6th Semester Project

Project Report

PATH INTEGRALS IN ONE-BODY AND MANY-BODY QUANTUM MECHANICS

Submitted By:

Bineet Kumar Dash

Roll No:1411025

School of Physical Sciences, NISER

Guided by: Dr. Anamitra Mukherjee

April 22, 2017

Acknowledgments

First and foremost, I would like to thank the School of Physical Sciences, NISER for a wonderful academic programme and the opportunity to work on a semester project. I am highly grateful to my guide Dr. Anamitra Mukherjee for having accepted me as a project student, guiding me through the project and providing me much needed help at many points of time. Also I am thankful to Chairperson Dr. Bedangadas Mohanty, for the valuable advice at the beginning of the project regarding research and our careers.

I am also very thankful to my classmates for their support, in particular, for several highly fruitful brainstorming sessions. Finally and customarily I must thank my family for their well-wishes and support.

Abstract

In this project, we begin with a overview of different kinds of path integrals and their application in one-body quantum mechanics, in particular, the equation of motion for low-energy electrons in Lowest Landau Level has been derived using path integral formalism. Especially we have explored the relation between quantum statistical mechanics and path integral in Euclidean coordinates. After a brief review of *ab-initio* mean field approximations such as Hartree-Fock method, we have used stationary phase approximation to extract the mean field Hamiltonian for Hubbard model from path integrals and shown its superiority over ab-initio formalisms with self-consistent calculation. Finally we have explored a framework, called Perturbed Static Path Approximation (PSPA) to improve the mean field results by introducing time-dependent fluctuations through auxiliary fields obtained from Hubbard Stratonovich transformation.

Contents

Chapter 1

Path Integrals

1.1 Introduction

Quantum mechanics was brought forth in the early 1900's by Max Planck's solution to Black Body radiation and A. Einstein's *annus mirabilis* paper that explained the photoelectric effect. The seminal works by Erwin Schroedinger and Werner Heisenberg in 1920s profoundly reconceived quantum mechanics by formulating the wave mechanics and matrix mechanics. Further foundations and application of quantum mechanics were contributed by Louis de Broglie, Wolfgang Pauli, Max Born, Niels Bohr, Enrico Fermi and so on. In 1930's P.A.M Dirac unified the formulations due to Heisenberg and Schroedinger, and further developments of operator theory by David Hilbert and John von Neumann formalized the mathematical basis of quantum mechanics.

In 1933, Dirac made the observation that the action plays a central role in classical mechanics unlike quantum mechanics as it was known at the time. His speculation on rectifying the situation was to introduce a quantity in quantum mechanics that corresponds to $\exp(iS/\hbar)$, where $S =$ the classical action evaluated along the classical path.

In 1948, Feynman developed on Diracs suggestion, and succeeded in deriving a third formulation of quantum mechanics, based on the fact that the propagator can be written as a sum over all possible paths connecting the initial and final points. Each path contributes $\exp(iS/\hbar)$ to the propagator. Feynman's formalism, called Path Integral formalism implies that quantum particle takes all possible paths, and the amplitudes for each path add according to the usual quantum mechanical rule for combining amplitudes.

1.2 Path Integral for free particle

Given a Hamiltonian, we can derive its propagator as a path-integral. Application of resolution of identity at different places and in different bases can result in many types of path integral, e.g. configuration space path integral, phase path integral etc.

For configuration space path integral, the propagator $U(x_N, t_N; x_0, t_0)$ is

$$U(x_N, t_N; x_0, t_0) = \int_{x_0}^{x_N} e^{iS[x(t)]/\hbar} \mathcal{D}[x(t)] \tag{1.1}$$

where, $x(t)$ = the path followed by particle when going from x_0 to x_N
$\mathcal{D}[x(t)]$ = measure for integration over all possible paths from x_N to x_0.
$S[x(t)]$ = classical action for following the path $x(t)$

The time span to cover the path can be sliced into N time slices, such that the possible values of $x(t)$ for time $t_1, t_2, \ldots, t_n$ can be from $-\infty$ to ∞. For large N, the particle is assumed to follow classical path for free particle,so that it has a constant velocity. Then the classical action can be expressed in terms of Riemann sum as:

$$S[x(t)] = \int_{t_0}^{t_N} \mathcal{L}(t)dt = \int_{t_0}^{t_N} \frac{1}{2}m\dot{x}^2 dt = \sum_{i=0}^{N-1} \frac{m}{2}\left(\frac{x_{i+1}-x_i}{\epsilon}\right)^2 \epsilon \qquad (1.2)$$

where, $t_0, t_1, \ldots, t_n$= the mesh for Riemann sum over dt
and $x_i = x(t_i)$

With A as normalization constant, the propagator can be evaluated as:

$$\begin{aligned} U(x_N, t_N; x_0, t_0) &= \int_{x_0}^{x_N} e^{iS[x(t)]/\hbar}\mathcal{D}[x(t)] \\ &= \lim_{\substack{N\to\infty \\ \epsilon\to 0}} A\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\left[\frac{1}{\hbar}\frac{m}{2}\sum_{i=0}^{N-1}\frac{(x_{i+1}-x_i)^2}{\epsilon}\right] dx_1 \ldots dx_{N-1} \end{aligned}$$

Changing the variables to $y_i = \left(\frac{m}{2\hbar\epsilon}\right)^{1/2} x$, the propagator becomes

$$U(x_N, t_N; x_0, t_0) = \lim_{\substack{N\to\infty \\ \epsilon\to 0}} A'\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\left[\sum_{i=0}^{N-1}\frac{(y_{i+1}-y_i)^2}{i}\right] dy_1 \ldots dy_{N-1}$$

The multiple integration is carried out by integrating from y_1 to y_n. The integration for y_1 is:

$$\begin{aligned} I_1 = \int_{-\infty}^{\infty} \exp\left[i\{(y_2-y_1)^2 + (y_1-y_0)^2\}\right] &= e^{\frac{i(y_2-y_0)^2}{2}} \int_{-\infty}^{\infty} e^{-\left(\sqrt{-2i}y_1 - \frac{y_0+y_2}{\sqrt{2i}}\right)^2} dy_1 \\ &= e^{\frac{i(y_2-y_0)^2}{2}} \times \sqrt{2i}\frac{\sqrt{\pi}}{2} = \left(\frac{i\pi}{2}\right)^{\frac{1}{2}} e^{\frac{i(y_2-y_0)^2}{2}} \end{aligned}$$

Then moving on to the integration of y_2:

$$\begin{aligned} I_2 &= \left(\frac{i\pi}{2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp[i\{2(y_3-y_2)^2 + (y_2-y_0)^2\}]dy_2 = \left(\frac{i\pi}{2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp[i\{2(y_3-y_2)^2 + (y_2-y_0)^2\}]dy_2 \\ &= \left(\frac{i\pi}{2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left[\frac{i}{2}(2y_3^2 + y_0^2 + 3y_2^2 - 2y_2(y_0+2y_3))\right] dy_2 = = \left(\frac{i\pi}{2}\right)^{\frac{1}{2}} \left(\frac{2\pi i}{3}\right)^{\frac{1}{2}} e^{-\frac{(y_3-y_0)^2}{3i}} \\ &= \left(\frac{(i\pi)^2}{3}\right)^{\frac{1}{2}} e^{-\frac{(y_3-y_0)^2}{3i}} \end{aligned}$$

Carrying out the integration recursively, by induction we have

$$I_N = \frac{(i\pi)^{(N-1)/2}}{N^{1/2}} e^{-\frac{(y_N - y_0)^2}{N i}}$$

Changing the variable back to x_i, and normalization constant to A:

$$U = A \left(\frac{2\pi\hbar\epsilon i}{m} \right)^{N/2} \left(\frac{m}{2\pi\hbar i N\epsilon} \right)^{1/2} \exp\left[\frac{im(x_N - x_0)^2}{2\hbar N\epsilon} \right]$$

Taking normalization constant to be $A = \left(\frac{2\pi\hbar\epsilon i}{m}\right)^{-N/2}$, $\epsilon \to 0$ and $N\epsilon \to t_N - t_0$:

$$U(x_N, t_N; x_0, t_0) = \left(\frac{m}{2\pi\hbar i N\epsilon} \right)^{1/2} \exp\left[\frac{im(x_N - x_0)^2}{2\hbar(t_N - t_0)} \right] \tag{1.3}$$

The normalization constant can be incorporated into the measure of the integration by defining [4]:

$$\mathcal{D}[x(t)] = \lim_{\substack{N\to\infty \\ \epsilon\to 0}} \frac{1}{B} \frac{dx_1}{B} \cdots \frac{dx_{N-1}}{B} \qquad \text{where, } B = \left(\frac{2\pi\hbar\epsilon i}{m} \right)^{1/2} \tag{1.4}$$

1.2.1 Time Evolution in Path Integral Formalism

In path-integral formalism, time evolution over an infinitesimal time interval ϵ is given as:

$$\psi(x, \epsilon) = \int_{-\infty}^{\infty} U(x, \epsilon; x')\psi(x', 0)dx' \tag{1.5}$$

It can be shown that this is consistent with the time evolution prescribed by Schroedinger's equation, i.e.

$$\psi(x, \epsilon) - \psi(x, 0) = \frac{-i\epsilon}{\hbar} \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, 0) \right] \psi(x, 0)$$

1.3 Configuration Space Path Integral

For a time-independent Hamiltonian $H = \frac{P^2}{2m} + V(x)$, the propagator is defined as:

$$U(x,t;x',0) = U(x,x',t) = \langle x| \exp\left(-\frac{i}{\hbar}Ht\right)|x'\rangle \tag{1.6}$$

Since P^2 and $V(x)$ do not commute, the exponential sum is not separable, so we resort to infinitesimal time evolution.

$$U(x,x',t) = \langle x| \left[\exp\left(-\frac{i}{\hbar}\frac{t}{N}H\right)\right]^N |x'\rangle = \langle x| \left[\exp\left(-\frac{i\epsilon}{\hbar}\left(\frac{P^2}{2m} + V(x)\right)\right)\right]^N |x'\rangle$$

where, $\epsilon = \frac{t}{N}$ and $N \to \infty$ so that $\epsilon \to 0$.

In first order approximation, for any two operators $\hat{A}$ and $\hat{B}$,

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]} \approxeq e^{\hat{A}+\hat{B}} \tag{1.7}$$

Therefore in the limit of $\epsilon \to 0$,

$$\exp\left(-\frac{i\epsilon}{\hbar}\left(\frac{P^2}{2m} + V(x)\right)\right) \approx \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right)\exp\left(-\frac{i\epsilon}{\hbar}V(x)\right)$$

$$\therefore U(x_N,x_0,t) = \langle x_N| \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right)\exp\left(-\frac{i\epsilon}{\hbar}V(x)\right)^{\text{N times}}_{\cdots\cdots}\exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right)\exp\left(-\frac{i\epsilon}{\hbar}V(x)\right)|x_0\rangle$$

Introducing resolution of identity as $I = \int_{-\infty}^{\infty} dx\,|x\rangle\langle x|$ between each instance of $\exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right)\exp\left(-\frac{i\epsilon}{\hbar}V(x)\right)$,

$$U(x_N,x_0,t) = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dx_1\ldots dx_{N-1}\,\langle x_N| \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right)\exp\left(-\frac{i\epsilon}{\hbar}V(x)\right)|x_{N-1}\rangle\ldots$$
$$\ldots\langle x_1| \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right)\exp\left(-\frac{i\epsilon}{\hbar}V(x)\right)|x_0\rangle$$

Each instance of the inner product can be evaluated as:

$$\langle x_N| \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right) \exp\left(-\frac{i\epsilon}{\hbar}V(x)\right) |x_{N-1}\rangle = \langle x_N| \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right) |x_{N-1}\rangle \exp\left(-\frac{i\epsilon}{\hbar}V(x_{N-1})\right)$$

$$\begin{aligned}\langle x_N| \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right) |x_{N-1}\rangle &= \int_{-\infty}^{\infty} \langle x|p\rangle \langle p|x'\rangle \, e^{-ip^2\epsilon/2m\hbar} dp \\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-x')/\hbar}.e^{-ip^2\epsilon/2m\hbar} dp \\ &= \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{1/2} e^{im(x-x')^2/2\hbar\epsilon}\end{aligned}$$

Therefore,

$$\langle x_N| \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right) \exp\left(-\frac{i\epsilon}{\hbar}V(x)\right) |x_{N-1}\rangle = \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{1/2} \exp\left[\frac{im(x-x')^2}{2\hbar\epsilon}\right] \exp\left[-\frac{i\epsilon}{\hbar}V(x_{N-1})\right]$$

The propagator thus can be expressed as:

$$U(x_N, x_0, t) = \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{1/2} \int \prod_{n=1}^{N-1} \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{1/2} dx_n \exp\left[\sum_{n=0}^{N-1} \frac{im(x_n - x_{n-1})^2}{2\hbar\epsilon} - \frac{i\epsilon}{\hbar}V(x_{n-1})\right] \tag{1.8}$$

In continuum notation, under the assumption of classical path with constant velocity for a time-slice of ϵ,

$$\begin{aligned}\exp\left[\sum_{n=0}^{N-1} \frac{im(x_n - x_{n-1})^2}{2\hbar\epsilon} - \frac{i\epsilon}{\hbar}V(x_{n-1})\right] &= \exp\frac{i\epsilon}{\hbar}\sum_{n=0}^{N-1}\left[\frac{m(x_n - x_{n-1})^2}{2\epsilon^2} - V(x_{n-1})\right] \\ &= \exp\frac{i}{\hbar}\epsilon\sum_{n=0}^{N-1}\left[\frac{1}{2}m\dot{x}^2 - V(x_{n-1})\right] = \exp\left[\frac{i}{\hbar}\int_0^t \mathcal{L}(x,\dot{x})dt\right]\end{aligned}$$

From the definition of the measure for the integration (Equation-1.4),

$$U(x, x', t) = \int [\mathcal{D}x] \exp\left[\frac{i}{\hbar}\int_0^t \mathcal{L}(x,\dot{x})dt\right] \tag{1.9}$$

1.4 Phase Space Path Integral

The propagator derived previously is evaluated on all possible paths in configuration space, as reflected in the measure $\mathcal{D}[x]$. For taking all the connecting paths in phase space, we need to perform phase space path integral. This is achieved by introducing another resolution of identity:

$$I = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} |p\rangle \langle p|$$

Under the resolution in both $|x\rangle$ and $|p\rangle$ basis,

$$U(x_N, x_0, t) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{n=1}^{N} dx_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \langle x_N | \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right) |p_N\rangle \langle p_N | \exp\left(-\frac{i\epsilon}{\hbar}V(x)\right) |x_{N-1}\rangle \dots$$
$$\dots \langle x_1 | \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right) |p_1\rangle \langle p_1 | \exp\left(-\frac{i\epsilon}{\hbar}V(x)\right) |x_0\rangle$$

$$\begin{aligned}
&\langle x_N | \exp\left(-\frac{i\epsilon}{2m\hbar}P^2\right) |p_N\rangle \langle p_N | \exp\left(-\frac{i\epsilon}{\hbar}V(x)\right) |x_{N-1}\rangle \\
&= \exp\left(-\frac{i\epsilon}{2m\hbar}p_N^2\right) \langle x_N | p_N\rangle \exp\left(-\frac{i\epsilon}{\hbar}V(x_{N-1})\right) \langle p_N | x_{N-1}\rangle \\
&= \exp\left[-\frac{i\epsilon}{2m\hbar}p_N^2 - \frac{i\epsilon}{\hbar}V(x_{N-1}) + \frac{ix_N p_N}{\hbar} - \frac{ip_{N-1}x_N}{\hbar}\right]
\end{aligned}$$

Collecting all such $(2N-1)$ instances,

$$U(x, x', t) = \int [\mathcal{D}p\mathcal{D}x] \exp\left[\sum_{n=0}^{N}\left(-\frac{i\epsilon}{2m\hbar}p_n^2 - \frac{i\epsilon}{\hbar}V(x_{n-1}) + \frac{ix_n p_n}{\hbar} - \frac{ix_{n-1}p_n}{\hbar}\right)\right]$$

In continuum notation,

$$\begin{aligned}
U(x, x', t) &= \int [\mathcal{D}p\mathcal{D}x] \exp\left[\frac{i}{\hbar}\epsilon \sum_{n=0}^{N}\left(-\left(\frac{1}{2m}p_n^2 + V(x_{n-1})\right) + p_n\left(\frac{x_n - x_{n-1}}{\epsilon}\right)\right)\right] \\
&= \int [\mathcal{D}p\mathcal{D}x] \exp\left[\frac{i}{\hbar}\int_0^t [p\dot{x} - \mathcal{H}(x,p)]dt\right]
\end{aligned} \tag{1.10}$$

1.5 Imaginary Time Path Integral

In imaginary time, we set $\tau = it$, therefore the Minkowski metric changes to $ds^2 = c^2 d\tau^2 + dx^2 + dy^2 + dz^2$. So the spacetime coordinates in imaginary time are called Euclidean Coordinates. The propagator for imaginary time is:

$$U(\tau) = \exp\left(-\frac{1}{\hbar} H\tau\right) \tag{1.11}$$

This satisfies the Schrodingers equation in imaginary time, i.e.

$$-\hbar \frac{d}{d\tau} |\psi(t)\rangle = H |\psi(t)\rangle$$

Therefore the eigenvalues and eigenfunctions for imaginary time Hamiltonian is the same as usual ones. So in terms of eigenfunctions $|n\rangle$, the propagator for imaginary time can be expressed as:

$$U(\tau) = \sum |n\rangle \langle n| \exp\left(-\frac{1}{\hbar} H\tau\right) \tag{1.12}$$

Since $U(\tau)$ is Hermitian, but not unitary it does not preserve the norm of the state. As $\tau \to \infty$, every state under the action of $U(\tau)$ evolves into the ground state $|0\rangle$. As shown in the following derivation, any state not orthonormal to ground state at $\tau = 0$ evolves into ground state over time.

$$\begin{aligned}
\lim_{\tau\to\infty} \langle x|U(\tau)|x'\rangle &= \lim_{\tau\to\infty} \sum \langle x|n\rangle \langle n|x'\rangle \exp\left(-\frac{1}{\hbar} E_n \tau\right) \\
&\approx \langle x|0\rangle \langle 0|x'\rangle \exp\left(-\frac{1}{\hbar} E_n \tau\right) \lim_{\tau\to\infty} \exp\left(-\frac{1}{\hbar} E_n \tau\right) \\
&= \psi_0(x)\psi_0(x')
\end{aligned}$$

To evaluate path integral in imaginary time, we need to evaluate the matrix element $U(x, x', t) = \langle x|U(\tau)|x'\rangle$. In imaginary time, the Lagrangian (Euclidean

Lagrangian) is given as:

$$\mathcal{L}_E = \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x) \tag{1.13}$$

The particle in imaginary time obeys Euclidean equation of motions and experiences a potential inverted with respect to the usual one. The imaginary time configuration space path integral can be derived similarly using Euclidean Lagrangian as:

$$U(\tau) = \sum |n\rangle \langle n| \exp\left(-\frac{1}{\hbar}H\tau\right) = \int [\mathcal{D}x] \exp\left[-\frac{1}{\hbar}\int_0^t \mathcal{L}_E(x,\dot{x})d\tau\right] \tag{1.14}$$

The imaginary time propagator can be analytically continued to obtain the usual propagator by setting $\tau = it$. The farther a path is from classical static path, the higher is its action, which is the argument of the exponential summed over in the path integral. The exponential factor ensures that rapidly varying (higher argument) nullifies on integration. So paths closer to classical path have higher contribution.

1.5.1 Path Integrals and Quantum Statistical Mechanics

The Euclidean coordinates used in imaginary time propagator can be exploited to derive the partition function for a quantum system. In terms of the eigenfunction of the Hamiltonian (with eigenvalues E_n), temperature T and Boltzmann's constant k, the partition function is defined as:

$$Z = \sum_n e^{-\beta E_n} = \text{Tr } e^{-\beta H}$$

Since trace is invariant with any change of basis, the trace can be evaluated in position basis as:

$$Z = \int_{-\infty}^{\infty} \langle x|e^{-\beta H}|x\rangle \, dx = \int_{-\infty}^{\infty} \exp\left(-\frac{1}{\hbar}\beta\hbar H\right) dx = U(x,x,\beta\hbar) \tag{1.15}$$

Thus the partition function of a system is the integral of the amplitude to go from and return to a point x in imaginary time $\tau = \beta\hbar$ over all possible position.

1.6 Application of Path Integral Formalism (to Landau Levels)

Path integrals is utilized in numerous cases of many-body physics, statistical mechanics, quantum field theory and so on. The kind of path integral chosen depends on the ease of resolution of identity operator in each case. Here we will find the equation of motion for electrons in magnetic field.

Consider an electron moving in $X-Y$ plane with uniform magnetic field B along Z direction. Using Gauge freedom, we choose the symmetric gauge of the vector potential so that

$$\overrightarrow{A} = \frac{B}{2}(-y\hat{i} + x\hat{j}) \tag{1.16}$$

The electromagnetic Hamiltonian for this system is

$$H = \frac{(p_x + \frac{qyB}{2c})^2}{2m} + \frac{(p_y - \frac{qxB}{2c})^2}{2m} = \frac{\Pi^2}{2m} + \frac{1}{2}m\left(\frac{qB}{mc}\right)^2 Q^2 \tag{1.17}$$

where $\Pi = p_y - \frac{eA_y}{c} = p_y - \frac{qxB}{2c}$ and $Q = \frac{c}{qB}\left(p_x + \frac{qyB}{2c}\right)$ are canonically transformed momentum and coordinate such that $[Q, \Pi] = i\hbar$. Therefore equation-1.17 suggests an analogous Harmonic Oscillator problem with $\omega = \frac{qB}{mc}$. The energy levels of the system is called Landau Levels. However the other pair of canonical momentum and coordinates $Q' = p_y + \frac{qxB}{2c}$ and $\Pi' = \frac{c}{qB}\left(p_x - \frac{qyB}{2c}\right)$ are cyclic coordinates as they commute with Π and Q but do not appear in the H. So the Landau levels are infinitely degenerate.

From the heuristic picture of Landau quantization, the energy of the Lowest Landau Level (LLL) $\approx \frac{\hbar qB}{mc}$. So a two dimensional electron gas in EM field, where spin is fixed along applied field (normal to the plane) and therefore

the spatial wavefunction suffices, we consider the case where electron-electron interaction is negligible compared to the interaction with the external potential $V(x,y)$. For interactions with scale smaller than $\frac{\hbar qB}{mc}$ at low temperature, the state of the system lies in the Hilbert space restricted to the LLL. For this system, path integral formalism gives the equation of motions with ease. Since the electron-electron interaction is negligible, electrons in the system can be considered independent and hence functional integral can be written for each electrons. The Lagrangian and action for the electron is:

$$\mathcal{L}(x,\dot{x},t) = \frac{1}{2}m\left(\dot{x}^2+\dot{y}^2\right) + \left(V(x,y) - \frac{q\overrightarrow{A}.\overrightarrow{v}}{c}\right) \tag{1.18}$$

$$\implies S = \int\left[\frac{1}{2}m\left(\dot{x}^2+\dot{y}^2\right) + \frac{eB}{2c}(-y\dot{x}+x\dot{y}) - V(x,y)\right]dt \tag{1.19}$$

As the energy lower than LLL, and higher levels do not contribute, the energy gap $\frac{\hbar qB}{mc}$ must be high, which translates to $m \to 0$, so kinetic energy is negligible.

$$\begin{aligned} S &= \frac{eB}{2c}\left[-\int(y\dot{x})dt + \int(x\dot{y})dt\right] + \int V(x,y)dt \\ &= \frac{eB}{2c}\left[-y\int(\dot{x})dt + \int\dot{y}dt(\int(\dot{x})dt)dt + \int(x\dot{y})dt\right] + \int V(x,y)dt \\ &= \frac{eB}{2c}\left[-xy + 2\int(x\dot{y})dt\right] + \int V(x,y)dt \\ \implies S_{LLL} &= \int\left(\frac{eB}{c}x\dot{y} + V(x,y)\right)dt \end{aligned} \tag{1.20}$$

So the configuration space path integral is [6] :

$$U(x,x',t) = \int[\mathcal{D}x]\exp\left[\frac{i}{\hbar}\int\left(\frac{eB}{c}x\dot{y} + V(x,y)\right)dt\right] \tag{1.21}$$

Interestingly this configuration space path integral is the phase space path integral for canonically conjugate variables y and $\bar{y} = \frac{eB}{c}x$, with $\mathcal{L} = V(x,y)$. So in this semiclassical limit, the orbits obey Hamilton's equation, i.e.

$$\dot{y} = \frac{\partial V}{\partial\bar{y}} = \frac{c}{eB}\frac{\partial V}{\partial x} \qquad \dot{\bar{y}} = -\frac{\partial V}{\partial y} \text{ or } \dot{x} = -\frac{c}{eB}\frac{\partial V}{\partial y} \tag{1.22}$$

Chapter 2

Mean Field Theory

Principles of statistical mechanics become excruciatingly complicated in interacting systems containing a large number of particles, in which case the motions of the particles become correlated. When the correlation is not very high, it suffices to include the average correlation, i.e. the the interaction of other particles being included as a mean-field, thus reducing the system to an effective one body problem. This approximation discards small time-dependent fluctuations of interactions, hence observables about the corresponding mean values. This approach is called Mean Field theory.

2.1 Mathematical Structure

For a system with two different types of particles, described by operators a_ν and b_μ, consider that only the interparticle interaction between the different kinds are significant. Then the Hamiltonian is given as:

$$H = \sum_\nu \zeta_\nu^a a_\nu^\dagger a_\nu + \sum_\mu \zeta_\mu^b b_\mu^\dagger b_\mu + \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} a_\nu^\dagger b_\mu^\dagger b_{\mu'} a_{\nu'}$$

Here the interaction is given by:

$$V_{int} = \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} a^\dagger_\nu b^\dagger_\mu b_{\mu'} a_{\nu'}$$

Here if the density operator $a^\dagger_\nu a_\nu$ and $b^\dagger_\mu b_\mu$ do not have high deviations from their mean values, then we can expand them about the mean values using the deviation operators.

$$d_{\nu\nu'} = a^\dagger_\nu a_\nu - \langle a^\dagger_\nu a_\nu \rangle \tag{2.1}$$

$$e_{\mu\mu'} = b^\dagger_\mu b_\mu - \langle b^\dagger_\mu b_\mu \rangle \tag{2.2}$$

Using the expansion in the Hamiltonian,

$$H = H_0 + \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} (a^\dagger_\nu a_\nu \langle b^\dagger_\mu b_\mu \rangle + b^\dagger_\mu b_\mu \langle a^\dagger_\nu a_\nu \rangle) - \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} \langle a^\dagger_\nu a_\nu \rangle \langle b^\dagger_\mu b_\mu \rangle + \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} d_{\nu\nu'} e_{\mu\mu'} \tag{2.3}$$

$$\text{where, } H_0 = \sum_\nu \zeta^a_\nu a^\dagger_\nu a_\nu + \sum_\mu \zeta^b_\mu b^\dagger_\mu b_\mu$$

Considering the deviations to be small, the second-order term $\sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} d_{\nu\nu'} e_{\mu\mu'}$ is ignored. By defining the mean-field interaction as:

$$V_{MF} = \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} (a^\dagger_\nu a_\nu \langle b^\dagger_\mu b_\mu \rangle + b^\dagger_\mu b_\mu \langle a^\dagger_\nu a_\nu \rangle) - \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} \langle a^\dagger_\nu a_\nu \rangle \langle b^\dagger_\mu b_\mu \rangle \tag{2.4}$$

the mean-field Hamiltonian is then defined as:

$$H_{MF} = H_0 + V_{MF}$$

H_{MF} now contains only single-body operators, hence a soluble problem, in principle. As suggested by equations- , if the interaction term is product of two operators ($H_{AB} = AB$), the mean-field approximation can be generalized as [2]

$$H_{MF} = A \langle B \rangle + \langle A \rangle B - \langle A \rangle \langle B \rangle \tag{2.5}$$

2.2 Self-Consistency Formula

The solution to one-body H_{MF} can be obtained only when the scalars $\bar{n}^a_{\nu\nu'} = \langle a^\dagger_\nu a_\nu \rangle$ and $\bar{n}^b_{\mu\mu'} = \langle b^\dagger_\mu b_\mu \rangle$ are known quantities. Due to thermodynamic consideration, the $n_{\nu\nu'}$ is chosen which minimizes the free-energy for mean-field Hamiltonian.

$$\begin{aligned}
\frac{d}{d\bar{n}^a_{\nu\nu'}} F_{MF} &= \frac{d}{d\bar{n}^a_{\nu\nu'}} \left(-\frac{1}{\beta} \ln Z_{MF} \right) = 0 \\
&\implies \frac{1}{Z_{MF}} Tr \left[e^{-\beta H_{MF}} \frac{d}{d\bar{n}^a_{\nu\nu'}} H_{MF} \right] = 0 \\
&\implies \frac{1}{Z_{MF}} Tr \left[e^{-\beta H_{MF}} \sum_{\mu\mu'} V_{\nu\mu,\nu'\mu'} (\langle b^\dagger_\mu b_\mu \rangle - \bar{n}^b_{\mu\mu'}) \right] = 0 \\
&\implies \sum_{\mu\mu'} V_{\nu\mu,\nu'\mu'} (\langle b^\dagger_\mu b_\mu \rangle_{MF} - \bar{n}^b_{\mu\mu'}) = 0
\end{aligned}$$

Since (ν, ν') is arbitrary, $\langle b^\dagger_\mu b_\mu \rangle_{MF} - \bar{n}^b_{\mu\mu'}$ must vanish. Following the same logic with $\bar{n}^a_{\nu\nu'}$,

$$\bar{n}^b_{\mu\mu'} = \langle b^\dagger_\mu b_\mu \rangle_{MF} = \frac{\mathrm{Tr}\left[e^{-\beta H_{MF}} a^\dagger_\nu a_\nu \right]}{\mathrm{Tr}\left[e^{-\beta H_{MF}} \right]} \tag{2.6}$$

$$\bar{n}^a_{\nu\nu'} = \langle a^\dagger_\mu a_\mu \rangle_{MF} = \frac{\mathrm{Tr}\left[e^{-\beta H_{MF}} b^\dagger_\mu b_\mu \right]}{\mathrm{Tr}\left[e^{-\beta H_{MF}} \right]} \tag{2.7}$$

These equations are called self-consistency equations as $\bar{n}^a_{\nu\nu'}$ and $\bar{n}^b_{\mu\mu'}$ depend on H_{MF} and Z_{MF}, which in turn depends on $\bar{n}^a_{\nu\nu'}$ and $\bar{n}^b_{\mu\mu'}$. The process is realized by choosing proper initial values and applying the equations recursively to obtain better approximations for $\bar{n}^a_{\nu\nu'}$ and $\bar{n}^b_{\mu\mu'}$.

The applicability of mean field approximation and the convergence of self-consistency formula relies on small deviation of interacting operators from their mean values. If the deviation is high, other mean-field parameters may be chosen or else the framework can not adopted.

2.3 Hartree-Fock Approximation

The previous discourse included two different kind of particles interacting in a system. For a system with identical interacting particles, more terms emerge in the interaction. The general scheme for applying mean-field theory in those cases is called Hartree-Fock approximation.

For a weakly interacting system of identical fermions, the Hamiltonian is given by

$$H = \sum_{\nu} \xi_{\nu} {c_{\nu}}^{\dagger} c_{\nu} + \frac{1}{2} \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} {c_{\nu}}^{\dagger} {c_{\mu}}^{\dagger} c_{\mu'} c_{\nu'} \tag{2.8}$$

Assuming the interaction is weak, Wick's theorem can be applied to resolve $\langle {c_{\nu}}^{\dagger} {c_{\mu}}^{\dagger} c_{\mu'} c_{\nu'} \rangle$ into two-term averages as follows (negative sign introduced for odd permutation of fermionic creation/annihilation operator)

$$\langle {c_{\nu}}^{\dagger} {c_{\mu}}^{\dagger} c_{\mu'} c_{\nu'} \rangle_{MF} = \langle {c_{\nu}}^{\dagger} c_{\nu'} \rangle_{MF} \langle {c_{\mu}}^{\dagger} c_{\mu'} \rangle_{MF} - \langle {c_{\nu}}^{\dagger} c_{\mu'} \rangle_{MF} \langle {c_{\mu}}^{\dagger} c_{\nu'} \rangle_{MF} \tag{2.9}$$

The mean-field approximation also satisfies Pauli-exclusion principle as $\nu = \nu'$ and $\mu = \mu'$ implies

$$\langle {c_{\nu}}^{\dagger} {c_{\mu}}^{\dagger} c_{\mu} c_{\nu} \rangle_{MF} = 0$$

In case of identical particles the self-consistency calculation must include the exchange terms which are absent in the interaction of non-identical or distinguishable fermions. So, the mean field approximation here is:

$$\begin{aligned} {c_{\nu}}^{\dagger} {c_{\mu}}^{\dagger} c_{\mu'} c_{\nu'} \approx \quad & {c_{\nu}}^{\dagger} c_{\nu'} \langle {c_{\mu}}^{\dagger} c_{\mu'} \rangle_{MF} + \langle {c_{\nu}}^{\dagger} c_{\nu'} \rangle_{MF} {c_{\mu}}^{\dagger} c_{\mu'} - {c_{\nu}}^{\dagger} c_{\mu'} \langle {c_{\mu}}^{\dagger} c_{\nu'} \rangle_{MF} - \langle {c_{\nu}}^{\dagger} c_{\mu'} \rangle_{MF} {c_{\mu}}^{\dagger} c_{\nu'} \\ & - \langle {c_{\nu}}^{\dagger} c_{\nu'} \rangle_{MF} \langle {c_{\mu}}^{\dagger} c_{\mu'} \rangle_{MF} + \langle {c_{\nu}}^{\dagger} c_{\mu'} \rangle_{MF} \langle {c_{\mu}}^{\dagger} c_{\nu'} \rangle_{MF} \end{aligned} \tag{2.10}$$

Here the first two terms can be identified as the direct interaction and second two terms are the exchange interaction.

Accordingly two mean-field interaction terms can be defined as:

$$V_{\mathrm{MF}}^{\mathrm{Hartree}} = \frac{1}{2}\sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'}\bar{n}_{\mu\mu'}{c_\nu}^\dagger c_{\nu'} + \frac{1}{2}\sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'}\bar{n}_{\nu\nu'}{c_\mu}^\dagger c_{\mu'} - \frac{1}{2}\sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'}\bar{n}_{\mu\mu'}\bar{n}_{\nu\nu'} \tag{2.11}$$

$$V_{\mathrm{MF}}^{\mathrm{Fock}} = \frac{1}{2}\sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'}\bar{n}_{\nu\mu'}{c_\mu}^\dagger c_{\nu'} + \frac{1}{2}\sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'}\bar{n}_{\mu\nu'}{c_\nu}^\dagger c_{\mu'} - \frac{1}{2}\sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'}\bar{n}_{\nu\mu'}\bar{n}_{\mu\nu'} \tag{2.12}$$

So, the mean-field Hamiltonian under Hartree-Fock approximation is given by:

$$H_{MF} = H_0 + V_{\mathrm{MF}}^{\mathrm{Hartree}} + V_{\mathrm{MF}}^{\mathrm{Fock}} \tag{2.13}$$

$$\text{where, } H_0 = \sum_\nu \xi_\nu {c_\nu}^\dagger c_\nu$$

So, Hartree-Fock approximation is a nearly free electron model, which predicts the band theory for crystalline solids. The band theory has successfully classified a number of materials as metals and insulators. However, since it does not include correlation effects and time-dependent fluctuation, certain predictions regarding metal-insulator problem fails when independent electron assumption is used.

A case where correlation effects are important and supersede other effects is Mott transition, which can be treated with the framework of Hubbard Model.

Chapter 3

Mott Transition and Hubbard Model

A material is called an insulator if its static electrical conductivity approaches zero as the temperature is lowered. If the material possesses finite conductivity at that stage, then it is called metallic. For N electrons, nearly free electron model and band theory predicts the $N/2$ lowest-lying band states occupied by two electrons each, and the ground state to be the corresponding Slater's determinant. This description predicts a metal if the density of states at the Fermi level is non-vanishing, i.e. $\rho(\epsilon_F) \neq 0$ If $\rho(\epsilon_F) = 0$, the material must be an insulator.

With the assumption of translational invariance and time-reversal symmtery of the Hamiltonian under periodic potential, band theory necessarily requires an even number of electrons per unit cell to have $\rho(\epsilon_F) = 0$, i.e. an insulator. Otherwise the band is partially filled, resulting in $\rho(\epsilon_F) \neq 0$, i.e. a metal. However this prediction fails spectacularly in many cases, e.g. CoO, an insulator (though, no of electrons per unit cell=9+6=15).

3.1 Failure of Band Theory

The failure of the band theory lies in the exclusion of correlation effect. Correlated systems have non-zero tunneling probability between at least some of the sites. In crystals, this leads to charge fluctuation and spin-pairing as electrons propagate through the lattice. The energy of the various configurations which arises because of the allowed transitions differs from the ground state and band theory or mean-field theories fail when the fluctuation is not negligible.

The competing effects that play role in deciding the Hamiltonian is minimization of kinetic energy and minimization of potential energy. Reduction in kinetic energy requires a more distributed wave function, as Kinetic energy operator $\propto \nabla^2$, resulting in higher value for more localized states. However, the delocalization of electrons in the lattice requires intrasite tunneling leading to higher intraatomic Coulomb energy, thus increasing the potential energy. The optimization for minimal energy configuration is decided by the lattice structures and the nature of valence shells.

The Hamiltonian for a band, according to tight-binding model with nearest neighbour approximation is given by:

$$H_{band} = \sum_{j}\sum_{\sigma} \epsilon_k \hat{n}_{j\sigma} - t\sum_{\langle j,l\rangle}\sum_{\sigma}(c_{j\sigma}{}^{\dagger} c_{l\sigma} + c_{j\sigma} c_{l\sigma}{}^{\dagger}) \tag{3.1}$$

The intraatomic Coulomb energy due to Coulomb repulsion from charge fluctuation is given by in terms of the ground state wavefunction $|\Phi\rangle$ as:

$$U = \int\int dr_1 dr_2 |\Phi(r_1)|^2 \frac{e^2}{|r_1 - r_2|} |\Phi(r_2)|^2 \tag{3.2}$$

U is the most important energy term for a system of interacting electrons moving in a narrow band or more localized orbitals, as $\langle r_1 - r_2\rangle \sim 1\text{A}^\circ$, resulting in very high potential energy.

3.2 Mott Transition

The discourse in the last section indicated that the minimization of kinetic energy is accompanied by charge transfer, which costs potential energy due to Coloumb repulsion. So above a certain critical value of the lattice parameter, the bands are so sufficiently narrow that the energy gain due to charge coupling outweighs the minimization of kinetic energy by electron delocalization. So, The charge fluctuations necessary for metallic conduction are suppressed by the intrasite Coulomb interaction, marking a transition from conducting metallic to an insulating state. These kinds of interaction-induced, collective localization of all the electrons is called Mott transition.

Since the electrons of a Mott insulator try to minimize the Coulomb potential by avoiding each other as much as possible. This is achieved by letting one electron stay per site, as far as possible. Therefore, spatial part of the insulator ground state is highly degenerate ($\sim 2^N$ for N singly occupied sites). This degeneracy is lifted by electron spins and the spin arrangement corresponding to the ground state of the effective spin Hamiltonian acting in the low-energy subspace of the large-U Hubbard model becomes the optimal configuration. Since the insulating state is highly correlated, this results in magnetism of Mott insulators.

Consider a periodic array of Na-atoms (monovalent), only the $3s$ shell of which is considered for analysis. If the number of lattice sites is L, and the Coulomb interaction energy for doubly occupied state is U_{3s} then the energy of the assembly can be expressed as:

$$H_{band} = \epsilon_{3s} \sum_{j} \sum_{\sigma} \hat{n}_{j\sigma} - t_{3s} \sum_{\langle j,l \rangle} \sum_{\sigma} (c_{j\sigma}{}^{\dagger} c_{l\sigma} + c_{j\sigma} c_{l\sigma}{}^{\dagger}) = L(\epsilon_{3s} - \alpha t_{3s}) \quad (3.3)$$

where, α is the lattice parameter. Due to homogeneity of the half-filled band ground state, the probability of occupation of a site by $\uparrow$-electron= the probability of occupation of a site by $\downarrow$-electron= $\frac{1}{2}$. So the probability of a site being doubly

occupied= $\frac{1}{4}$, resulting in potential energy gain of $\frac{LU_{3s}}{4}$. So the total energy density corresponding to the uncorrelated band (Fermi Sea) is:

$$E_d = \frac{1}{L}\langle FS|\mathcal{H}_{3s}|FS\rangle = \epsilon_{3s} - \alpha t_{3s} + \frac{U_{3s}}{4} \tag{3.4}$$

As the lattice constant a is increased, U_{3s} remains invariant, while t_{3s}, the overlap integral between adjacent sites, falls off exponentially. So the $\frac{U_{3s}}{t_{3s}}$ steeply increases with a, and after $\frac{U_{3s}}{t_{3s}} \geq 4\alpha$, $E_d \geq \epsilon_{3s}$. This implies that after the critical value of $\frac{U_{3s}}{t_{3s}}_{cr} = 4\alpha$, the formation of an itinerant ground state is no longer favourable as compared to one electron localize exactly at each site.

This naive picture of Na-lattice predicts an itinerant ground state for $\frac{U_{3s}}{t_{3s}} \leq 4\alpha$ and an array of neutral atoms for $\frac{U_{3s}}{t_{3s}} \geq 4\alpha$, indicating two extremes for the ground state. This transition from a delocalized metallic state to fully localized insulating state is a simple example of Mott transition.

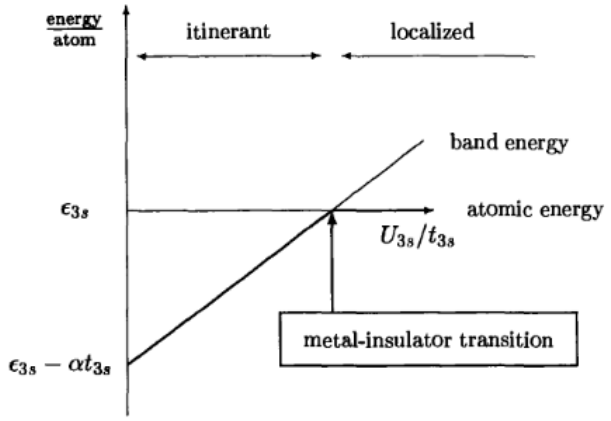

Figure 3.1: Transition of Na lattice from metal to insulator [3]

3.3 Hubbard Model

To overcome the lacunae of band theory and to explain the magnetism of transition metals, the Hubbard model was propounded by John. H. Hubbard, Gutzwiller and Kanamori by inclusion of correlation effects into tight binding model. It is the simplest many-body Hamiltonian which takes into account both the opposing factors of kinetic energy minimization by electron delocalization and potential energy minimization by minimizing electron-electron interaction. The one-band fermion Hubbard model is expressed as:

$$\mathcal{H} = -t \sum_{\langle j,l \rangle} \sum_{\sigma} ({c_{j\sigma}}^{\dagger} c_{l\sigma} + c_{j\sigma} {c_{l\sigma}}^{\dagger}) + U \sum_{j} \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} \tag{3.5}$$

Here $({c_{j\sigma}}^{\dagger}$ and $(c_{j\sigma}$ are fermionic creation and annihilation operators, i.e. $({c_{j\sigma}}^{\dagger}$ creates an electron in the Wannier state $\phi(r - R_j)$ with spin σ, at site with index j. The first term is the tight-binding model, centered about atomic energy, taken at level zero. It describes the electron hopping and kinetic energy. The second term is the interaction term which assigns an amount U to the doubly occupied sites, counted by the number operators $\hat{n}_{j\uparrow}$, and $\hat{n}_{j\downarrow}$, the product of which is nonzero only for doubly occupied states.

The interaction term Hubbard U is defined as:

$$U = \int \int dr_1 dr_2 |\phi(r_1 - R_j)|^2 \frac{e^2}{|r_1 - r_2|} |\phi(r_2 - R_j)|^2 \tag{3.6}$$

By definition, U is usually positive, and correspondingly the model is called positive-U Hubbard Model. Each lattice site in the Hubbard model can be found in any of the four local basis states: $|0\rangle_j$ (empty site), ${c_{j\uparrow}}^{\dagger} |0\rangle_j$ (site with $\uparrow$-electron), ${c_{j\downarrow}}^{\dagger} |0\rangle_j$ (site with $\downarrow$-electron), and ${c_{j\downarrow}}^{\dagger} {c_{j\uparrow}}^{\dagger} |0\rangle_j$ (site doubly occupied).

3.4 Mean Field Hamiltonian for Hubbard Model

3.4.1 Hatree-Fock Decomposition

To derive the mean-field Hamiltonian for Hubbard model, the quartic term is decoupled into Hartree and Fock terms. The Hartree-Fock decomposition gives:

Hartree Terms

By definition of $\hat{n}$ and $\hat{S}_{iz} = \overrightarrow{S_i}.\hat{z}$, and taking $\hbar = 1$

$$\hat{n}_i = \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow} \tag{3.7}$$

$$\hat{S}_{iz} = \frac{1}{2}[\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow}] \tag{3.8}$$

Here using equation-2.11 and 3.7:

$$\begin{aligned} {c_{i,\uparrow}}^{\dagger} c_{i,\uparrow} {c_{i,\downarrow}}^{\dagger} c_{i,\downarrow} = n_{i,\uparrow} n_{i,\downarrow} &= [\langle n_{i,\uparrow} \rangle n_{i,\uparrow} + \langle n_{i,\downarrow} \rangle n_{i,\downarrow} - \langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle] \\ &= \frac{1}{2}\left[n_i \langle n_i \rangle - 4 S_{iz} \langle S_{iz} \rangle - \left(\frac{\langle n_i \rangle^2}{2} - 2 \langle S_{iz}^2 \rangle \right) \right] \end{aligned} \tag{3.9}$$

Fock Terms

Using $\overrightarrow{S}_j = \frac{1}{2} \sum_{\alpha,\beta} c_{j,\alpha}^{\dagger} \overrightarrow{\sigma}_{\alpha,\beta} c_{j,\beta}$,

$$\begin{aligned} {c_{i,\uparrow}}^{\dagger} c_{i,\uparrow} {c_{i,\downarrow}}^{\dagger} c_{i,\downarrow} &= -{c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} {c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} \\ &= -{c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} \langle {c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} \rangle - \langle {c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} \rangle {c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} + \langle {c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} \rangle \langle {c_{i,\uparrow}}^{\dagger} c_{i,\downarrow} \rangle \\ &= -S_{i,+} \langle S_{i,-} \rangle - \langle S_{i,+} \rangle S_{i,-} + \langle S_{i,+} \rangle \langle S_{i,-} \rangle \end{aligned} \tag{3.10}$$

where, $S_{i,\pm} = S_{ix} \pm S_{iy}$

Adding equations 3.9 and 3.10,

$$U n_{i,\uparrow} n_{i,\downarrow} = \frac{U}{2}[n_i \langle n_i \rangle - 4 \overrightarrow{S_i} \langle \overrightarrow{S_i} \rangle] - \frac{U}{4}[\langle n_i \rangle^2 - 4 \langle S_i \rangle^2]$$

Using $\overrightarrow{S_i} = \frac{1}{2}\overrightarrow{\sigma_i}$ and $\overrightarrow{m_i} = \langle\overrightarrow{\sigma_i}\rangle$ the mean-field Hamiltonian is obtained as:

$$H = H_0 + \frac{U}{2}[n_i \langle n_i\rangle - \overrightarrow{\sigma_i}.\overrightarrow{m_i}] - \frac{U}{4}[\langle n_i\rangle^2 - \overrightarrow{m_i}^2] \tag{3.11}$$

3.4.2 Stationary Phase Approximation

The mean-field Hamiltonian can also be obtained from the imaginary time path integral by integrating about the saddle point using method of steepest descent. The saddle point for the path integral is given by the field configuration that extremizes the action on the exponential, and this stationary phase contributes the most to the integral.

Thus the partition function is approximated by the trace of the extracted stationary phase, instead of the complete integral. Since the free energy is given by the logarithm of the partition function, the stationary phase approximation gives the free energy as action in imaginary time evaluated at the saddle point. The Hamiltonian can be obtained thereby as a function of chemical potential μ.

By squaring equations-3.7 and taking an arbitrary unit vector $\hat{\Omega}$,

$$n_{i,\uparrow}n_{i,\downarrow} = \frac{1}{4}\hat{n}_i^2 - \left(\overrightarrow{S_i}.\hat{\Omega}\right)^2 \tag{3.12}$$

To obtain the partition function for $\beta = \frac{1}{kT}$, action in imaginary time is given in terms of imaginary time Lagrangian as

$$S = \int_0^\beta d\tau \mathcal{L}(\tau) \tag{3.13}$$

By Legendre transformation of $H(\tau)$,

$$\begin{aligned}\mathcal{L}(\tau) &= \sum_{i,\sigma} c^\dagger_{i,\sigma}(\tau)\partial_\tau c_{i,\sigma}(\tau) + H(\tau) \\ &= \sum_{i,\sigma} c^\dagger_{i,\sigma}(\tau)\partial_\tau c_{i,\sigma}(\tau) - t\sum_{\langle j,l\rangle}\sum_{\sigma}(c_{j\sigma}{}^\dagger c_{l\sigma} + c_{j\sigma}c_{l\sigma}{}^\dagger) + U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\end{aligned}$$

By dividing $\tau = \beta\hbar$ into $\epsilon = \frac{\tau}{N}$ time slices for large N,

$$U'(\beta\hbar) = e^{-\beta(H_0 + U n_{i\uparrow} n_{i\downarrow})} = \left[e^{\epsilon H_0 + \epsilon U n_{i\uparrow} n_{i\downarrow}}\right]^N$$

In the limit of $\epsilon \to 0$, Suzuki-Trotter decomposition and $\overrightarrow{S_i}.\hat{z} = \frac{1}{2}\overrightarrow{m_i}$ gives

$$U'(\beta\hbar) = \prod_{k=1}^{N} \exp\left[-H_0\epsilon\right] \exp\left[\frac{-U\epsilon}{4} \sum_{i=1,2} n_i^2\right] \exp\left[\frac{U\epsilon}{4} \sum_{i=1,2} m_i^2\right]$$

By Hubbard-Stratonovich transformation, two auxiliary fields can be introduced: ξ_i that couples with n_i and ϕ_i that couples with m_i. The transformation is:

$$e^{\lambda \hat{a}^2} = \begin{cases} \sqrt{\frac{\lambda}{\pi}} \int_{-\infty}^{\infty} dx e^{-\lambda x^2 + 2\lambda x}, & (\lambda > 0) \\ \sqrt{\frac{\lambda}{\pi}} \int_{-\infty}^{\infty} dx e^{-\lambda x^2 - 2i\lambda x}, & (\lambda < 0) \end{cases} \tag{3.14}$$

$$\begin{aligned} U'(\beta\hbar) &= \lim_{N\to\infty} \prod_{k=1}^{N} e^{-H_0\epsilon} \frac{U\epsilon}{4\pi} \int_{-\infty}^{\infty} \prod_{j=1,2} d\xi_j e^{\frac{-U\epsilon}{4}\sum_j \xi_j^2} e^{\frac{-U\epsilon i}{2}\sum_j \xi_j n_j} \frac{U\epsilon}{4\pi} \int_{-\infty}^{\infty} \prod_{j=1,2} d\phi_j e^{\frac{-U\epsilon}{4}\sum_j \phi_j^2} e^{\frac{-U\epsilon}{2}\sum_j \phi_j n_j} \\ &= \int \mathcal{D}[\xi_1\xi_2\phi_1\phi_2] \exp\left[-\int_0^\beta d\tau \left(H_0 + \frac{U}{4}\sum_{j=1,2}(\xi_j^2 + \phi_j^2) + \frac{U}{2}\sum_{j=1,2}(in_j\xi_j - \phi_j m_j)\right)\right] \\ (i\xi_j \to \chi_j) &= \int \mathcal{D}[\chi_1\chi_2\phi_1\phi_2] \exp\left[-\int_0^\beta d\tau \left(H_0 + \frac{U}{4}\sum_{j=1,2}(\phi_j^2 - \chi_j^2) + \frac{U}{2}\sum_{j=1,2}(n_j\chi_j - \phi_j m_j)\right)\right] \end{aligned} \tag{3.15}$$

The function on the exponential $G(\chi, \phi)$ can be extremized by calculus of variation using the equations:

$$\frac{d}{dt}\left(\frac{\partial G}{\partial \dot{\chi_j}}\right) = \frac{\partial G}{\partial \chi_j} \implies \chi_j|_{\text{statn}} = i\xi_j|_{statn} = n_{j_0} \tag{3.16}$$

$$\frac{d}{dt}\left(\frac{\partial G}{\partial \dot{\phi_j}}\right) = \frac{\partial G}{\partial \phi_j} \implies \phi_j|_{\text{statn}} = m_{j_0} \tag{3.17}$$

We can take saddle point values n_{j_0} and m_{j_0} as the mean-fields $\langle n_j \rangle$ and $\langle m_j \rangle$.

As per method of steepest descent, the deviation is negligible, so the τ-dependence is dropped. The stationary phase can be extracted by using as:

$$U'(\beta\hbar) = \exp\left[-\beta\left(H_0 + \frac{U}{4}\sum_{j=1,2}(\langle m_j\rangle^2 - \langle n_j\rangle^2) + \frac{U}{2}\sum_{j=1,2}(n_j\langle n_j\rangle - \langle m_j\rangle m_j)\right)\right]$$

$$\implies H_{eff} = H_0 + \frac{U}{4}\sum_{j=1,2}(\langle m_j\rangle^2 - \langle n_j\rangle^2) + \frac{U}{2}\sum_{j=1,2}(n_j\langle n_j\rangle - \langle m_j\rangle m_j) - \mu\sum_i n_i$$

Since $m = \overrightarrow{\sigma}.\hat{z}$, defining $\overrightarrow{a_j} = \langle m_j\rangle\,\hat{z} = (\langle\overrightarrow{\sigma_j}\rangle.\hat{z})\hat{z}$ and noting that $(\overrightarrow{a_j})^2 = \langle m_j\rangle^2$:

$$H_{eff} = -t\sum_{\langle j,l\rangle}\sum_{\sigma}({c_{j\sigma}}^{\dagger}c_{l\sigma} + c_{j\sigma}{c_{l\sigma}}^{\dagger}) + \frac{U}{4}\sum_{j=1,2}(\overrightarrow{a_j}^2 - \langle n_j\rangle^2) + \frac{U}{2}\sum_{j=1,2}(n_j\langle n_j\rangle - \overrightarrow{a_j}.\overrightarrow{\sigma_j}) - \mu\sum_i n_i \tag{3.18}$$

At $T = 0$, this result from static path approximation perfectly agrees with the Hartree-Fock mean field (equation-3.9). [5] However self-consistent calculation like Hartree-Fock approximation fails in cases where there is significant departure from the mean values.

Chapter 4

Beyond Static Path Approximation

The Static Path Approximation (SPA) for the partition function has been obtained when the path integral is approximated by summing over the time-independent fields only, weighted by the appropriate Boltzmann factor. This amounts to averaging over all possible static mean-field configurations rather than the self-consistent ones alone.

Further we will try to incorporate the time-dependent fluctuations in auxiliary fields in the approximated many-body propagator.

4.1 Perturbed Static Path Approximation

From equation 3.15,

$$U(\beta\hbar) = \int \mathcal{D}[\xi_1\xi_2\phi_1\phi_2] \exp\left[-\int_0^\beta d\tau \left(\frac{U}{4}\sum_{j=1,2}(\xi_j^2+\phi_j^2)\right)\right] U_{\xi_1,\xi_2,\phi_1,\phi_2} \quad (4.1)$$

$$\text{where, } U_{\xi_1,\xi_2,\phi_1,\phi_2} = \exp\left[-\int_0^\beta d\tau \left(H_0 + \frac{U}{2}\sum_{j=1,2}(in_j\xi_j - \phi_j m_j)\right)\right] \quad (4.2)$$

By expanding the auxiliary fields in an odd number of Fourier basis [1],

$$\xi_j(\tau = n\epsilon) = \sum_r \sigma_{jr} e^{i\omega_r \tau} \quad (4.3)$$

$$\phi_j(\tau = n\epsilon) = \sum_r \pi_{jr} e^{i\omega_r \tau} \quad (4.4)$$

where, $\omega_r = \frac{2\pi r}{\beta}$ are Matsubara frequencies. Also $\sigma_{j-r} = \sigma_{jr}^*$ and $\pi_{j-r} = \pi_{jr}^*$, to keep ξ_j and ϕ_j real. The odd number of basis ensures time-independent components σ_0 and π_0. In terms of the Fourier basis,

$$U(\beta\hbar) = \int \mathcal{D}[\sigma_1\sigma_2\pi_1\pi_2] \exp\left[-\frac{U\beta}{4}\left(\sum_{r;j=1,2}(|\sigma_{jr}|^2 + |\pi_{jr}|^2)\right)\right] U_{\sigma_1\sigma_2\pi_1\pi_2} \quad (4.5)$$

$$U_{\sigma_1\sigma_2\pi_1\pi_2} = \exp\left[-\int_0^\beta d\tau \left(H_0 + \frac{U}{2}\sum_{j=1,2}(in_j\sigma_{j0} - m_j\pi_{j0}) + \frac{U}{2}\sum_{\substack{r\neq 0\\ j=1,2}}(in_j\sigma_{jr} - m_j\pi_{jr})\right)\right] \quad (4.6)$$

Here the time-dependent fluctuations can be split as:

$$H_{\sigma_1\sigma_2\pi_1\pi_2} = h_0 + h_1 \quad (4.7)$$

$$\text{where, } h_0 = H_0 + \frac{U}{2}\sum_{j=1,2}(in_j\sigma_{j0} - m_j\pi_{j0}) \quad (4.8)$$

$$h_1 = \frac{U}{2}\sum_{\substack{r\neq 0\\ j=1,2}}(in_j\sigma_{jr} - m_j\pi_{jr}) \quad (4.9)$$

Extracting the static components from $U_{\sigma_1\sigma_2\pi_1\pi_2}$,

$$U_{\sigma_1\sigma_2\pi_1\pi_2} = e^{-\int_0^\beta d\tau(h_0+h_1)} = e^{-\beta h_0}\mathcal{U}_{\sigma_1\sigma_2\pi_1\pi_2} \quad (4.10)$$

$$\text{where, } \mathcal{U}_{\sigma_1\sigma_2\pi_1\pi_2} = e^{-\int_0^\beta d\tau h_1}$$

After collecting all static parts in the many body propagator

$$U = \left(\frac{U\beta}{2\pi}\right)^2 \int \prod_{j=1,2} d\sigma_{j0} d\pi_{j0} \exp\left[-\frac{U\beta}{4} \sum_{j=1,2} \left(\sigma_{j0}^2 + \pi_{j0}^2\right) - \beta h_0\right] \int \mathcal{D}[\sigma_1\sigma_2\pi_1\pi_2] \exp\left[-\frac{U\beta}{4} \left(\sum_{\substack{r>0 \\ j=1,2}} \left(|\sigma_{jr}|^2 + |\pi_{jr}|^2\right)\right)\right] \mathcal{U}_{\sigma_1\sigma_2\pi_1\pi_2} \tag{4.11}$$

This expresses the manybody evolution operator as a Gaussian-weighted average of one-body evolutions contributed by to static fields (σ_{j0}, π_{j0}), multiplied by a correction factor contributed by the time-dependent fluctuations of the auxiliary fields about the mean values. Finally the partition function is given by:

$$Z = \mathrm{Tr}\ U = \left(\frac{U\beta}{2\pi}\right)^2 \int \prod_{j=1,2} d\sigma_{j0} d\pi_{j0} \exp\left[-\frac{U\beta}{4} \sum_{j=1,2} \left(\sigma_{j0}^2 + \pi_{j0}^2\right)\right] \mathrm{Tr}\left(e^{-\beta h_0}\right) \int \mathcal{D}[\sigma_1\sigma_2\pi_1\pi_2] \exp\left[-\frac{U\beta}{4} \left(\sum_{\substack{r>0 \\ j=1,2}} \left(|\sigma_{jr}|^2 + |\pi_{jr}|^2\right)\right)\right] \frac{\mathrm{Tr}\left(e^{-\beta h_0} \mathcal{U}_{\sigma_1\sigma_2\pi_1\pi_2}\right)}{\mathrm{Tr}\left(e^{-\beta h_0}\right)}$$

$$= \left(\frac{U\beta}{2\pi}\right)^2 \int \prod_{j=1,2} d\sigma_{j0} d\pi_{j0} \exp\left[-\frac{U\beta}{4} \sum_{j=1,2} \left(\sigma_{j0}^2 + \pi_{j0}^2\right)\right] \zeta_0 {\zeta_0}' = \left(\frac{U\beta}{2\pi}\right)^2 \int \prod_{j=1,2} d\sigma_{j0} d\pi_{j0} e^{-\beta F(\beta, \sigma_j, \pi_j)}$$

where, $\zeta_0 = \mathrm{Tr}\left(e^{-\beta h_0}\right)$

and ${\zeta_0}' = \int \mathcal{D}[\sigma_1\sigma_2\pi_1\pi_2] \exp\left[-\frac{U\beta}{4} \left(\sum_{\substack{r>0 \\ j=1,2}} \left(|\sigma_{jr}|^2 + |\pi_{jr}|^2\right)\right)\right] \frac{\mathrm{Tr}\left(e^{-\beta h_0} \mathcal{U}_{\sigma_1\sigma_2\pi_1\pi_2}\right)}{\mathrm{Tr}\left(e^{-\beta h_0}\right)}$

The free energy in this framework is given by:

$$F(\beta, \sigma_j, \pi_j) = \frac{U}{4} \sum_{j=1,2} \left(\sigma_{j0}^2 + \pi_{j0}^2\right) - \frac{1}{\beta} \log \zeta_0 - \frac{1}{\beta} \log {\zeta_0}' \tag{4.12}$$

4.2 Future Outlook

In this project, we explored the role of path integrals in many-body problems like mean field theories, and have found that similar but superior result can be obtained from path integral formalism. The fundamental reason for this is explained after deriving SPA:" averaging over all possible static mean-field configurations rather than the self-consistent ones alone". Also the proposed framework PSPA takes into account time-dependent fluctuations in mean-field .

The time-independent part of the free energy constitutes the Static Path Approximation, and generates the same result as mean field calculation, as already shown. It is obtained by setting $h_1 = 0$, i.e. ${\zeta_0}' = 1$. The time-dependent fluctuations can be incorporated by using evaluating ${\zeta_0}'$.

ζ_0 has already been evaluated and shown equivalent to Hartree-Fock mean field in earlier section. In future, we will try to estimate ${\zeta_0}'$ by calculating of $\log \langle \mathcal{U} \rangle_0$. It can be performed by choosing a Fock Space basis where h_0 is diagonal, and expanding $\log \langle \mathcal{U} \rangle_0$ up to a certain order in σ_{jr}, π_{jr}. This PSPA framework is expected to get better insights into several exotic phenomena, driven by quantum fluctuation.

Bibliography

[1] H Attias and Y Alhassid. The perturbed static path approximation at finite temperature: observables and strength functions. *Nuclear Physics A*, 625(3):565–597, 1997.

[2] Henrik Bruus and Karsten Flensberg. *Many-body quantum theory in condensed matter physics: an introduction*. Oxford University Press, 2004.

[3] Patrick Fazekas. *Lecture notes on electron correlation and magnetism*, volume 5. World scientific, 1999.

[4] Richard P Feynman, Albert R Hibbs, and Daniel F Styer. *Quantum mechanics and path integrals*. Courier Corporation, 2010.

[5] Anamitra Mukherjee, Niravkumar D Patel, Shuai Dong, Steve Johnston, Adriana Moreo, and Elbio Dagotto. Testing the monte carlo-mean field approximation in the one-band hubbard model. *Physical Review B*, 90:205133, 2014.

[6] R. Shankar. *Principles of Quantum Mechanics*. Springer US, 2012.