periodic potential is stabilized for small U (case a), and the $4k_f$ -periodic potential (case c) for large U , as found for the Hubbard-Holstein model. This energy gain is mainly due to the prefactors. A more detailed analysis of the algebraic behavior for $W \rightarrow 0$ shows that $E_a \propto W^{1.68}$ and $E_c \propto W^2$ if $U=2t$, but $E_a \propto W^{1.76}$ and $E_c \propto W^{1.76}$ if $U = 10t$. In case (a) the exponent increases with interaction, in case (c) it decreases.

For all interactions, however, term (d), $h_i S_i$ is dominant. Of course, in a real system, a potential coupled to the density is much bigger than a magnetic field. It leads—similar to potential (c)—to $4k_f$ oscillations in the charge density and $2k_f$ oscillations in the magnetization. In the non-interacting system the data points for potentials (a) and (d) lie nearly on top of each other [by use of open boundary conditions the exact equivalence of (a) and (d) is waived], but in the interacting system the energy gain due to potential (d) grows faster with interaction than in all other cases. To be more specific, we find $E_d \propto W^{1.62}$ for $U=2t$ and $E_d \propto W^{1.44}$ for $U=6t$.

The excitation gaps:

$$\Delta_c = \frac{1}{2} [E(N_e + 1) + E(N_e - 1) - 2E(N_e)]$$

And:

$$\Delta_s = \frac{1}{2} [E(S^z = 1) + E(S^z = -1) - 2E(S^z = 0)]$$

Are calculated for finite systems only. An extrapolation to the thermodynamic limit, $\Delta = \Delta_0 + f(N)$ with $f(N) \rightarrow 0$ for $N \rightarrow \infty$, is not performed, for the following reasons: for small gap Δ_0 the accuracy of the DMRG away from half filling is not accurate enough and for large Δ_0 we have $f(N) \approx 0$ for the considered system sizes. The dependence of the excitation gaps on the potential strength. In cases (a), (b), and (c) we see that $\Delta_s \sim \Delta_c$ according to the band insulating. An almost linear dependence on W , as for non-interaction particles, is recovered in the interacting system for the charge gap in cases (a), (b), and (c). The saturation of the gaps in case (b) is obtained for the spin gap in the considered parameter regime. The influence of the interaction in the band insulating suite can be summarized as follows. In case (a) the charge gap becomes smaller with interaction, the spin gap even more. In case (b) the charge gap increases with interaction for small U , but saturates for strong interaction. The spin gap decreases rapidly with interaction. In case (d) the charge gap increases but does not saturate. The spin gap shows a maximum for inter- mediate interaction strength. For $U=10t$ it is even smaller than in the noninteracting system. On the contrary, we find for potential (c) a linear increase of Δ_c with U and W as well as $\Delta_3(W, U, N) \sim 1/U, / W, 1/N \rightarrow 0$, indicating the Mott insulating state. Due to the finite system size, we are not able to obtain exponents for small W . As a consequence, a comparison with bosonization or the energy data, is not possible. To conclude, for strong interaction and small potential we find a

large charge gap but a small spin gap.

In order to calculate the spin –spin correlation function $\langle \mathbf{S}_i^z \mathbf{S}_j^z \rangle$ within DMRG we gain use open boundary conditions and the Parzen filter function to reduce the Friedel oscillations. In the Mott insulating regime, the Friedel oscillations in the spin sector are long ranged, but decay fast in spin gap systems. The main question concerns the correspondence of the spin –spin correlation functions of the $2a$ -periodic potential (case c) and the Heisenberg model. For comparison, we calculate the spin –spin correlation function of the half-filled Hubbard model, which can be mapped onto a Heisenberg chain in case of strong interaction. In the Heisenberg model we have.

$$\langle \mathbf{S}_i^z \mathbf{S}_0^z \rangle = \frac{1}{4\pi(a_i)^2} + \frac{a_{2k_f} \cos(2k_f a i)}{a_i}$$

Correlation function decreases exponentially in cases (a) and (b), which show a spin gap without spin order. In case (d) the spins fixed by the potential. The exponentially decaying part is hard to extract from the mean magnetization in the numerical data due to the incomplete suppression of the boundary oscillations.

In the Mott insulating regime, however, the linear decrease of the spin-spin correlation function with distance is obtained already for small potential W . For better comparison with the data of the half-filled Hubbard chain obviously, the quarter-filled Hubbard chain with $4k_f$ -periodic distortion can be mapped onto the Heisenberg model. One note that in case (d) already a weak potential—connected with a small spin gap – leads to significant structures in $\langle \mathbf{S}_i^z \mathbf{S}_j^z \rangle$, whereas in case (c) the potential has to be much stronger to yield effects of similar size. The increase of $S(q) \propto q$ appears

both in the half-filled Hubbard chain and in the quarter-filled Hubbard chain with $4k_f$ - periodic potential. $S(q)$ has a sharp maximum at $q = \pi/2$ in case (d).

Studying the effects of periodic potentials on a chain one is interested in particular, we have considered the one-dimensional Hubbard model at quarter filling. We have compared periodic potentials yielding different types of behavior: (a) a $2k_f$ - periodic potential leading to a band insulator, (b) a $2K_f$ - periodic leading to a band insulator with cluster like arrangements of the charges, (c) a $4k_f$ -periodic potential leading to a Mott insulator with anti of Heisenberg type spins on next-nearest neighbor sites, and (d) a $2K_f$ -periodic magnetic field leading to a band insulator with antiferromagnetic alignment of ising type spins. Cases (c) and (d) reveal the same charge and spin distribution but different spin excitations. In the Heisenberg case the spin excitations are gapless, whereas in the ising case they are gapped.

In non-interacting systems, one find $E_a = E_d > E_b > E_c$, thus the band insulator. The charge distribution is quite homogeneous, and the cluster like arrangement is not minimal in energy. Turning on the interaction, potential (d) results in the largest energy gain, while the order of the remaining potentials depends on both the potential strength and the interaction. The interaction strongly supports the spin order, where double occupancy is suppressed.

For weak interaction and weak *potential*, one recover the behavior of the noninteracting system, with $E_a > E_b > E_c$. Turning to intermediate values ($U \approx 3t$, $W \approx t$) the cluster like arrangement of potential (b) gains more energy than the homogeneous distribution of case (a). $E_b < E_a > E_c$. For strong $W \rightarrow t$,

also a $4k_f$ pattern is favored against the homogeneous case. $E_b > E_c > E_a$ Thus, for small or intermediate interaction and potential, the gain of energy due to the hopping is stronger than the effects of the repulsive interaction or the underlying potential. With increasing potential, however, the effects of the potential dominates.

On the other hand, regarding a weak potential but increasing interaction, one find that a pattern related to potential (a) is established only at small interaction. The cluter like arrangement is formed at intermediate interaction ($U \approx 3 - 5t$), but at strong interaction the $4k_f$ - periodic interaction ($U \approx 3 - 5t$), but at $4k_f$ -periodic pattern dominates.

Concerning the spin chain compound $(Ca,Sr)_{14}Cu_{24}O_{41}$, we have applied the potential only in order to clarify the leading instability of the system. For comparison with a real material, which shows no lattice effects, the limit $W \rightarrow 0$ is relevant. In addition, for Copper oxides usually a correlation parameter of $U \approx 8$ ev is assumed. Together with the bandwidth of about 1 ev, we have $U > 15t$.In this parameter region, we find-neglecting the magnetic field—the $4k_f$ -periodic charge pattern with anti-ferromagnetism to be the most probable ground state. The energetic order found for weak potentials extends to strong potentials. For strong interaction. We always have $E_c > E_b > E_a$, The tendency of the repulsive interaction to separate the charges dominates the phase diagram in this region, the influence of the potential is weaker, leading to a preference of the cluster over the homogeneous distribution.

Finally, one remark that adding electrons stabilizes the cluster formation. This observation likewise agrees with experimental results, obtained for the $(Ca, La)_{14}Cu_{24}O_{41}$ series, where the cluster size grows on additional charge.

Therefore, we conclude, that the anti-ferromagnetism is due to the band filling, thus a commensurability effect [60].

3.7 Anomalous Self-Energy Features in the 2D Hubbard Model:

The two –dimensional Hubbard model is generally believed to be the minimal model sufficient to describe the behavior of high T_c cuprate superconductors [61].

The Hamiltonian of the two –dimensional Hubbard model reads as

$$H = -4t \sum_{ij} \alpha_{ij} c^\dagger(i)c(j) + U \sum_i n_\uparrow(i)n_\downarrow(i) - \mu \sum_i n(i) \quad (3.7.1)$$

Where $c^\dagger(i) = (c_\uparrow^\dagger(i), c_\downarrow^\dagger(i))$ is the electronic creation operator in spinorial notation at the site i , $n_\sigma(i) = c_\sigma^\dagger(i) c_\sigma(i)$ is the charge density operator for spin σ at the site i , $n(i) = \sum_\sigma n_\sigma(i)$ is the charge density operator at the site i , μ is the chemical potential, U is the on-site coulomb interaction strength, t is the hopping integral, α_{ij} is the projection operator on the nearest-neighbor sites. (For a generic operator $\Psi(i)$, we will often use the following definition:

$$\Psi^\alpha(i) = \sum_j \alpha_{ij} \Psi(j). \quad (3.7.2)$$

The equation of motion for the electronic operator $c(i)$ in the Heisenberg picture ($i = (i, t)$):

$$i \frac{\partial}{\partial t} c(i) = -\mu c(i) - 4t c^\alpha(i) + U \eta(i) \quad (3.7.3)$$

With $\eta(i) = n(i) c(i)$ and decompose $c(i)$ as $c(i) = \xi(i) + \eta(i)$, where $\xi(i) = [1 - n(i)]c(i)$ and choose $\xi(i)$ and $\eta(i)$ as Components of the basic field $\Psi^+(i) = (\xi^+(i), \eta^+(i))$.

The basic field then satisfies the following equations of motion:

$$i \frac{\partial}{\partial t} \Psi(i) \sum_j \varepsilon_{ij} \Psi(j, t) + \delta J(i) \quad (3.7.4)$$

With:

$$\varepsilon_{ij} = \delta_{ij} \varepsilon_0 - 4t \alpha_{ij} I (1 + \sigma_1)$$

$$\delta J(i) = \sigma_3 \boldsymbol{\pi}(i), \quad \boldsymbol{\pi}(i) = \frac{1}{2} \sigma^\mu \delta n_\mu(i) c^\alpha(i) + c^\dagger \alpha(i) c(i) c(i),$$

$$\varepsilon_0 = \begin{pmatrix} -\mu & 0 \\ 0 & U - \mu \end{pmatrix}, \quad I = \mathcal{F} \langle \{ \psi(i), \psi^\dagger(i) \} \rangle = \begin{pmatrix} 1 - \frac{n}{2} & 0 \\ 0 & n/2 \end{pmatrix},$$

Where n is the filling, $\delta n_\mu(i) = c^\dagger(i) \sigma_\mu c(i) - \delta_{\mu 0}^n$ is the charge ($\mu = 0$) and spin ($\mu = 1, 2, 3$) density fluctuation operator at the site i , $\sigma_\mu = (1, \sigma)$, $\sigma^\mu = (-1, \sigma)$, σ are the Pauli matrices, $\langle \dots \rangle$ stands for the thermal average in the grand-canonical ensemble and \mathcal{F} denotes the Fourier transform.

One here find the thermal retarded Green function $G(\mathbf{k}, \omega) = \mathcal{F} \langle R[\psi(i) \psi^\dagger(j)] \rangle$ in terms of the self-energy $\Sigma(\mathbf{K}, \omega)$ and, in turn, of the scattering matrix $T(\mathbf{K}, \omega) = I^{-1} [m(\mathbf{k}) + \mathcal{F} \langle R[\delta J(t) \delta J^\dagger(j)] \rangle] I^{-1}$:

$$G(\mathbf{K}, \omega) = \frac{1}{\omega - \varepsilon(\mathbf{k}) - \Sigma(\mathbf{k}, \omega)} I, \quad \Sigma(\mathbf{k}, \omega) = I \frac{1}{T^{-1}(\mathbf{k}, \omega) + G_0(\mathbf{K}, \omega)},$$

Where $G_0(\mathbf{K}, \omega) = \frac{1}{\omega - \varepsilon(\mathbf{k})} I$ is just the 0-th approximation ($\delta J(i) = 0$) and

$$m(\mathbf{k}) = \mathcal{F} \langle [\delta J(i), \psi^\dagger(j)] \rangle = -4t [\alpha(\mathbf{k}) \rho + \Delta] (1 - \sigma_1) \text{ with } \Delta = C_{11}^\alpha - C_{22}^\alpha, \quad P = \frac{1}{4} (C_0^\alpha + 3 C_3^\alpha) - C_P^\alpha, \quad C^\alpha = \langle \psi^\alpha(i) \psi^\dagger(i) \rangle, \quad C_\mu^\alpha = \langle \delta n_\mu^\alpha(i) \delta n_\mu(i) \rangle, \quad C_P^\alpha = \langle [C_\uparrow(i) C_\downarrow(i)]^\alpha C_\downarrow^\dagger(i) C_\uparrow^\dagger(i) \rangle.$$

In the pole approximation, we would have just $\Sigma(\mathbf{k}, \omega) \approx m(\mathbf{k}) I^{-1}$ as we would replace $\delta J(i)$ by its projection on the chosen basis $\psi(i)$: $\delta J(\mathbf{k}) \approx m(\mathbf{k}) I^{-1}(\mathbf{k})$. In the non-crossing approximation, we take advantage of the possibility of exactly rewriting $\delta J(i)$ in terms of bosonic field multiplied by

fermionic ones. Accordingly, we can approximate the scattering matrix $T(k, \omega_n)$ and retain pole contribution plus the non-crossing diagrams that is diagrams containing the convolution of charge and spin. (Here we choose neglect the pair term propagators compared to the electronic one:

$$\Sigma(k, \omega_n) \approx m(k) I^{-1} - 4t^2(1 - \sigma_1) \times \mathcal{F} \{ \mathcal{F}^{-1} [S(k, \omega_n)] \mathcal{F}^{-1} [\alpha^2(k) G_{cc}(k, \omega_n)] \} I^{-1},$$

Where:

$$G_{cc}(k, \omega_n) = \mathcal{F} \langle T_T [C(i) C^\dagger(i)] \rangle$$

And:

$$S(k, \omega_n) = \mathcal{F} \langle T_T [\delta n_\mu(i) \delta n_\mu(j)] \rangle$$

Here, the parameter P has been fixed through the algebraic constraint $\langle \xi(i) \eta^\dagger(i) \rangle = 0$ and charge and spin propagators have been computed in the two-pole approximation. It is worth noticing that this approach is completely microscopic, exclusively analytical, and fully self-consistent.

One can see that the imaginary part of the self-energy $\Sigma''(k, \omega_n)$ shows two different behavior as a function of frequency when computed at the nodal point $\underline{K} = S$ and at its companion position on the phantom half of the hole pocket $\underline{K} = \underline{S}$. In particular, at $\underline{K} = S$, a parabolic –like (i.e., Fermi-liquid –like) behavior is apparent, whereas at $\underline{K} = \underline{S}$, the dependence shows a predominance of the linear term [61].

3.8 Summary and Critique:

The attempts exhibited here and most of attempts made to describe superconductor behavior [43, 57, 58]. Specially HTSC [61], are based on very complex mathematical structure. These models can describe partially

the behavior of HTSC [43, 61] .One needs simple general quantum model that can describe HTSC behavior.

Chapter 4

Quantum Schrodinger Model in Energy Space

4.1 Introduction

The main recent approach, in describing the behavior of bulk matter and new materials, is based mainly on production and destruction operators.

The Heisenberg picture is mainly used in these models. This chapter is concerned with describing the behavior of matter in terms the energy wave function in the coordinate space. This approach is based on the analogy of such wave function with production and destruction operator.

4.2 The Equation of motion:

The transition probability of electrons in atoms depends on the probability of existence of electrons in energy levels. Thus it is important to find the time and spatial evolution of the wave function in the energy space.

4.2.1 In the energy space:

The wave function can be expressed in terms of the energy eigenfunction u and energy wave function c , in the form:

$$|\Psi\rangle = \sum c_K |u_K\rangle \quad (4.2.1.1)$$

Thus:

$$\Psi(x) = \sum c_K u_k \quad (4.2.1.2)$$

The eigenfunction satisfies:

$$\hat{H}|u_k\rangle = E_k |u_k\rangle \quad (4.2.1.3)$$

Which is the energy eigen equation in the coordinate

Space:

$$\hat{H}u_k = E_k u_k \quad (4.2.1.4)$$

u_k : is the energy eigenfunction, equation (4.2.1.4) can be written in the form:

$$i\hbar \frac{\partial u_k}{\partial t} = E_k u_k \quad (4.2.1.5)$$

Which gives the time evolution of the eigenfunction.

4.2.2 Spatial dependent Energy Wave function:

Schrodinger equation which is based on Newtonian energy relation is given by:

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V \Psi \quad (4.2.2.1)$$

To make use of equation (4.2.2.1) consider:

$$c_k = c_k(E, x) \quad (4.2.2.2)$$

i.e., the energy wavefunction depends on E and x only, where:

$$u_k = u_k(E, t) = A e^{iE_k t/\hbar} \quad (4.2.2.3)$$

Substituting equation (4.2.1.2) in (4.2.2.1) yields:

$$i\hbar \sum_k c_k \frac{\partial u_k}{\partial t} = \frac{-\hbar^2}{2m} \sum \nabla^2 c_k u_k + \sum_k V u_k c_k \quad (4.2.2.4)$$

$$i\hbar \sum_k c_k \frac{\partial u_k}{\partial t} = \frac{-\hbar^2}{2m} \sum \nabla^2 c_k u_k + \sum_k V u_k c_k \quad (4.2.2.5)$$

$$\sum_k E_k c_k u_k = \frac{-\hbar^2}{2m} \sum_k u_k \nabla^2 c_k + \sum_k V u_k c_k \quad (4.2.2.6)$$

Multiply equation (4.2.2.6) by \bar{u}_n , then integrating, yields:

$$\sum_k E_k c_k \int u_k \bar{u}_n \cdot dr = \frac{-\hbar^2}{2m} \sum_k (\int u_k \bar{u}_n dr) \nabla^2 c_k + \sum_k c_k \int \bar{u}_n V u_k dr$$

$$\sum_k E_k c_k \delta_{kn} = \frac{-\hbar^2}{2m} \sum_k (\nabla^2 c_k) \delta_{kn} + \sum_k c_k V_{nk}$$

$$\delta_{kn} = \delta_{nn} = 1 \quad (n=k)$$

Thus Schrödinger equation for energy wave function is given by:

$$c_n E_n = \frac{-\hbar^2}{2m} \nabla^2 c_n + \sum_k c_k V_{nk} \quad (4.2.2.7)$$

Multiplying equation (4.2.2.7) by c_n^+ :

$$c_n^+ c_n E_n = \frac{-\hbar^2}{2m} (\nabla^2 c_n) c_n^+ + \sum_k c_n^+ c_k V_{nk} \quad (4.2.2.8)$$

Taking the complex conjugate of the equation (4.2.2.7), one gets:

$$c_n^+ E_n = \frac{-\hbar^2}{2m} \nabla^2 c_n^+ + \sum_k c_k^+ V_{nk} \quad (4.2.2.9)$$

Multiplying by c_n , yields:

$$c_n c_n^+ E_n = \frac{-\hbar^2}{2m} c_n \nabla^2 c_n^+ + \sum_k c_n c_k^+ V_{nk} \quad (4.2.2.10)$$

But since:

$$\nabla(c_n c_k^+) = c_n \nabla c_k^+ + c_k^+ \nabla c_n$$

$$\nabla^2(c_n c_k^+) = \nabla c_n \nabla c_k^+ + c_n \nabla^2 c_k^+ + \nabla c_k^+ \nabla c_n + c_k^+ \nabla^2 c_n = 2\nabla c_n \nabla c_k^+ + c_n \nabla^2 c_k^+ + c_k^+ \nabla^2 c_n$$

$$\nabla^2(c_n c_k^+) - 2\nabla c_n \nabla c_k^+ = c_n \nabla^2 c_k^+ + c_k^+ \nabla^2 c_n \quad (4.2.2.11)$$

Taking:

$$n=k$$

One gets:

$$\nabla^2(c_n c_n^+) - 2\nabla c_n \nabla c_n^+ = c_n \nabla^2 c_n^+ + c_n^+ \nabla^2 c_n \quad (4.2.2.12)$$

Using (4.2.2.11) and adding equations (4.2.2.8), (4.2.2.10) yields:

$$2E_n |c_n|^2 = \frac{-\hbar^2}{2m} [\nabla^2 |c_n|^2 - 2\nabla c_n \nabla c_n^+] + \sum_k c_n^+ c_k v_{nk} + c_n c_k^+ V_{kn} \quad (4.2.2.13)$$

Where:

$$|c_n|^2 = c_n c_n^+ \quad (4.2.2.14)$$

However, if one can use equation (4.2.1.2):

$$\Psi = \sum_i c_i u_i \quad (4.2.2.15)$$

$$\int u_i^+ u_j dr = \delta_{ij}; \langle E \rangle = \int \Psi^+ \hat{H} \Psi dr \quad (4.2.2.16)$$

To get average energy in the form:

$$\langle E \rangle = \int (\sum_i c_i^+ u_i^+) \hat{H} (\sum_j c_j u_j) dr = \int (\sum_i c_i^+ u_i^+) (\sum_j c_j u_j) dr = \sum_i c_i^+ (\sum_j c_j E_j) \int u_i^+ u_i. dr = \sum_i c_i^+ c_j E_i \delta_{ij} \quad (4.2.2.17)$$

Put:

$$E_j = t \quad (4.2.2.18)$$

$$\therefore \langle E \rangle = \sum t c_i^+ c_j \quad (4.2.2.19)$$

This expression resembles that of Hubbard model.

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H}\Psi \quad (4.2.2.20)$$

$$|\Psi_n\rangle = \sum_i c_i |u_i\rangle$$

$$\langle \Psi | = \sum_i c_i^+ \langle u_i |, |\Psi_m\rangle = \sum_i c_i |u_i\rangle = \sum_{ij} c_i^+ c_j \langle u_i | \hat{H} | u_j \rangle = \sum_{ij} c_i^+ c_j H_{ij} \quad (4.2.2.21)$$

$$H_{ij} = \langle u_i | \hat{H} | u_j \rangle = E_j \langle u_i | u_j \rangle = E_j \delta_{ij} \quad (4.2.2.22)$$

4.2.3 The time and Spatial Evolutions:

It is very interesting to see how the energy wave function can evolve with time and coordinates. Thus:

c_k is a function of x and t :

$$|\Psi\rangle = \sum c_k |u_k\rangle \quad (4.2.3.1)$$

Where:

$$c_k = c_k(x, t) \quad (4.2.3.2)$$

In this case Schrodinger equation becomes:

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = \hat{H} |\Psi\rangle \quad (4.2.3.3)$$

$$i\hbar \frac{\partial}{\partial t} \sum_k c_k |u_k\rangle = \sum_k \hat{H} c_k |u_k\rangle$$

$$i\hbar \frac{\partial}{\partial t} \sum_k c_k u_k = \sum_k \hat{H} c_k u_k$$

$$\sum \left[i\hbar \left(\frac{\partial c_k}{\partial t} \right) u_k + i\hbar c_k \left(\frac{\partial u_k}{\partial t} \right) \right] = \sum_k \hat{H} c_k u_k \quad (4.2.3.4)$$

But according to equation (4.2.3.1):

$$i\hbar \frac{\partial u_k}{\partial t} = E_k u_k \quad (4.2.3.5)$$

Thus:

$$\sum_k \left[i\hbar \left(\frac{\partial c_k}{\partial t} \right) u_k + c_k E_k u_k \right] = \sum_k \hat{H} c_k u_k = \sum_k \frac{-\hbar^2}{2m} \nabla^2 (c_k u_k) + V c_k u_k \quad (4.2.3.6)$$

For two level systems n and m, equation (4.2.3.6) becomes:

$$i\hbar \frac{\partial c_n}{\partial t} u_n + E_n u_n c_n + i\hbar \frac{\partial c_m}{\partial t} u_m + E_m u_m c_m = \frac{-\hbar^2}{2m} u_n \nabla^2 c_n + V u_n c_n - \frac{\hbar^2}{2m} (\nabla^2 c_m) u_m + V u_m c_m \quad (4.2.3.7)$$

If one assumes that the particles is initially at level n. This means that

$$c_m = 0, t \rightarrow 0$$

Thus equation (4.2.3.7) reduced to:

$$\left[i\hbar \frac{\partial c_n}{\partial t} + E_n c_n \right] u_n = \left[\frac{-\hbar^2}{2m} \nabla^2 c_n + V c_n \right] u_n$$

Hence:

$$i\hbar \frac{\partial c_n}{\partial t} + E_n u_n = \frac{-\hbar^2}{2m} \nabla^2 c_n + V c_n \quad (4.2.3.8)$$

To prove equivalence of schrodinger. And Heisenberg picture:

$$i\hbar \frac{\partial \hat{C}}{\partial t} = [\hat{H}, \hat{C}]$$

$$i\hbar \frac{\partial \hat{C}}{\partial t} \Psi = \hat{H} \hat{C} \Psi - \hat{C} \hat{H} \Psi \quad (4.2.3.9)$$

$$\text{Let } \hat{C} \Psi = c \Psi \quad (4.2.3.10)$$

$$i\hbar \left(\frac{\partial \hat{C}}{\partial t} \right) \Psi = \hat{H} (c \Psi) - \hat{C} \hat{H} \Psi = c \hat{H} \Psi - (\hat{H} c) \Psi - \hat{C} \hat{H} \Psi \quad (4.2.3.11)$$

If:

$$\hat{C} \hat{H} \Psi = \hat{C} \Phi = c \Phi = c \hat{H} \Psi \quad (4.2.3.12)$$

$$\Rightarrow i\hbar \left(\frac{\partial \hat{C}}{\partial t} \right) \Psi = c \hat{H} \Psi - (\hat{H} c) \Psi - c \hat{H} \Psi = (\hat{H} c) \Psi = \hat{H} \hat{C} \Psi$$

$$\therefore i\hbar \frac{\partial \hat{c}}{\partial t} = \hat{H} \hat{c} = \frac{-\hbar^2}{2m} \nabla^2 \hat{c} + V \hat{c} \quad (4.2.3.13)$$

This is true for time independent potential:

$$V = V(r)$$

Where:

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V\Psi = E\Psi$$

4.2.4 Harmonic oscillator:

For harmonic oscillator:

$$V_1 = c_1 x^2 = \frac{1}{2} K x^2 \quad (4.2.4.1)$$

Substituting (4.2.4.1) in (4.2.3.8), yields:

$$i\hbar \frac{\partial c_n}{\partial t} + E_n c_n = \frac{-\hbar^2}{2m} \nabla^2 c_n + c_1 x^2 c_n \quad (4.2.4.2)$$

Solution:

Let:

$$c_n = A e^{+\frac{i}{\hbar} E_0 t - \alpha x^2} \quad (4.2.4.3)$$

$$\frac{\partial c_n}{\partial t} = +\frac{i}{\hbar} E_0 c_n, \quad \nabla c_n = \frac{\partial c_n}{\partial x} = -2\alpha x c_n$$

$$\begin{aligned} \nabla^2 c_n &= \frac{\partial^2 c_n}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial c_n}{\partial x} \right) = \frac{\partial}{\partial x} (-2\alpha x c_n) = -2\alpha c_n - 2\alpha x \left(\frac{\partial c_n}{\partial x} \right) = \\ &= -2\alpha c_n - 2\alpha x (-2\alpha x c_n) = -2\alpha c_n + 4\alpha^2 x^2 c_n \end{aligned} \quad (4.2.4.4)$$

By subs. in equation (4.2.4.2):

$$(-E_0 + E_n) c_n = \frac{-\hbar^2}{2m} (-2\alpha c_n) - \frac{\hbar^2}{2m} (4\alpha^2 x^2) c_n + c_1 x^2 c_n$$

$$\Rightarrow (-E_0 + E_n) c_n = \frac{\hbar^2}{m} \alpha c_n + c_1 x^2 c_n - \frac{2\hbar^2 \alpha^2}{m} x^2 c_n$$

$$(E_n - E_0) = \frac{\hbar^2}{m} \alpha + \left[c_1 - \frac{2\hbar^2}{m} \alpha^2 \right] x^2$$

Comparing free terms coefficients and coefficient of x^2 :

$$-E_0 + E_n = \frac{\hbar^2}{m} \alpha ; \quad \alpha = \frac{m}{\hbar^2} (E_0 + E_n)$$

$$\frac{2\hbar^2 \alpha^2}{m} = C_1 = \frac{1}{2} K = \frac{1}{2} m \omega^2 ; \quad \alpha = \frac{m \omega}{2\hbar}$$

$$\therefore -E_0 + E_n = \frac{\hbar^2}{m} \left(\frac{m \omega}{2\hbar} \right) = \frac{1}{2} \hbar \omega$$

$$\therefore E_n - E_0 = \frac{\hbar \omega}{2}$$

$$E_n = \frac{1}{2} \hbar \omega + E_0 \tag{4.2.4.5}$$

To find E_0 , one can use the periodicity condition of c_n . With the aid of (4.2.4.3):

$$c_n = A e^{\frac{i}{\hbar} E_0 t - \alpha x^2} = f e^{\frac{i}{\hbar} E_0 t}$$

Where:

$$f = A e^{-\alpha x^2}$$

Since the motion is periodic. It follows that:

$$c_n(t + T) = c_n(t)$$

$$f e^{\frac{i}{\hbar} E_0 (t+T)} = f e^{\frac{i}{\hbar} E_0 t}$$

$$\cos \frac{E_0}{\hbar} T = 1$$

$$\frac{E_0}{\hbar} T = 2n\pi$$

$$E_0 = n \hbar \omega$$

On the other side:

$$\sin \frac{E_0}{\hbar} T = 0$$

$$E_0 = \frac{\hbar(2\pi)n}{T}$$

Therefore:

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

This resembles the ordinary quantum expression of harmonic oscillator, but by using simple mathematics.

To find A:

$$\int |c_n|^2 dE_n = N \quad ; \quad c_n = A e^{\frac{i}{\hbar}E_0 t - \alpha x^2} = A e^{i\theta t - \alpha x^2}$$

$$\bar{c}_n = A e^{-i\frac{1}{\hbar}E_0 t - \alpha x^2} = A e^{-i\theta t - \alpha x^2}$$

$$\int \bar{c}_n c_n dE_n = N = \int_0^\infty A^2 (e^{(-i\theta t - \alpha x^2)})(e^{(i\theta t - \alpha x^2)}) dE_n = N$$

$$\therefore \int_0^\infty \bar{c}_n c_n dE_n = N =$$

$$A^2 \int_0^\infty e^{-\frac{2m(E_0 + E_n)x^2}{\hbar^2}} dE_n = \left[A^2 e^{-\frac{\frac{2m}{\hbar^2}E_0 x^2}{\frac{-2mx^2}{\hbar^2}}} e^{-\frac{-2mE_n x^2}{\hbar^2}} \right]_0^\infty$$

$$= \left[A^2 e^{-\frac{2mE_0 X^2}{\hbar^2} - \frac{-\hbar^2}{2mx^2}} \right]_0^\infty = -\frac{\hbar^2}{2mx^2} |C_n|^2$$

4.2.5 Crystal field:

$$i\hbar \frac{\partial c_n}{\partial t} + c_n E_n = \frac{-\hbar}{2m} \nabla^2 c_n + V_0 c_n \quad (4.2.5.1)$$

Let:

$$c_n = A e^{i/\hbar E_0 t} e^{i\alpha x} \quad (4.2.5.2)$$

$$\frac{\partial c_n}{\partial t} = \frac{i}{\hbar} E_0 c_n, \quad \nabla c_n = \frac{\partial c_n}{\partial x} = i\alpha c_n ;$$

$$\nabla^2 c_n = -\alpha^2 c_n \quad (4.2.5.3)$$

Subs. (4.2.5.3) in (4.2.5.1), we get:

$$(-E_0 + E_n)c_n = \left(\alpha^2 \frac{\hbar^2}{2m} + V_0\right) c_n \quad (4.2.5.4)$$

$$\Rightarrow E_n - E_0 = \frac{\hbar^2}{2m} \alpha^2 + V_0 \quad (\alpha = k = \text{Wave number})$$

$$\therefore E_n - E_0 = \frac{\hbar^2}{2m} k^2 + V_0 \quad (4.2.4.5)$$

$$E_n - E_0 = n\hbar\omega, k \leq k_0 \quad (4.2.4.6)$$

Let:

$$C_n = e^{i/\hbar E_0 t} e^{-\alpha x}$$

$$\frac{\partial C_n}{\partial t} = \frac{i}{\hbar} E_0 C_n, \quad \nabla C_n = -\alpha C_n, \quad \nabla^2 C_n = \alpha^2 C_n \quad (4.2.5.7)$$

$$\Rightarrow (-E_0 + E_n)C_n = -\frac{\hbar^2}{2m} \alpha^2 C_n + V_0 C_n \quad (4.2.5.8)$$

$$\therefore E_n - E_0 = V_0 - \frac{\hbar^2}{2m} \alpha^2 \quad (4.2.5.9)$$

$$\int \bar{C}_n C_n dE_n = N, \quad C_n = A e^{i/\hbar E_0 t} e^{i\alpha x} = A e^{i\left(\frac{1}{\hbar} E_0 t + \alpha x\right)} = A e^{i\theta t + i\alpha x} = A e^{i(\theta t + \alpha x)} \quad (4.2.5.10)$$

$$\bar{C}_n = A e^{-i(\theta t + \alpha x)} \quad (4.2.5.11)$$

$$\therefore \int A^2 e^{-i(\theta t + \alpha x)} e^{i(\theta t + \alpha x)} dE_n = N \quad (4.2.5.12)$$

$$A^2 \int dE_n = N$$

$$A^2 E_n = N$$

$$A^2 = \frac{N}{E_n} \quad (4.2.5.13)$$

So, as:

$$C_n = e^{i/\hbar E_0 t} e^{-\alpha x} = e^{i\theta t - \alpha x} ; \bar{C}_n = e^{-i\theta t - \alpha x}$$

$$\int \bar{C}_n C_n dE_n = N = \int A^2 (e^{i\theta t - \alpha x}) e^{(-i\theta t - \alpha x)} dE_n = N$$

$$\begin{aligned}
&= A^2 \int e^{-2\alpha x} dE_n = N \\
&\Rightarrow A^2 e^{-2\alpha x} E_n = N \\
\therefore A^2 &= \frac{N}{e^{-2\alpha x E_n}} \tag{4.2.5.14}
\end{aligned}$$

4.2.6 Dirac Equation:

Dirac equation can be written as:

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(c\alpha \cdot \frac{\hbar}{i} \nabla \Psi + m_0^2 c^4 \beta \Psi \right)$$

Let $\Psi = \sum c_k u_k$

$$\begin{aligned}
\sum_k i\hbar \frac{\partial c_k u_k}{\partial t} &= c \frac{\hbar}{i} \alpha \sum_k \nabla (u_k c_k) + m_0^2 c^4 \beta \sum u_k c_k \\
\sum_i i\hbar \left(\frac{\partial c_k}{\partial t} \right) u_k + i\hbar \sum c_k \frac{\partial u_k}{\partial t} &= c \frac{\hbar}{i} \alpha \sum_i [u_k \nabla c_k + c_k \nabla u_k] + m_0^2 c^4 \beta \sum u_k c_k \\
&= c \frac{\hbar}{i} \alpha \sum_i u_k \nabla c_k + \sum \left[c \frac{\hbar}{i} (\nabla u_k) + m_0^2 c^4 \beta u_k \right] c_k
\end{aligned}$$

But:

$$i\hbar \frac{\partial u_k}{\partial t} = E_k u_k = c \frac{\hbar}{i} \alpha \nabla u_k + m_0^2 c^4 \beta u_k$$

Thus:

$$\begin{aligned}
\sum_i i\hbar u_k \frac{\partial c_k}{\partial t} + \sum_k E_k u_k c_k &= c \frac{\hbar}{i} \alpha \sum u_k \nabla c_k + \sum E_k u_k c_k \\
\sum_i \left[i\hbar \frac{\partial c_k}{\partial t} - \frac{c\hbar}{i} \alpha \nabla c_k \right] u_k &= 0
\end{aligned}$$

Thus one of the possible solutions is:

$$i\hbar \frac{\partial c_k}{\partial t} - \frac{c\hbar}{i} \alpha \nabla c_k = 0 \tag{4.2.6.1}$$

Take complex conjugate:

$$\begin{aligned}
-i\hbar \frac{\partial c_k^*}{\partial t} + \frac{c\hbar}{i} \alpha \nabla c_k^* \\
= 0 \tag{4.2.6.2}
\end{aligned}$$

Multiply (4.2.6.1) by c_k^* and (4.2.6.2) by c_k to get:

$$i\hbar c_k^* \frac{\partial c_k^*}{\partial t} - \frac{c\hbar}{i} \alpha c_k^* \nabla c_k = 0$$

$$i\hbar c_k \frac{\partial c_k^*}{\partial t} - \frac{c\hbar}{i} \alpha c_k \nabla c_k^* = 0$$

$$i\hbar \frac{\partial |c_k|^2}{\partial t} - \frac{c\hbar}{i} \alpha \nabla |c_k|^2 = 0$$

Multiply by $\frac{i}{\hbar}$:

$$\frac{\partial |c_k|^2}{\partial t} + \alpha c \nabla |c_k|^2 = 0$$

But:

$$n = |c_k|^2$$

$$\frac{\partial n}{\partial t} + \alpha c \nabla n = 0$$

Multiply by m_0 :

$$\frac{\partial m_0 n}{\partial t} + \alpha \nabla m_0 n = 0$$

But the mass density ρ is given by:

$$\frac{\partial \rho}{\partial t} + \alpha \nabla \rho c = 0$$

This equation is the continuity equation for a particle moving.

Then:

$$\sum_k E_k c_k u_k = c \frac{\hbar}{i} \alpha \cdot \sum_k u_k \nabla c_k + m_0^2 c^4 \beta \sum_k u_k c_k \quad (4.2.6.3)$$

Multiply equation (4.2.5.3) by \bar{u}_n , yield:

$$\sum_k E_k c_k \int \bar{u}_n u_k dt = c \frac{\hbar}{i} \alpha \cdot \nabla c_k \int \bar{u}_n u_k dt + m_0^2 c^4 \beta \int \bar{u}_n u_k dt$$

$$E_k c_k \delta_{nk} = c \frac{\hbar}{i} \alpha \cdot \nabla c_k \delta_{nk} + m_0^2 c^4 \beta \delta_{nk}$$

$$n = k \Rightarrow \delta_{nk} = 1$$

$$\therefore E_n c_n = c \frac{\hbar}{i} \alpha \cdot \nabla c_n + m_0^2 c^4 \beta \quad (4.2.6.4)$$

Let:

$$c_n = A e^{\gamma x}, \nabla c_n = \frac{dc_n}{dx} = \gamma A e^{\gamma x} = \gamma c_n$$

$$E_n c_n = c \frac{\hbar}{i} \alpha \cdot \gamma c_n + m_0^2 c^4 \beta$$

$$E_n c_n = c \frac{\hbar}{i} \alpha \gamma c_n + m_0^2 c^4 \beta$$

$$E_n c_n - c \frac{\hbar}{i} \alpha \gamma c_n = m_0^2 c^4 \beta$$

$$\left(E_n - c \frac{\hbar}{i} \gamma \alpha \right) = m_0^2 c^4 \beta$$

$$\therefore E_n = m_0^2 c^4 \beta + c \frac{\hbar}{i} \alpha \gamma \quad (4.2.6.5)$$

$$\gamma = \frac{(E_n - \beta m_0^2 c^4) i}{c \hbar \alpha} = \frac{i(E_n - \beta m_0^2 c^4)}{c \hbar \alpha} = i\theta \quad (4.2.6.6)$$

To find A:

$$\int |c_n|^2 dE_n = N; \int \bar{c}_n c_n dE_n = N = \int A^2 e^{-i\theta x} e^{i\theta x} dE_n = N$$

$$A^2 \int_0^{E_m} dE_n = N; A^2 E_m = N; A^2 = \frac{N}{E_m} = \frac{N(8ml)}{n^2 \hbar^2}$$

$$A = \frac{\sqrt{N(8ml)}}{n \hbar} \quad (4.2.6.7)$$

4.2.7 Klein-Gordon:

$$-\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} = -c^2 \hbar^2 \nabla^2 \Psi + m_0^2 c^4 \Psi \quad (4.2.7.1)$$

$$-\hbar^2 \sum_k \frac{\partial^2 c_k u_k}{\partial t^2} = -c^2 \hbar^2 \sum_k \nabla^2 c_k u_k + \sum_k m_0^2 c^4 c_k u_k \quad (4.2.7.2)$$

$$-\hbar^2 \frac{\partial^2 u_k}{\partial t^2} = E_k^2 u_k$$

Then:

$$\sum_k E_k^2 c_k u_k = -c^2 \hbar^2 \sum_k u_k \nabla^2 c_k + \sum m_0^2 c^4 c_k u_k \quad (4.2.7.3)$$

Multiply equation (4.2.6.3) by \bar{u}_n , yields:

$$\begin{aligned} \sum_k E_k^2 c_k \int \bar{u}_n u_n dt &= -c^2 \hbar^2 \sum_k \nabla^2 c_k \int \bar{u}_n u_n dt + \sum m_0^2 c^4 c_k \int \bar{u}_n u_n dt \\ \sum E_k^2 c_k \delta_{nk} &= -c^2 \hbar^2 \nabla^2 c_k \delta_{nk} + m_0^2 c^4 \delta_{nk} \end{aligned}$$

Thus:

$$E_n^2 c_n = -c \hbar^2 \nabla^2 c_n + m_0^2 c^4 c_n \quad (4.2.7.4)$$

But:

$$c_n = A e^{\gamma x}$$

$$\therefore \nabla c_n = \frac{dc_n}{dx} = \gamma c_n ; \nabla^2 c_n = \gamma^2 c_n$$

By substituting in equation (4.2.6.4), we get:

$$E_n^2 c_n = -c^2 \hbar^2 \gamma^2 c_n + m_0^2 c^4 c_n$$

$$E_n^2 = -c^2 \hbar^2 \gamma^2 + m_0^2 c^4$$

$$E_n^2 = m_0^2 c^4 - c^2 \hbar^2 \gamma^2$$

$$\gamma^2 = \frac{E_n^2 - m_0^2 c^4}{c^2 \hbar^2} = \frac{m_0^2 c^4 - E_n^2}{c^2 \hbar^2}$$

$$\gamma = \frac{\sqrt{m_0^2 c^4 - E_n^2}}{c \hbar} ; m_0^2 c^4 \geq E_n^2$$

$$\Rightarrow \gamma = m_0^2 c^4 \sqrt{1 - \frac{E_n^2}{m_0^2 c^4}} \approx \frac{m_0^2 c^4}{c \hbar} \left(1 - \frac{1}{2} \frac{E_n^2}{m_0^2 c^4}\right) \quad (4.2.7.5)$$

To find A:

$$\int |c_n|^2 dE_n = \int A^2 e^{2\gamma x} dE_n = N = A^2 \int e^{2 \frac{m_0 c^2 x}{c \hbar}} dE_n = N \quad (4.2.7.6)$$

$$A^2 e^{\frac{2m_0 c x}{\hbar}} E_n = N$$

$$A^2 = \frac{N}{E_n e^{2m_0 c x/\hbar}} = \frac{8 m l N}{n^2 \hbar^2 e^{2m_0 c x/\hbar}} \quad (4.2.7.7)$$

4.2.8 A relationship between state vector and many particle system:

$$i\hbar \frac{dc_k}{dt} = i\hbar \frac{d|c_j|^2}{dt} = i\hbar \frac{d}{dt} c_j c_j^* = i\hbar \left[c_j \frac{dc_j^*}{dt} + \left(\frac{dc_j}{dt} \right) c_j^* \right] \quad (4.2.8.1)$$

$$i\hbar \frac{dc_j^*}{dt} = \sum_k (H_1)_{jk}^* e^{-j\omega_{jk}t} c_k^*$$

$$i\hbar \frac{dc_j}{dt} = \sum_k (H_1)_{jk} e^{j\omega_{jk}t} c_k$$

$$i\hbar c_j \frac{dc_j^*}{dt} = \sum_k (H_1)_{jk}^* e^{-j\omega_{jk}t} c_j c_k^*$$

$$i\hbar c_j^* \frac{dc_j}{dt} = \sum_k (H_1)_{jk} e^{j\omega_{jk}t} c_j^* c_k$$

Hence, the number of particles in state j is given by:

$$i\hbar \frac{d|c_j|^2}{dt} = \sum_k \left[(H_1)_{jk}^* e^{-j\omega_{jk}t} c_j c_k^* + (H_1)_{jk} e^{i\omega_{jk}t} c_j^* c_k \right]$$

$$\therefore i\hbar \frac{dn}{dt} = \sum_k \left[(H_1)_{jk}^* e^{-j\omega_{jk}t} c_j c_k^* + (\hat{H}_1)_{jk} e^{i\omega_{jk}t} c_j^* c_k \right] \quad (4.2.8.2)$$

$$|\Psi\rangle = \sum_k c_k |u_k\rangle \quad (4.2.8.3)$$

$$\langle\Psi| = \sum_k c_k^+ \langle u_k| \quad (4.2.8.4)$$

$$\langle\Psi|\Psi\rangle = \sum_k \sum_{\tilde{k}} c_k c_{\tilde{k}}^+ \langle u_k | u_{\tilde{k}} \rangle = \sum_k c_k \left(\sum_{\tilde{k}=1}^n c_{\tilde{k}}^+ \delta_{k\tilde{k}} \right) = \sum_k c_k (c_k^+ \delta_{kk}) = \sum_k c_k c_k^+ = \sum_k |c_k|^2 \quad (4.2.8.5)$$

Also:

$$|\Psi\rangle = \sum_k a_k |\dots n_k\rangle$$

$$\langle\Psi| = \sum_{\tilde{k}} a_{\tilde{k}}^+ \langle \dots n_{\tilde{k}}| = \sum_{\tilde{k}} \langle \dots n_{\tilde{k}} | a_{\tilde{k}}^+$$

$$\langle\Psi|\Psi\rangle = \sum_{k,\tilde{k}} \langle n_{\tilde{k}} | a_{\tilde{k}}^+ a_k | n_k \rangle = \sum_{k,\tilde{k}} \langle n_{\tilde{k}} | a_{\tilde{k}}^+ \sqrt{n_k} | \dots n_{k-1} \rangle = \sum_{k,\tilde{k}} \sqrt{n_k} \langle n_{\tilde{k}} | a_{\tilde{k}}^+ | n_{k-1} \rangle$$

$$[a_k | n_k \rangle = \sqrt{n_k} | \dots n_{k-1} \rangle, \langle n_k | a_k^+ = \langle n_{k-1} | \sqrt{n_k}]$$

$$\begin{aligned} \sum_{\hat{k},k}(\sqrt{n_k})\langle n_{\hat{k}-1}|(\sqrt{n_{\hat{k}}})|n_{k-1}\rangle &= \sum_{\hat{k},k} \sqrt{n_k} \sqrt{n_{\hat{k}}} \langle n_{\hat{k}-1}|n_{k-1}\rangle \\ \langle \Psi|\Psi\rangle &= \sum_k \sqrt{n_k} \sum_{\hat{k}} \sqrt{n_{\hat{k}}} \delta_{\hat{k}-1,k-1} = \sum_k \sqrt{n_k}(\sqrt{n_k}) = \sum_k n_k \end{aligned} \quad (4.2.8.6)$$

Comparing (4.2.8.5) and (4.2.8.6), yields:

$$\sum_k |C_k|^2 = \sum_k n_k \quad (4.2.8.7)$$

$$n_k = |C_k|^2 \quad (4.2.8.8)$$

=number of particle in state k.

$$|\Psi\rangle = \sum_j c_j |u_j\rangle \quad (4.2.8.9)$$

$$\langle \Psi| = \sum_i c_i^+ \langle u_i| \quad (4.2.8.10)$$

$$\begin{aligned} \hat{H} &= \langle \Psi|H|\Psi\rangle = \sum_j \sum_i c_i^+ c_j \langle u_i|\hat{H}|u_j\rangle = \\ &= \sum_i \sum_j c_j^+ c_j t_{ij} = \sum_{i,j} c_i^+ c_j t_{ij} \end{aligned}$$

$$t_{ij} = \langle u_i|\hat{H}|u_j\rangle$$

$$\hat{H} = \hat{H}_0 + V_1$$

For the Hamiltonian which is not perturbed:

$$\hat{H} = \hat{H}_0$$

And if u_j is not the eigenvalue of the Hamiltonian:

$$t_{ij} = \langle u_i|\hat{H}_0|u_j\rangle$$

Thus the matrix of the Hamiltonian becomes:

$$H_0 = \sum_{ij} c_i^+ c_j t_{ij}$$

Which the Hubbard Hamiltonian.

$$t_{ij} = t, \text{ For all } i, j \quad (4.2.8.11)$$

$$\hat{H}_0 = \sum_{ij} t C_i^+ C_j = t \sum_{ij} C_i^+ C_j \quad (4.2.8.12)$$

From (4.2.8.5):

$$|\Psi\rangle = \sum C_k |u_k\rangle = \sum_i C_i |u_i\rangle \quad (4.2.8.12)$$

$$H_0|\Psi\rangle = \sum_i C_i \hat{H}_0 |u_i\rangle$$

$$\hat{H}_0|u_i\rangle = E_i|u_i\rangle = t_i|u_i\rangle$$

$$\langle\Psi|\hat{H}_0|\Psi\rangle = \sum_j C_j^+ \langle u_i|H_0|\Psi\rangle = \sum_{ij} C_j^+ t_i C_j \langle u_j|u_i\rangle = t \sum_{ij} C_j^+ C_i \delta_{ij}$$

$$\langle u_j|u_i\rangle = \delta_{ji}$$

From (4.2.8.8):

$$= t \sum |C_i|^2 = t \sum_i n_i = t N = E_T, \sum_k n_k = N$$

Thus Hubbard model and our model are equivalent, but our model is very simple compared to Hubbard model.

4.2.9 Harmonic Oscillator Critical Temperature:

Consider the equation:

$$i\hbar \frac{\partial c_k}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 c_k + V_1 c_k \quad (4.2.9.1)$$

For time independent potential, let:

$$c_k = e^{\frac{-iE_k t}{\hbar}} u_k \quad (4.2.9.2)$$

To get:

$$E_k u_k = \frac{\hbar^2}{2m} \nabla^2 u_k + V_1 u_k \quad (4.2.9.3)$$

For harmonic oscillator perturbation by electromagnetic field:

$$V_1 = \frac{1}{2} kx^2 = c_1 x^2$$

(4.2.9.4)

Thus:

$$\frac{\hbar^2}{2m} \nabla^2 u_k + c_1 x^2 = -E_k c_k \quad (4.2.9.5)$$

Substituting:

$$u_k = A e^{-\alpha x^2} \quad (4.2.9.6)$$

$$\nabla u_k = -2\alpha x e^{-\alpha x^2} = -2\alpha x u_k$$

$$\nabla^2 u_k = -2\alpha u_k - 2\alpha x \nabla u_k = -2\alpha u_k + 4\alpha^2 x^2 u_k \quad (4.2.9.7)$$

$$\frac{\hbar^2}{2m} [-2\alpha + 4\alpha^2 x^2 + c_1 x^2] u_k = -E_k u_k \quad (4.2.9.8)$$

$$E_k = \frac{\hbar^2}{m} \alpha; 4\alpha^2 = -c_1 \quad (4.2.9.9)$$

$$\alpha = \frac{1}{2} \sqrt{-\frac{k}{2}} = \frac{i}{\sqrt{2}} \sqrt{k} = \frac{i\sqrt{m}}{2\sqrt{2}} \omega$$

Thus from (4.2.9.2) and (4.2.9.6) beside (4.2.9.9):

$$c_k = A e^{-\frac{iE_k T}{\hbar}} e^{\frac{i\sqrt{k}}{2\sqrt{2}} x^2} \quad (4.2.9.10)$$

Which represents non localized travelling wave.

However for particles affected by additional perturbing potentials like applying sound wave with frequency ω_s and electron magnetic wave with frequency ω_e , such that the two forces apposes each other; in this case:

$$-\nabla V = F = m \ddot{x} = F_e - F_s = -k_e x + k_s x$$

$$-\frac{\partial V}{\partial x} = -m\omega_e^2 x + m\omega_s^2 x$$

Thus:

$$\begin{aligned} V &= \frac{1}{2} m\omega_s^2 x^2 - \frac{1}{2} m\omega_e^2 x^2 \\ &= \frac{1}{2} m(\omega_s^2 - \omega_e^2) x^2 \\ &= \frac{1}{2} m(\omega_s + \omega_e)(\omega_s - \omega_e) x^2 \\ &= -\frac{1}{2} k x^2 \end{aligned}$$

$$K = m(\omega_s + \omega_e)(\omega_s - \omega_e) = c_1 \quad (4.2.9.11)$$

When:

$$\omega_s > \omega_e$$

In this case:

$$c_2 = -c_1 = m(\omega_s + \omega_e)(\omega_s - \omega_e) > 0 \quad (4.2.9.12)$$

Thus equation (4.2.9.9) gives:

$$\alpha = \frac{1}{2} \sqrt{c^2} \quad (4.2.9.13)$$

Due to the periodicity of c_k in (4.2.9.2):

$$c_k(t + T) = c_k(t)$$

Thus:

$$e^{+\frac{i}{\hbar}E_k T} = 1$$

$$\cos \frac{E_k T}{\hbar} = 1; \sin \frac{E_k T}{\hbar} = 0 \quad (4.2.9.14)$$

Hence:

$$\frac{TE_k}{\hbar} = 2n\pi$$

$$E_k = n\pi \left(\frac{2\pi}{T} \right) = n\hbar\omega$$

Thus from equation (4.2.9.9):

$$\alpha = \frac{m}{\hbar^2} E_k = \frac{nm\omega}{\hbar} \quad (4.2.9.15)$$

From equation (4.2.9.6):

$$u_k = A e^{-\alpha x^2}$$

Thus the energy is quantized, and is highly localized thus move by hopping.

4.2.10 Spatial Dependent Energy wavefunction and Particles in a box:

Schrödinger equation which is based on Newtonian energy relation is gives by:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \quad (4.2.10.1)$$

To make use of equation (4.2.10.1) consider:

$$c_k = c_k(E, x) \quad (4.2.10.2)$$

i.e., the energy wave function depends on E and x only, where:

$$u_k = u_k(E, t) = A e^{\frac{iE_k T}{\hbar}} \quad (4.2.10.3)$$

Substituting equation (4.2.10.2) in (4.2.10.1) yields:

$$i\hbar \sum_k c_k \frac{\partial u_k}{\partial t} = -\frac{\hbar^2}{2m} \sum \nabla^2 c_k u_k + \sum_k V u_k c_k \quad (4.2.10.4)$$

$$\sum_k c_k \frac{\partial u_k}{\partial t} = -\frac{\hbar^2}{2m} \sum \nabla^2 c_k u_k + \sum_k V u_k c_k \quad (4.2.10.5)$$

In view of equation:

$$i\hbar \frac{\partial u_k}{\partial t} = E_k u_k$$

Thus:

$$\sum_k E_k c_k u_k = -\frac{\hbar^2}{2m} \sum_k u_k \nabla^2 c_k + \sum_k V u_k c_k \quad (4.2.10.6)$$

Multiply equation (4.2.10.6) by \overline{u}_n , then integrating, yields:

$$\sum_k E_k c_k \int u_k \overline{u}_n \cdot dr = -\frac{\hbar^2}{2m} \sum_k (\int u_k \overline{u}_n \cdot dr) \nabla^2 c_k + \sum_k c_k \int \overline{u}_n V u_k dr$$

$$\sum_k E_k c_k \delta_{nk} = -\frac{\hbar^2}{2m} \sum_k (\nabla^2 c_k) \delta_{nk} + \sum_k c_k V_{nk}$$

$$\delta_{nk} = \delta_{nn} = 1 \quad (n=k)$$

Thus Schrodinger equation for energy wave function is given by:

$$c_n E_n = -\frac{\hbar^2}{2m} \nabla^2 c_n + \sum_k c_k V_{nk} \quad (4.2.10.7)$$

For constant potential V_0 equation (4.2.10.7) reduces to:

$$c_n E_n = -\frac{\hbar^2}{2m} \nabla^2 c_n + \sum_k c_k V_0 \delta_{kn}$$

Thus:

$$-\frac{\hbar^2}{2m} \nabla^2 c_n = (E_n - V_0) c_n \quad (4.2.10.8)$$

To solve this equation consider the solution of equation (4.2.10.8) to be:

$$c_n = A e^{ikx} \quad (4.2.10.9)$$

Thus:

$$K = \sqrt{2m(E_n - V_0)} \quad (4.2.10.10)$$

For highly localized electrons:

$$E_n < V_0 \quad (4.2.10.11)$$

In this case:

$$K = i\alpha = i \sqrt{2m(V_0 - E_n)} \quad (4.2.10.12)$$

Thus:

$$c_n = Ae^{i^2\alpha x} = Ae^{-\alpha x} \quad (4.2.10.13)$$

Thus the probability of existence of electrons in level n:

$$|c_n|^2 = A^2 e^{-2\alpha x} \quad (4.2.10.14)$$

This probability highly decays as $x \rightarrow \infty$. Thus the electron is highly localized at $x = 0$, when:

$$E_n < V_0 \quad (4.2.10.15)$$

If one considers energy to be thermal, then:

$$E_n = KT$$

Thus:

$$kT < V_0 \quad (4.2.10.16)$$

$$T < \frac{V_0}{k} \quad (4.2.10.17)$$

The critical temperature beyond which the electrons are highly localized is:

$$T_c = \frac{V_0}{k} \quad (4.2.10.18)$$

Thus:

$$T < T_c \quad (4.2.10.19)$$

The fact that electrons are highly localized indicates that electron current does not result from electron motion in the whole super conductivity. This localization confirms the fact that electron conduction mechanism in super conductivity is by hopping of electrons from atom to adjacent one. This forces the next atom to eject another electron to hop to third one.

Another solution is of the form:

$$c_n = A \sin \alpha x \quad (4.2.10.20)$$

Substituting equation (4.2.10.20) in equation (4.2.10.8) yields:

$$\begin{aligned}
& + \frac{\hbar^2}{2m} \alpha^2 = (E_n - V_0) \\
\alpha & = \frac{\sqrt{2m(E_n - V_0)}}{\hbar} \tag{4.2.10.21}
\end{aligned}$$

Where:

$$E_n < V_0$$

Thus the electrons are bound to adjacent atoms. Only for particle in a box which, indicates that electrons in super conductivity does not move freely but hop just to the adjacent atom,

$$|c_n(x = d)|^2 = 0 \tag{4.2.10.22}$$

Hence from (4.2.10.20):

$$\text{Sin} \alpha d = 0 \tag{4.2.10.23}$$

Therefore:

$$\alpha d = 2n \pi$$

$$\alpha = \frac{2n\pi}{d} \tag{4.2.10.24}$$

Thus from equation (4.2.10.21) and (4.2.10.24):

$$E_n = \frac{\hbar^2}{2md^2} n^2 + V_0 \tag{4.2.10.25}$$

This means that the energy is quantized in a superconductivity temperature material.

4.2.11 Complex Quantum Resistance Model:

Plasma equation describes ionized particles in a gaseous or liquid form.

This equation can thus describes the electron motion easily. This is since the electrons be behaves as ionized particles in side matter. For pressure exerted by the gas plasma equation becomes:

$$mn \frac{dv}{dt} = -\nabla P + F \tag{4.2.11.1}$$

But for pressure exerted by the medium on the electron gas, the equation become:

$$mn \frac{dv}{dt} = \nabla P + \nabla F = \nabla P - n \nabla V \quad (4.2.11.2)$$

In one dimensions, the equation becomes:

$$mn \frac{dv}{dx} \frac{dx}{dt} = \frac{d(nkT)}{dx} - \frac{dnV}{dx}$$

$$mn \frac{v dv}{dx} = \frac{d}{dx} [nkT - nV]$$

Where V is the potential for one particle.

$$mn \frac{d \frac{1}{2} v^2}{dx} = \frac{d}{dx} [nkT - nV]$$

Thus in integrating both sides by assuming n to be constant, or in- dependent of K, yields:

$$\frac{n}{2} m v^2 = nkT - nV + c$$

$$\frac{1}{2} m v^2 + V - kT = \frac{c}{n} = \text{constant} = E$$

This constant of motion stands for energy, thus:

$$E = \frac{p^2}{2m} + V - kT \quad (4.2.11.3)$$

Multiplying by, yields:

$$E\psi = \frac{p^2}{2m} \psi + V\psi - kT\psi \quad (4.2.11.4)$$

According to the wave nature of particles:

$$\psi = A e^{\frac{i}{\hbar}(px - Et)}$$

$$i\hbar \frac{\partial \psi}{\partial t} = E\psi$$

$$-\hbar^2 \nabla^2 \psi = p^2 \psi \quad (4.2.11.5)$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi - kT\psi \quad (4.2.11.6)$$

The time in dependent equation becomes:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi - kT\psi = E\psi \quad (4.2.11.7)$$

Consider the case when these electrons wave subjected to constant crystal field V_0 . This assumption is quite natural as far as particles are distributed homogenously. Thus, equation (4.2.11.7) becomes:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V_0\psi - kT\psi = E\psi \quad (4.2.11.8)$$

One can suggest the solution to be:

$$\psi = Ae^{ikx} \quad (4.2.11.9)$$

A direct substitution yields:

$$\left(\frac{\hbar^2}{2m} k^2 + V_0 - kT\right)\psi = E\psi$$

Therefore:

$$K = \frac{\sqrt{2m(E+kT-V_0)}}{\hbar} \quad (4.2.11.10)$$

This wave number K is related to the momentum according to the relation:

$$P = mv = \hbar k = \sqrt{2m(E + KT - V_0)} \quad (4.2.11.11)$$

This relation can be used to find the quantum resistance R of a certain material. According to classical laws:

$$R = \frac{V}{I} \quad (4.2.11.12)$$

For electrons accelerated by the potential. The wave done is related to the potential V and kinetic energy K according to the relation:

$$K = V = 1/2 mv^2 \quad (4.2.11.13)$$

But since the current I is gives by:

$$I = nev A \quad (4.2.11.14)$$

$$R = \frac{mv^2}{2nevA} = \frac{mv}{2neA} = \frac{P}{2neA} \quad (4.2.11.15)$$

From (4.2.11.11) and (4.2.11.15):

$$R = \frac{\sqrt{2m(E+kT-V_0)}}{2neA} \quad (4.2.11.16)$$

Splitting R to real part R_s and imaginary part R_i :

$$R = R_s + R_i \quad (4.2.11.17)$$

According to equation (4.2.11.16) R becomes pure imaginary, when:

$$E + kT - V_0 < 0$$

$$kT < V_0 - E$$

$$T < (V_0 - E)/K \quad (4.2.11.18)$$

Thus the critical temperature is given by:

$$T_c = \frac{V_0 - E}{K}$$

Which requires:

$$V_0 > E \quad (4.2.11.19)$$

In this case (see equation (4.2.11.17)):

$$R = jR_i$$

$$R_s = 0 \quad (4.2.11.20)$$

Thus the superconductivity resistance R_s becomes zero beyond a certain critical temperature given by equation (4.2.11.17). Which requires binding energy to dominate.

Another direct approach can also be found by considering the pressure exerted by the electrons. In this case the Hamiltonian becomes:

$$\hat{H} = \frac{\hat{p}^2}{2m} + kT + V \quad (4.2.11.21)$$

For spin repulsive force:

$$V = -V_0$$

Thus:

$$\hat{H} = \frac{\hat{p}^2}{2m} + kT - V_0 \quad (4.2.11.22)$$

Thus the average energy which is equal to the classical energy is given by:

$$\langle \hat{H} \rangle = \langle \hat{p}^2 / 2m \rangle + kT - V_0 = E_0 + kT - V_0 \quad (4.2.11.23)$$

Using the quantum definition of R :

$$R = \frac{\langle \hat{H} \rangle}{I} = \frac{E_0 + kT - V_0}{I} \quad (4.2.11.24)$$

Where one splits R to positive and negative one.

When:

$$E_0 + kT - V_0 < 0 \quad (4.2.11.25)$$

$$R_- = \frac{E_0 + kT - V_0}{I}, \quad R_+ = 0 \quad (4.2.11.26)$$

From equations (4.2.11. 25) and (4.2.11.26) the super conductivity resistance R_s Vanishes i.e.:

$$R_+ = R_s = 0$$

When:

$$kT < V_0 - E_0$$

$$T < \frac{V_0 - E_0}{K} \quad (4.2.11.27)$$

Thus the critical temperature is given by:

$$T_C = \frac{V_0 - E_0}{K} \quad (4.2.11.28)$$

Again for T_c to be positive $V_0 > E_0$

Thus for:

$$T < T_c$$

$$R_{sc} = R_+ = 0$$

4.3 Discussion:

According to equation (4.2.9.1) the energy wave function is affected by perturbed potential only. This is similar to that happens for time dependent perturbation ordinary equation. The harmonic oscillator solution in section (4.2.9) shows according to equation (4.2.9.10) that electrons travel in the whole superconductivity. This agrees with cooper pair model. However when the atoms vibrate due to effect of two sources the electrons are localized and move by hopping to adjacent atoms only [see equations (4.2.10.16), (4.2.10.17), (4.2.10.18), (4.2.10.19)].

For spatial dependent energy wave function and by considering electrons hope only to adjacent atoms, one can consider electrons as particle in a box. The solution (4.2.10.13) indicates that the electrons are highly localized thus hope only to adjacent atoms. The temperature dependent Schrodinger equation shows that T_c in equation(4.2.10.18) to be dependent on binding energy V_0 .

However equation (4.2.10.20) predicts standing wave solution. Thus the particles are localized at:

$$x = \frac{(n + \frac{1}{2})}{\alpha}$$

The energy is shown to be quantized [see equation (4.2.10.25)]. Since one assume that:

$$C_n(x = a) = 0$$

This confirms that the electrons are localized and hope only to adjacent atoms.

Using plasma equation (4.2.11.1) a useful energy expression containing thermal energy is found in equation (4.2.11.3). Assuming electrons are free. Free wave solution is given by equation (4.2.11.9). This gives quantum momentum relation in equation (4.2.11.11). This relation is used in quantum resistances R . Expression (4.2.11.17) which splits R to real and imaginary part. Thus one gets condition for zero resistance in equations (4.2.11.18) and (4.2.11.19). This happens beyond a critical temperature given by equation (4.2.11.19). This critical temperature T_c requires binding energy domination, which means that condition takes place by hopping. Another quantum resistance expression, which splits R to positive and negative terms is also proposed in equation (4.2.11.24). The superconductivity positive resistance vanishes beyond critical temperature given by equation (4.2.11.27). Again this T_c requires binding energy domination and hopping mechanism.

3.5 Conclusion:

The solution of Schrodinger equation by using energy approach suggests that the electrons in most cases conduct by hopping mechanism. Another solution shows electrons can move as a travelling wave, which agrees with Cooper-pairs model.

The solution of temperature dependent Schrodinger equation explains easily while the Sc resistance vanishes beyond a critical temperature.

3.6 Future Work:

The new quantum model need to be used for the following systems and applications:

1. The Super fluidity behavior.
2. Thermodynamic properties of Sc.
3. The behavior of nano material.

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