Application of Perturbed Static Path Approximation to Lattice Models

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DECLARATION

I hereby declare that I am the sole author of this thesis in partial fulfillment of the requirements for a postgraduate degree from National Institute of Science Education and Research (NISER). I authorize NISER to lend this thesis to other institutions or individuals for the purpose of scholarly research.

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ABSTRACT

Path-integral based mean field formalisms, based on saddle point approximations, has been popular since 1970s. In this project we are trying to incorporate dynamic correction to mean-field Hamiltonian by keeping leading order contribution of Fourier-decomposed auxiliary field around saddle points; with which we make a connection to the generalized RPA fluctuations. So far we have applied it on Fermi-Hubbard model at half-filling and studied the interplay of quantum and thermal fluctuations at small, exactly solvable system sizes.

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Chapter 1

Introduction

Mathematical structure of mean-field theory

A general many-body Hamiltonian for multiple species system can be expressed as:

$$H = \sum_{\nu} \zeta^a_\nu a^\dagger_\nu a_\nu + \sum_{\mu} \zeta^b_\mu b^\dagger_\mu b_\mu + \sum_{\nu\nu^\dagger,\mu\mu^\dagger} V_{\nu\mu,\nu'\mu'} a^\dagger_\nu b^\dagger_\mu b_{\mu'} a_{\nu'} \tag{1.1}$$

The mean-field approximation rests on the assumption that if the density operators $a^\dagger_\nu a_\nu$ and $b^\dagger_\mu b_\mu$ do not have high deviations from their mean values, then we can ignore the fluctuations beyond first order to have the effective Hamiltonian

$$H_{MF} = \sum_{\nu} \zeta^a_\nu a^\dagger_\nu a_\nu + \sum_{\mu} \zeta^b_\mu b^\dagger_\mu b_\mu + V_{MF} \tag{1.2}$$

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

H_{MF} is now comprised of only single-body operators, hence a solvable problem in principle. If the interaction term is product of two operators ($H_{AB} = AB$), the mean-field approximation can be generalized as [1]

$$H_{MF} = A \langle B \rangle + \langle A \rangle B - \langle A \rangle \langle B \rangle \tag{1.3}$$

For the formal solution to one-body H_{MF}, we must choose the value of $\bar{n}^a_{\nu\nu'} = \langle a^\dagger_\nu a_\nu \rangle$ and $\bar{n}^b_{\mu\mu'} = \langle b^\dagger_\mu b_\mu \rangle$ which minimizes the free-energy for mean-field Hamiltonian.

$$\frac{d}{d\bar{n}^a_{\nu\nu'}} F_{MF} = \frac{d}{d\bar{n}^a_{\nu\nu'}} \left(-\frac{1}{\beta} \ln Z_{MF} \right) = 0$$

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

So the mean field solutions for the density operators is given by

$$\bar{n}^b_{\mu\mu'} = \langle b^\dagger_\mu b_\mu \rangle_{MF} = \frac{\mathrm{Tr}\left[e^{-\beta H_{MF}} a^\dagger_\nu a_\nu\right]}{\mathrm{Tr}\left[e^{-\beta H_{MF}}\right]} \tag{1.4}$$

$$\bar{n}^a_{\nu\nu'} = \langle a^\dagger_\mu a_\mu \rangle_{MF} = \frac{\mathrm{Tr}\left[e^{-\beta H_{MF}} b^\dagger_\mu b_\mu\right]}{\mathrm{Tr}\left[e^{-\beta H_{MF}}\right]} \tag{1.5}$$

These equations are self-consistent 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 $\bar{n}^b_{\mu\mu'}$, which is solved by choosing proper initial values and applying the equations iteratively to find the fixed point of convergence for $\bar{n}^a_{\nu\nu'}$ and $\bar{n}^b_{\mu\mu'}$. Therefore the reliability of mean field approximation and the convergence of self-consistency formula relies on small deviation of interacting operators from their mean values, which is better realized in weakly interacting systems and at higher dimensions.

Hartree-Fock Approximation

Hartree Fock Approximation is a standard application of mean field theory for a weakly interacting fermionic system with the Hamiltonian

$$H = \sum_\nu \xi_\nu c^\dagger_\nu c_\nu + \frac{1}{2} \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} c^\dagger_\nu c^\dagger_\mu c_{\mu'} c_{\nu'} \tag{1.6}$$

For weak interaction, the interaction term can be decomposed by Wick's theorem as

$$\langle c^\dagger_\nu c^\dagger_\mu c_{\mu'} c_{\nu'} \rangle_{MF} = \langle c^\dagger_\nu c_{\nu'} \rangle_{MF} \langle c^\dagger_\mu c_{\mu'} \rangle_{MF} - \langle c^\dagger_\nu c_{\mu'} \rangle_{MF} \langle c^\dagger_\mu c_{\nu'} \rangle_{MF} \tag{1.7}$$

This mean-field approximation takes care of Pauli-exclusion principle since

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

Here the self-consistent equations include the "exchange terms" arising from fermionic commutation relation. The mean field decomposition of interaction term is:

$$\begin{aligned} c^\dagger_\nu c^\dagger_\mu c_{\mu'} c_{\nu'} \approx \quad & c^\dagger_\nu c_{\nu'} \langle c^\dagger_\mu c_{\mu'} \rangle_{MF} + \langle c^\dagger_\nu c_{\nu'} \rangle_{MF} c^\dagger_\mu c_{\mu'} - c^\dagger_\nu c_{\mu'} \langle c^\dagger_\mu c_{\nu'} \rangle_{MF} - \langle c^\dagger_\nu c_{\mu'} \rangle_{MF} c^\dagger_\mu c_{\nu'} \\ & - \langle c^\dagger_\nu c_{\nu'} \rangle_{MF} \langle c^\dagger_\mu c_{\mu'} \rangle_{MF} + \langle c^\dagger_\nu c_{\mu'} \rangle_{MF} \langle c^\dagger_\mu c_{\nu'} \rangle_{MF} \end{aligned} \tag{1.8}$$

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

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

$$H_{MF} = \sum_{\nu} \xi_\nu c_\nu^\dagger c_\nu + \frac{1}{2} V^{\text{Hartree}} - \frac{1}{2} V^{\text{Fock}} \tag{1.9}$$

where the two mean-field potentials are

$$V_{\text{MF}}^{\text{Hartree}} = \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} \bar{n}_{\mu\mu'} c_\nu^\dagger c_{\nu'} + \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} \bar{n}_{\nu\nu'} c_\mu^\dagger c_{\mu'} - \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} \bar{n}_{\mu\mu'} \bar{n}_{\nu\nu} \tag{1.10}$$

$$V_{\text{MF}}^{\text{Fock}} = \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} \bar{n}_{\nu\mu'} c_\mu^\dagger c_{\nu'} + \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} \bar{n}_{\mu\nu'} c_\nu^\dagger c_{\mu'} - \sum_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} \bar{n}_{\nu\mu'} \bar{n}_{\mu\nu} \tag{1.11}$$

Hartree-Fock approximations provide reliable results for weakly interacting systems and low-lying excitations such as uniform electron gas, plasmonic modes, multielectron atoms, molecules with s and p hybridization and so on. However the approximation may fail to describe the physics of systems with strong interaction, such as Hubbard Model.

Hubbard Model: a paradigm of strong correlation

Traditionally band theory has been successful in describing the structural, thermodynamic and optical properties of many metallic and crystalline material. For instance, for N electrons, nearly free electron model and band theory predicts the $N/2$ lowest-lying band states occupied. 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. Under translational invariance and time-reversal symmtery of the Hamiltonian, band theory requires an even number of electrons per unit cell to havei.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[2], e.g. CoO is an insulator though, number of electrons per unit cell is 15 .

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.

Hubbard model, propounded by John. H. Hubbard, Gutzwiller and Kanamori facilitates the inclusion of correlation into tight binding model through electron-electron interaction. The model takes into account the competing 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:

$$\mathcal{H} = -t \sum_{\langle j,l \rangle} \sum_{\sigma} (c^{\dagger}_{j\sigma} c_{l\sigma} + c^{\dagger}_{l\sigma} c_{j\sigma}) + U \sum_{j} \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} \tag{1.12}$$

Here $c^{\dagger}_{j\sigma}$ and $c_{j\sigma}$ are fermionic creation and annihilation operators, i.e. $c^{\dagger}_{j\sigma}$ 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:

$$U = \int \int dr_1 dr_2 |\phi(r_1 - R_j)|^2 \frac{e^2}{|r_1 - r_2|} |\phi(r_2 - R_j)|^2 \tag{1.13}$$

In general, the mean field approximation is closer to an exact solution of the model at weak U. At larger U, the deviation becomes significant and at best the mean field approximation can describe some of the qualitative behavior.In the Hubbard model, the minimization of kinetic energy through delocalization is accompanied by charge transfer, which costs potential energy due to Coloumb repulsion. So above a certain critical value of the ratio of the interaction to lattice parameter,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.

The electrons of a Mott insulator minimize the Coulomb potential by letting one electron stay per site resulting in an exponentially growing ensemble of singly occupied sites. The ground state is decided by the ground state spin arrangement the effective spin Hamiltonian acting in the low-energy subspace of the large-U Hubbard model. This gives rise to the magnetic property and strong correlation of the insulating state. A naive mean-field decomposition using 1.3 can be expressed as

$$\mathcal{H} = -t\sum_{\langle j,l\rangle}(c^{\dagger}_{j\uparrow}c_{l\uparrow} + c.c.) + U\sum_{j}\hat{n}_{j\uparrow}\langle\hat{n}_{j\downarrow}\rangle - t\sum_{\langle j,l\rangle}(c^{\dagger}_{j\downarrow}c_{l\downarrow} + c.c.) \tag{1.14}$$

$$+U\sum_{j}\hat{n}_{j\downarrow}\langle\hat{n}_{j\uparrow}\rangle - U\sum_{j}\langle\hat{n}_{j\downarrow}\rangle\langle\hat{n}_{j\uparrow}\rangle \tag{1.15}$$

Though this effective Hamiltonian is computationally feasible to solve and flexible, it breaks $SU(2)$ symmetry and only long wavelength modes of the correlation has been accounted for. We can construct a rotationally symmetric mean field Hamiltonian by using Hartree Fock decomposition. However this way of mean field approximation does not naturally admit a prescription for adding further correction coming from the fluctuations.

Chapter 2

Static Path Approximation

As an alternative to the mean-field decoupling 1.3, we are going to develop a path integral based approach which reduces to Hartree-Fock like result as $T \to 0$.

Path Integral in imaginary time

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:[3]

$$U(\tau) = \exp\left(-\frac{1}{\hbar} H\tau\right) \tag{2.1}$$

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

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

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:

$$U(\tau) = \sum |n\rangle \langle n| \exp\left(-\frac{1}{\hbar} E_n \tau\right) \tag{2.2}$$

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. This lets imaginary time be interpreted

as temperature in thermal field theory.

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

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[4]:

$$\mathcal{L}_E = \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x) \tag{2.3}$$

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

$$U(\tau) = \sum|n\rangle\langle n|\exp\left(-\frac{1}{\hbar}H\tau\right) = \int[\mathcal{D}x]\exp\left[-\frac{1}{\hbar}\int_0^t\mathcal{L}_E(x,\dot{x})d\tau\right] \tag{2.4}$$

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

$$Z = \int_{-\infty}^{\infty}\langle x|e^{-\beta H}|x\rangle\,dx = \int_{-\infty}^{\infty}U(x,x,\beta\hbar)dx = \text{Tr } U \tag{2.5}$$

HS Transformation and Auxiliary field PI

Let us consider the general interacting Hamiltonian 1.6. We note that any arbitrary potential can be expressed as a sum of separable potential by [5]

$$\begin{aligned}\sum_{ijkl} u_{ijkl} a_i^\dagger a_j^\dagger a_l a_k &= \sum_{ij}\left(\sum_k u_{ikjk}\right) a_i^\dagger aj - \sum_{ijkl} u_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \\ &= \sum_{\alpha=1}^{q} \tilde{u}_\alpha \rho_\alpha - \sum_{\alpha\beta=1}^{q} u_{\alpha\beta}\rho_\alpha\rho_\beta\end{aligned}$$

The matrix $u_{\alpha\beta}$ can be diagonalized to obtain at most q^2 separable terms, so we consider a general Hamiltonian of the form

$$H = K - \frac{1}{2}\sum_\alpha \chi_\alpha V_\alpha^2 \tag{2.6}$$

where, $K = \sum_{ij} K_{ij} a_i^\dagger a_j$ and $V^\alpha = \sum_{ij} v_{ij}^{(\alpha)} a_i^\dagger a_j$ (one-body operators)
Using Suzuki-Trotter decomposition, the propagator for 2.6 can be decomposed into N imaginary time slices of sub-interval length $\epsilon = \beta/N$

$$U = e^{-\beta H} = \prod_{n=1}^{N} \exp\left(-K\epsilon + \frac{1}{2}\sum_\alpha \chi_\alpha V_\alpha^2 \epsilon\right) = \prod_{n=1}^{N} e^{-K\epsilon} e^{\sum_\alpha \chi_\alpha V_\alpha^2 \epsilon}(1+\mathcal{O}(\epsilon^2)) \tag{2.7}$$

The complexity of the problem is manifested from the two body term in the action. So we perform a Hubbard Stratonovich transformation for $\lambda > 0$, given by [6][7]

$$\exp\left(\lambda \hat{a}^2\right) = \sqrt{\frac{\lambda}{\pi}} \int_{-\infty}^{\infty} d\xi e^{-\lambda\xi^2} e^{\pm 2\lambda\xi\hat{a}} \tag{2.8}$$

We perform the HS transformation at each time slices for each α to obtain

$$U = \left(\frac{\prod_\alpha \chi_\alpha \epsilon}{2\pi}\right)^{N/2} \int \prod_{n=1,\alpha}^{N} d\xi_n^\alpha \exp\left(-\frac{1}{2}\epsilon \sum_{n=1,\alpha}^{N} \chi_\alpha \xi_{n\alpha}^2\right) \prod_{n=1}^{N} \exp\left(-K\epsilon + \sum_\alpha \chi_\alpha \xi_{n\alpha} V_\alpha \epsilon\right) \tag{2.9}$$

Here we have ignored contributions beyond $\mathcal{O}(\epsilon)$ in 2.7, which is better justified for $\beta \to 0$, so the analysis becomes exact at high temperature.

In the continuum limit of $N \to \infty$, for each α, ξ_α becomes a classical field with $\xi_\alpha(\tau = n\epsilon) = \xi_{n\alpha}$. Defining measure $\mathcal{D}[\xi] \equiv \prod_{n\alpha} d\xi_n^\alpha (\frac{\chi_\alpha \epsilon}{2\pi})^{1/2}$,

$$U = \int \mathcal{D}[\xi] \exp\left[-\frac{1}{2}\sum_\alpha \int_0^\beta d\tau \chi_\alpha \xi_\alpha^2(\tau)\right] \mathrm{T} \exp\left[-\int_0^\beta d\tau \left(K - \sum_\alpha \chi_\alpha \xi_\alpha(\tau) V_\alpha\right)\right] \tag{2.10}$$

This is still an almost exact picture of the original Hamiltonian. It shows that the many-body evolution operator U is an Gaussian weighted average of single particle evolution operator $U_\xi = \mathrm{T}\exp[-\int_0^\beta d\tau (K - \sum_\alpha \chi_\alpha \xi_\alpha(\tau) V)]$, while the single particle evolution operator describes a non-interacting system of particle moving in potential V_α, modulated by a (imaginary) time dependent fluctuating field $\xi_\alpha(\tau)$. Since this contains all the information of the fully interacting system, it is not possible to solve equation-2.10 in general. Therefore we employ saddle point approximation to extract the effective propagator.

Saddle point approximation of auxiliary field PI

If $f(x)$ is a C^∞ function with a global minimum at $x = x_0$ so that $f'(x_0) = 0$, then an integral of the form $I = \lim_{\lambda\to\infty} \int_{-\infty}^{\infty} dx e^{-\lambda f(x)}$ can be approximated as

$$I \approx \lim_{\lambda\to\infty} e^{-\lambda f(x_0)} \int_{-\infty}^{\infty} dx e^{-\frac{\lambda}{2} f''(x_0)(x-x_0)^2} = \lim_{\lambda\to\infty} \left[\frac{2\pi}{\lambda f''(x_0)}\right]^{1/2} e^{-\lambda f(x_0)}$$

For equation 2.10, we assume commutation of $V(\tau)$ for different τ, so that the propagator can be expressed as

$$U = \int \mathcal{D}[\xi] \exp\left[-\int_0^\beta d\tau \left(K - \sum_\alpha \chi_\alpha \xi_\alpha(\tau) V_\alpha + \frac{1}{2}\sum_\alpha \chi_\alpha \xi_\alpha^2(\tau)\right)\right] \tag{2.11}$$

Here the minima of the function $S(\xi_1, ...\xi_q) = -\int_0^\beta d\tau \left(K - \sum_\alpha \chi_\alpha \xi_\alpha(\tau) V_\alpha + \frac{1}{2}\sum_\alpha \chi_\alpha \xi_\alpha^2(\tau)\right) = \int_0^\beta d\tau \mathcal{L}(\tau)$ contribute to the effective propagator as saddle points, which can be determined by calculus of variation.

The saddle points are given by

$$\left.\frac{\partial \mathcal{L}}{\partial \xi_\alpha}\right|_{\xi_\alpha^0} = \frac{d}{d\tau}\left(\frac{\partial \mathcal{L}}{\partial \dot{\xi}_\alpha}\right) = 0 \implies -\chi_\alpha V_\alpha^0 + \chi_\alpha \xi_\alpha^0 \mathcal{I} = 0 \implies \xi_\alpha^0 = \langle V \rangle_0 \tag{2.12}$$

Using the saddle point values for each ξ_α, the effective propagator can be written as

$$U_{eff} = \exp\left[-\int_0^\beta d\tau \left(K - \sum_\alpha \chi_\alpha \xi_{\alpha 0} V_\alpha + \frac{1}{2}\sum_\alpha \chi_\alpha \xi_{\alpha 0}^2\right)\right] S_0 \tag{2.13}$$

where

$$S_0 = \int \mathcal{D}[\xi] \prod_\alpha \left[\frac{2\pi}{\beta S_\alpha''(\xi_0)}\right]^{1/2} = \int \mathcal{D}[\xi] \prod_\alpha \left[\frac{2\pi}{\beta \chi_\alpha}\right]^{1/2} = 1 \text{ (normalized measure in 2.10)}$$

Moreover in 2.13, there is no τ-dependence, so the Static Path Approximated (SPA) propagator can be expressed as

$$U_{eff} = e^{-\beta H_{SPA}}, \text{ where, } H_{spa} = K - \sum_\alpha \chi_\alpha \xi_{\alpha 0} V_\alpha + \frac{1}{2}\sum_\alpha \chi_\alpha \xi_{\alpha 0}^2 \tag{2.14}$$

Mean field solution as a limiting case of SPA

As $\beta \to \infty$, i.e. as the temperature is lowered, the saddle point approximation holds better. At $T = 0$, each $\xi_{\alpha 0}$ assume exactly the saddle point values and 2.14 becomes exact insofar as the Suzuki-Trotter decomposition in 2.7 remains valid. Therefore at zero temperature H_{spa} becomes

$$H_{spa} = K - \sum_\alpha \chi_\alpha \langle V_\alpha \rangle V_\alpha + \frac{1}{2}\sum_\alpha \chi_\alpha \langle V_{\alpha 0} \rangle^2 \tag{2.15}$$

A mean-field decomposition of 2.6 according to 1.3 gives

$$H_{MF} = K - \frac{1}{2}\sum_\alpha \chi_\alpha \left(2V_\alpha \langle V_\alpha \rangle - \langle V_\alpha \rangle^2\right) = K - \sum_\alpha \chi_\alpha \langle V_\alpha \rangle V_\alpha + \frac{1}{2}\sum_\alpha \chi_\alpha \langle V_{\alpha 0} \rangle^2$$

So the zero temperature Hartree-Fock solutions are a limiting case of SPA. In fact at finite temperature, 2.12 generalizes to finite temperature Hartree-Fock equation [8]

$$\xi_\alpha^0 = \langle V \rangle_0 = \sum_i \frac{v_{ii}}{e^{\beta e_i} + 1} \tag{2.16}$$

Static Path Approximation for Hubbard Model

We are going to work with Fermi-Hubbard model at half-filling, i.e. the particle hole symmetric case. The Hubbard Hamiltonian is given by

$$\mathcal{H} = -t \sum_{\langle j,l \rangle} \sum_{\sigma} (c^{\dagger}_{j\sigma} c_{l\sigma} + c^{\dagger}_{l\sigma} c_{j\sigma}) + U \sum_{j} c^{\dagger}_{j\uparrow} c_{j\uparrow} c^{\dagger}_{j\downarrow} c_{j\downarrow} \tag{2.17}$$

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

$$\hat{n}_i = \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow} \tag{2.18}$$

$$\hat{S}_{iz} = \frac{1}{2}[\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow}] \tag{2.19}$$

By squaring equations-2.18 and taking an arbitrary unit vector $\hat{\Omega}$,

$$n_{i,\uparrow} n_{i,\downarrow} = \frac{1}{4}\hat{n}_i^2 - \left(\overrightarrow{S_i}.\hat{\Omega}\right)^2 \tag{2.20}$$

For half-filling case, we assume that $\langle n_i \rangle = 1$ for each lattice site i and $\hat{\Omega} = \hat{z}$. So the effective Hamiltonian is[9]

$$\mathcal{H} = \mathcal{H}_{TB} - \frac{U}{4} \sum_{j} \sigma_{zi}^2 - \mu \hat{n}_i \tag{2.21}$$

So in this case $\chi_\alpha = \frac{U}{2}$ and $V_\alpha = \sigma_{z\alpha}$. If the auxiliary field that couples to σ_{zi} is m_i, then the SPA Hamiltonian is given by

$$H_{spa} = -t \sum_{\langle j,l \rangle} \sum_{\sigma} (c^{\dagger}_{j\sigma} c_{l\sigma} + c^{\dagger}_{l\sigma} c_{j\sigma}) - \frac{U}{2} \sum_{i} m_i \sigma_{zi} + \frac{U}{4} \sum_{i} m_i^2 - \mu \hat{n}_i \tag{2.22}$$

As the temperature is lowered, we have $m_{i0} = \langle \sigma_{zi} \rangle$; the auxiliary field can be interpreted as magnetic moment coupled to each site. So as the temperature decreases further, the saddle point value of the m_i at each site indicates the preferred spin arrangement. As expected from the behavior of the Hamiltonian, at zero temperature, an antiferromagnetic ordering of m_i results in the ground state.

SPA and Mean field solution of Hubbard model

Hartree Terms

Here using equation-1.10 and 2.18:

$$\begin{aligned} c^{\dagger}_{i,\uparrow}c_{i,\uparrow}c^{\dagger}_{i,\downarrow}c_{i,\downarrow} = n_{i,\uparrow}n_{i,\downarrow} &= [\langle n_{i,\uparrow}\rangle n_{i,\uparrow} + \langle n_{i,\downarrow}\rangle n_{i,\downarrow} - \langle n_{i,\uparrow}\rangle \langle n_{i,\downarrow}\rangle] \\ &= \frac{1}{2}\left[n_i \langle n_i\rangle - 4S_{iz}\langle S_{iz}\rangle - \left(\frac{\langle n_i\rangle^2}{2} - 2\langle S_{iz}^2\rangle\right)\right] \end{aligned} \tag{2.23}$$

Fock Terms

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

$$\begin{aligned} c^{\dagger}_{i,\uparrow}c_{i,\uparrow}c^{\dagger}_{i,\downarrow}c_{i,\downarrow} &= -c^{\dagger}_{i,\uparrow}c_{i,\downarrow}c^{\dagger}_{i,\uparrow}c_{i,\downarrow} \\ &= -c^{\dagger}_{i,\uparrow}c_{i,\downarrow}\langle c^{\dagger}_{i,\uparrow}c_{i,\downarrow}\rangle - \langle c^{\dagger}_{i,\uparrow}c_{i,\downarrow}\rangle c^{\dagger}_{i,\uparrow}c_{i,\downarrow} + \langle c^{\dagger}_{i,\uparrow}c_{i,\downarrow}\rangle\langle c^{\dagger}_{i,\uparrow}c_{i,\downarrow}\rangle \\ &= -S_{i,+}\langle S_{i,-}\rangle - \langle S_{i,+}\rangle S_{i,-} + \langle S_{i,+}\rangle\langle S_{i,-}\rangle \end{aligned} \tag{2.24}$$

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

Adding equations 2.23 and 2.24,

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

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:

$$H = H_0 + \frac{U}{2}[n_i\langle n_i\rangle - \overrightarrow{\sigma_i}.\overrightarrow{m_i}] - \frac{U}{4}[\langle n_i\rangle^2 - \overrightarrow{m_i}^2] \tag{2.25}$$

At half-filling level with the assumption $\langle n_i\rangle = 1$, 2.25 reduces to

$$H_{HF} = -t\sum_{\langle j,l\rangle}\sum_{\sigma}(c^{\dagger}_{j\sigma}c_{l\sigma} + c^{\dagger}_{l\sigma}c_{j\sigma}) - \frac{U}{2}\sum_i \overrightarrow{\sigma_i}.\overrightarrow{m_i} + \frac{U}{4}\sum_i m_i^2 - \mu\hat{n}_i \tag{2.26}$$

So at $T = 0$, the Hartree-Fock Hamiltonian perfectly agrees with the SPA Hamiltonian with $\mu = \frac{U}{2}$

Chapter 3

Corrections to Mean Field Theory

From the last discourse, we have observed that irrespective of the formulation, any mean-field theory ignores fluctuations in the degree of freedoms from their average values. For ab-initio formulations like 1.3, second order deviations are neglected. For variational formulation of techniques like Hartree-Fock equation, the effective potentials are functions of densities averaged over several states. For path-integral and auxiliary field based formulation the saddle point approximation admits contribution only from τ-independent, static auxiliary field at the free energy minima, which effectively means constraining the path integral only along the path of steepest descent, resulting in a 'static' path approximation. Therefore correction to any mean-field theory seeks to recover parts of these fluctuations up to a certain order.

Origin of fluctuations

Fluctuations in the relevant degree of freedom implies the departure from the suggested average value. The origin of fluctuation can be either thermal or quantum effects. Thermal fluctuation is simply a result of finite probability of transitions from one macrostate to other in an ensemble. The probabilistic description of thermal fluctuations in observables (e.g. number density etc) is handled effectively by statistical mechanics using ensemble theory. At near zero temperature thermal fluctuations are obviously diminished. For finite temperature, stochastic techniques such as Monte Carlo algorithms can be used with Boltzmann's weight as transition probability to capture the effect of thermal fluctuations, at least in ergodic systems.

The quantal fluctuations arise from quantum correlation correlation induced by interactions, which can not be trivially captured by classical models and stochastic techniques. The mean field theories effectively describe single particle dynamics in a dressed potential averaged over the rest of the particles. Therefore the states described by a mean field Hamiltonian are single particle states, and to recover the many-body picture one needs to consider the relevant direct product space composed of these one body Hilbert spaces. For instance let us consider the ensemble of energy macrostates of a mean-field Hamiltonian, which while certainly allows thermal fluctuations among the states with probability $\alpha\ e^{-\beta\Delta E}$, can not admit any quantum correlation between them (since the states are orthonormal to each other). However under the action of real many-body interaction these states can have non-zero matrix elements; giving rise to quantum correlation that eludes the mean field theory.

Thermal fluctuations are effectively handled by obtaining the partition function and taking ensemble averages weighted by free energy of the relevant configurations. On the other hand to account for quantum correlation, one needs to find the action of the original interaction potentials on many body mean field state, composed out of the single particle states. As an alternative premise, we explore the use of auxiliary field path integral developed in last chapter to account for small fluctuations from the static path, by keeping leading order contributions from Fourier decomposed auxiliary field. This method gives a systematic way of adding corrections of different orders to the static-path propagator, therefore so called as perturbed static path approximation. All these techniques try to describe small fluctuations in the free energy landscape.

Variational approach to study correlation

Variational techniques such as Hartree-Fock equations are constructed by choosing an appropriate set of parametrized basis in the Hilbert space acted on by the Hamiltonian, and then minimizing the energy expectation to obtain the parameters of the ground state. Consider a general interacting Hamiltonian

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \tag{3.1}$$

To build a variational theory for correlation for N particles induced by such many body interaction, we have to choose a set of orthonormal many body states. We begin with lowest N Hartree-Fock (HF) levels filled denoted as $|HF\rangle$ and given by the Slater determinant of corresponding single particle states.The next basis states are particle-holes excitations on $|HF\rangle$. So the trial basis state can be expressed as:[10]

$$|\nu\rangle = C_0^\nu |HF\rangle + \sum_{mi} C_{mi}^\nu a_m^\dagger a_i |HF\rangle + \frac{1}{4} \sum_{mnij} C_{mn,ij}^\nu a_m^\dagger a_n^\dagger a_i a_j |HF\rangle + \dots \tag{3.2}$$

Here we assume m, n as index above Fermi level and i, j below the level, and $a^\dagger |\Omega\rangle$ are HF eigenstates. So each successive terms represents different orders of particle-hole excitations on $|HF\rangle$. The coefficients $C_{mi}^\nu, C_{mn,ij}^\nu, \dots$ need to be fixed through variational minimization. The solution becomes exact if all such possible particle hole fluctuation is considered in the trial state, which however can not be solved since it amounts up to full diagonalization of the problem. However 3.2 provides a way to implement order by order correction.

Tamm Dancoff Approximation (TDA)

If we consider only up to single particle hole fluctuation, then the excited states is

$$|\nu\rangle \approx C_0^\nu |HF\rangle + \sum_{mi} C_{mi}^\nu a_m^\dagger a_i |HF\rangle \tag{3.3}$$

Since $\langle HF|Ha_m^\dagger a_i|HF\rangle = 0$, Tamm Dancoff Approximation does not correct the ground state energy. Therefore it suffices to consider

$$|\nu\rangle \approx \sum_{mi} C_{mi}^{\nu} a_m^\dagger a_i \,|HF\rangle \tag{3.4}$$

After transforming the Hamiltonian to the Hartree-Fock basis, we have

$$H = H_0 + V = \sum_{\nu\mu} h_{\mu\nu} a_\mu^\dagger a_\nu + \sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'} c_\mu^\dagger c_\nu^\dagger c_{\nu'} c_{\mu'} \tag{3.5}$$

Now $\langle mi|H|nj\rangle = \langle mi|H_0|nj\rangle + \langle mi|V|nj\rangle$ can be evaluated using Wick's theorem as

$$\langle mi|H_0|nj\rangle = \sum_{\nu\mu} h_{\mu\nu} \langle a_i^\dagger a_m a_n^\dagger a_j a_\mu^\dagger a_\nu\rangle = -\delta_{mn} h_{ji} + \delta_{ij} h_{mn} + \delta_{ij}\delta_{mn} \sum_k h_{kk} \tag{3.6}$$

$$\langle mi|V|nj\rangle = v_{mjin} - v_{mjni} + \delta_{ij} \sum_k (v_{mknk} - v_{mkkn}) - \delta_{mn} \sum_k (v_{jkik} - v_{jkki}) + \frac{1}{2}\delta_{ij}\delta_{mn} \sum_{kl} (v_{klkl} - v_{kllk}) \tag{3.7}$$

We note that the Hartree-Fock energy eigenvalues are given by

$$\epsilon_k = h_{kk} + \frac{1}{2} \sum_{kl} (v_{klkl} - v_{kllk}) \tag{3.8}$$

Therefore from 3.6, with antisymmetrized $\hat{v}_{mjin} = v_{mjin} - v_{mjni}$, we obtain

$$\langle mi|H|nj\rangle = \delta_{mn}\delta_{ij}(E_{HF} + \epsilon_m - \epsilon_i) + \hat{v}_{mjin} \tag{3.9}$$

Then the TDA secular equation is given by:

$$H\,|\nu\rangle = E_\nu\,|\nu\rangle \implies \sum_{nj} \langle mi|H|nj\rangle\, C_{nj}^{\nu} = E^{\nu} C_{mi}^{\nu}$$

$$\implies \sum_{nj} \left(\delta_{mn}\delta_{ij}(\epsilon_m - \epsilon_i) + \hat{v}_{mjin}\right) C_{nj}^{\nu} = (E^{\nu} - E_{HF}) C_{mi}^{\nu} \tag{3.10}$$

While TDA equation does introduce correlation among ph-excited state under the action of H in 3.9, it fails to produce any correction to the ground state $|HF\rangle$.But considering further terms in 3.2 makes the computation exponentially larger.

Equation of motion approach

To build correlation in the ground state without resorting to higher order particle-hole fluctuations, we must consider a general approach to constructing trial basis sets rather than taking $|HF\rangle$. Since we are trying to describe small fluctuations around a free energy configuration, like an oscillator state we consider the general state as

$$|\nu\rangle = Q_\nu^\dagger |\Omega\rangle , \quad Q |\Omega\rangle = 0 \tag{3.11}$$

The properties of the basis $|\nu\rangle$, especially the correlations contained is decided by $Q_\nu^\dagger$. Therefore in this formalism, rather than using variational techniques on $|\nu\rangle$, we have to use the equation of motion for $Q_\nu^\dagger$:

$$[H, Q_\nu^\dagger] |0\rangle = (E_\nu - E_0) Q_\nu^\dagger |0\rangle \tag{3.12}$$

$$\implies \langle 0| Q_{\nu'} [H, Q_\nu^\dagger] |0\rangle = (E_\nu - E_0) \langle 0| Q_{\nu'} Q_\nu^\dagger |0\rangle \qquad \text{(For an arbitrary } Q_{\nu'}^\dagger\text{)}$$

Since $\langle 0| Q_\nu^\dagger = 0 = \langle 0| H Q_\nu^\dagger$, we can cast 3.12 as

$$\langle 0| [Q_{\nu'}, [H, Q_\nu^\dagger]] |0\rangle = (E_\nu - E_0) \langle 0| [Q_{\nu'}, Q_\nu^\dagger] |0\rangle \tag{3.13}$$

Random Phase Approximation

It can be clearly seen that choosing $Q_\nu^\dagger = \sum_{mi} C_{mi}^\nu a_m^\dagger a_i$ results in a TDA approximation. To go beyond the TDA formalism of creation of a $1p-1h$ pair, without including the $2p-2h$ fluctuation; we need to both create and destroy $1p-1h$ pair in the ground state. Therefore we choose

$$Q_\nu^\dagger = \sum_{mi} X_{mi}^\nu a_m^\dagger a_i - \sum_{mi} Y_{mi}^\nu a_i^\dagger a_m \tag{3.14}$$

The RPA ground state is defined from 3.11 as

$$Q_\nu |RPA\rangle = 0 \tag{3.15}$$

Since the ground state $|RPA\rangle$ is not known so far, the expectation of commutation relations of fermion operators can not be determined. Here we make the so-called "quasi-Boson approximation" that the correlated ground state is not very different than the non-interacting HF ground state; which implies

$$\langle RPA|\left[a_m^\dagger a_i, a_n^\dagger a_j\right]|RPA\rangle \approx \langle HF|\left[a_m^\dagger a_i, a_n^\dagger a_j\right]|HF\rangle = \delta_{ij}\delta_{mn} \tag{3.16}$$

This approximation ignores the some of the fermionic commutation terms and hence violates Pauli exclusion principle. It can be argued that as long as $|Y_{mi}^\nu| << |X_{mi}^\nu|$, the approximation holds true. In fact putting $|Y_{mi}^\nu| = 0$ restores the TDA solution, i.e. uncorrelated HF ground state. Under the quasi-boson approximation, the spectrum of the excited states $a_m^\dagger a_i|0\rangle$ and $a_i^\dagger a_m|0\rangle$ can be determined using 3.13 by choosing $Q_\nu^\dagger = a_m^\dagger a_i$ and $a_i^\dagger a_m$, respectively:

$$\langle RPA|\left[a_i^\dagger a_m, [H, Q_\nu^\dagger]\right]|RPA\rangle = \Omega_\nu \langle RPA|\left[a_i^\dagger a_m, Q_\nu^\dagger\right]|RPA\rangle \tag{3.17}$$

$$\langle RPA|\left[a_m^\dagger a_i, [H, Q_\nu^\dagger]\right]|RPA\rangle = \Omega_\nu \langle RPA|\left[a_m^\dagger a_i, Q_\nu^\dagger\right]|RPA\rangle \tag{3.18}$$

Solution of RPA spectrum (at T=0)

Using the definition of $Q_\nu^\dagger$, 3.17 can be cast into a matrix form as

$$\langle HF|\, a_i^\dagger a_m[H, a_n^\dagger a_j]\,|HF\rangle\, X_{nj}^\nu - \langle HF|\, a_i^\dagger a_m[H, a_j^\dagger a_n]\,|HF\rangle\, Y_{nj}^\nu = \Omega_\nu X_{nj}^\nu$$
$$-\langle HF|\, a_m^\dagger a_i[H, a_n^\dagger a_j]\,|HF\rangle\, X_{nj}^\nu + \langle HF|\, a_m^\dagger a_i[H, a_j^\dagger a_n]\,|HF\rangle\, Y_{nj}^\nu = -\Omega_\nu Y_{nj}^\nu$$

Therefore with the definitions

$$A_{minj} = \langle HF|\, a_i^\dagger a_m[H, a_n^\dagger a_j]\,|HF\rangle = (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \hat{v}_{mjin} \tag{3.19}$$

$$B_{minj} = -\langle HF|\, a_m^\dagger a_i[H, a_n^\dagger a_j]\,|HF\rangle = \hat{v}_{mnij} \tag{3.20}$$

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \Omega_\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} \tag{3.21}$$

If the basis is transformed as

$$P^\nu = i\sqrt{\frac{\Omega_\nu}{2}}(X^\nu + Y^\nu); \quad Q^\nu = \sqrt{\frac{1}{2\Omega_\nu}}(X^\nu - Y^\nu) \tag{3.22}$$

then 3.21 reduces to

$$(A+B)(A-B)Q^\nu = \Omega_\nu^2 Q^\nu \tag{3.23}$$

Stability matrix and imaginary RPA eigenvalues

Even though A and B matrix are symmetric, 3.23 implies that $(A+B)(A-B)$ must be positive definite to have real RPA spectrum. If the matrix $(A-B)$ is positive definite, then $\exists$ square root matrix T such that $A-B = T^T T$, so that for $R^\nu = TQ^\nu$

$$T(A+B)T^T R^\nu = \Omega_\nu^2 R^\nu \tag{3.24}$$

Since $T(A+B)T^T$ is also positive definite, this is sufficient to yield real RPA spectrum. The origin of real and imaginary root is better explained through the stability matrix:

$$\delta = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \tag{3.25}$$

It can be shown that the eigenvalues of Hermitian matrix δ characterizes the nature of HF solution. For a stable HF solution, i.e. a minimum in free energy landscape, δ must be positive definite. In that case, 3.21 can be modified as

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \delta^{1/2}\delta^{1/2} \begin{pmatrix} X \\ Y \end{pmatrix} = \Omega_\nu \begin{pmatrix} X \\ Y \end{pmatrix} \implies \delta^{1/2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \delta^{1/2} \begin{pmatrix} \tilde{X} \\ \tilde{Y} \end{pmatrix} = \Omega_\nu \begin{pmatrix} \tilde{X} \\ \tilde{Y} \end{pmatrix} \tag{3.26}$$

This is a Hermitian eigenvalue equation, so the spectrum is real. This implies that the RPA frequencies for configurations corresponding to Hartree-Fock minimum are real. While the converse is not true, imaginary RPA frequency indicates unstable configuration in HF free energy landscape.

Calculation of correction to ground state

Inspired by the quasi-boson approximation, let us use the p-h creation and annihilation operators as Bosonic operators, i.e. $a_m^\dagger a_i \equiv B_{mi}^\dagger$ and $a_i^\dagger a_m \equiv B_{mi}$. Using this substitution in 3.19, the Hamiltonian can be expressed as

$$H_B = E_{HF} + \sum_{minj} A_{minj} B_{mi}^\dagger B_{nj} + \frac{1}{2}\sum_{minj}(B_{minj}B_{mi}^\dagger B_{nj}^\dagger + c.c) \tag{3.27}$$

Breaking the sums into (m,i) and (n,j) pairs and then using the bosonic commutation relation, it can be reduced to

$$H_B = E_{HF} - \frac{1}{2}\sum_{mi} A_{mimi} + \frac{1}{2}\begin{pmatrix} B^\dagger & B \end{pmatrix}\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} B \\ B^\dagger \end{pmatrix} \tag{3.28}$$

By introducing a Bogoliubov transformation

$$O_\nu^\dagger = \sum_{mi}\left(X_{mi}^\nu B_{mi}^\dagger - Y_{mi}^\nu B_{mi}\right) \tag{3.29}$$

3.28 can be diagonalized easily with the transformation, as

$$H_B = E_{HF} - \frac{1}{2}\,\mathrm{Tr}A + \frac{1}{2}\begin{pmatrix} O^\dagger & O \end{pmatrix}\chi^\dagger\delta\chi\begin{pmatrix} O \\ O^\dagger \end{pmatrix} = E_{RPA} + \sum_\nu \Omega_\nu O_\nu^\dagger O_\nu \tag{3.30}$$

From 3.30, it can be clearly seen that the RPA correction is an harmonic correction. Moreover E_{RPA} is given as [10]

$$E_{RPA} = E_{HF} - \frac{1}{2}\mathrm{Tr}\ A + \frac{1}{2}\sum_{\nu>0}\Omega_\nu \tag{3.31}$$

So RPA indeed captures correlation in ground state and renormalizes the ground state energy. It can be shown that $E_{rpa} < E_{hf}$, which happens because RPA accounts for higher correlation. However RPA is not a variational technique, so the corrections provided by RPA may be overestimated, leading to lower than exact energy. The validity of this premise rests on the validity of quasi boson approximation.

Correction at finite temperature

The finite temperature expectation value of an observable $\hat{O}$ in a system in thermal equilibrium is given by the thermal average:

$$\langle \hat{O} \rangle = \frac{\text{Tr } [e^{-\beta(H-\mu N)}\hat{O}]}{\text{Tr } e^{-\beta(H-\mu N)}} \tag{3.32}$$

At finite temperature, the system is described a temperature dependent density matrix. Consequently the Hartree-Fock equation or RPA equation at finite temperature is derived from finite temperature variational methods or thermal field theory using imaginary time Green's function. The finite temperature Hartree-Fock equation is given by

$$\langle i|H|j\rangle + \sum_k f_k \langle ik|\widetilde{V}|jk\rangle = \varepsilon_i \delta_{ij} \tag{3.33}$$

$$\text{where, } f_i = \frac{1}{1+\mathrm{e}^{\beta(\varepsilon_i-\mu)}}$$

Finite temperature RPA equations are used to determine the small amplitude collective vibrations about these states, just as zero temperature. As a finite temperature generalization of 3.19, the RPA equations at $T \neq 0$ for a general two body interaction u_{ijkl} can be expressed as [11]

$$-\Delta_{ij}\xi^{\nu}_{ij} + \sum_{k,l} u_{iljk}\left(f_k - f_l\right)\xi^{\nu}_{kl} = \Omega_\nu \xi^{\nu}_{ij} \tag{3.34}$$

where $\Delta_{ij} = \epsilon_i - \epsilon_j$ and f_i are the Fermi-Dirac occupation numbers $f_i = \left(1 + e^{\beta\epsilon_i}\right)^{-1}$. This gives rise to an eigenvalue problem of which Ω_ν are RPA frequencies and ξ^{ν}_{ij} is the amplitude associated with the p-h pair (i, j). As $T \to 0$, $f_k - f_l = 0$ for $k, l > \mu$ or $k, l < \mu$. So the sum is reduced to only pairs above and below the Fermi-level. Then 3.34 reduces to zero temperature RPA equation 3.21 with the map

$$\xi_{x_1x_2} = X(m,n) = \begin{cases} X_{x_1x_2}, & x_1 > \mu, x_2 < \mu \\ -Y_{x_2x_1}, & x_1 < \mu, x_2 > \mu \end{cases}$$

Finite temperature RPA correction for separable potential

As explained in chapter-1, any two body potential can be expressed as a sum of separable potentials, without loss of generality. So let's consider $u_{iljk} = -\sum_\alpha \chi_\alpha U^\alpha_{ij} v^\alpha_{lk}$. Then equation 3.34 can be written as

$$\xi^\nu_{ij} = -\sum_\alpha \chi_\alpha \frac{v^\alpha_{ij}}{\Delta_{ij} + \Omega_\nu} \left[\sum_{kl} v^\alpha_{lk} \left(f_k - f_l\right) \xi^\nu_{kl} \right] \tag{3.35}$$

Let's define $\zeta^\nu_\alpha \equiv \sum_{kl} v^\alpha_{lk} \left(f_k - f_l\right) \xi^\nu_{kl}$, so that for each $\alpha' = 1, \ldots, q$

$$\sum_{ij} v^{\alpha'}_{ji} \left(f_i - f_j\right) \zeta^\nu_\alpha = \sum_{ij} v^{\alpha'}_{ji} \left(f_i - f_j\right) \sum_{kl} v^\alpha_{lk} \left(f_k - f_l\right) \xi^\nu_{kl}$$

$$\implies \sum_\alpha \left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v^{\alpha'}_{ji} v^\alpha_{ij} \frac{f_i - f_j}{\Delta_{ij} + \Omega_\nu} \right] \zeta^\nu_\alpha = 0, \quad \alpha' = 1, \ldots, q \tag{3.36}$$

For any nontrivial solution to exist, the determinant of the matrix has to be zero. So

$$\det \left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v^{\alpha'}_{ji} v^\alpha_{ij} \frac{f_i - f_j}{\Delta_{ij} + \Omega_\nu} \right] = 0 \tag{3.37}$$

Consider the function given by

$$P(\omega) = \det \left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v^{\alpha'}_{ji} v^\alpha_{ij} \frac{f_i - f_j}{\Delta_{ij} + \omega} \right] \tag{3.38}$$

Clearly from 3.37, we see that $\omega = \pm\Omega_\nu$ are the roots of $P(\omega)$. On the other hand, if $v^{\alpha'}_{ji} v^\alpha_{ij} (f_i - f_j) \neq 0$ and continuity conditions are satisfied, then $\pm\Delta_{ij}$ is a pole. Since the poles and roots are known as $\{\pm\Delta_{ij}, \ldots\}$ and $\{\pm\Omega_\nu, \ldots\}$, then the function is

$$\det \left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v^{\alpha'}_{ji} v^\alpha_{ij} \frac{f_i - f_j}{\Delta_{ij} + \Omega_\nu} \right] = \frac{\prod_\nu \left(\Omega^2_\nu - \omega^2\right)}{\prod'_{ij} \left(\Delta^2_{ij} - \omega^2\right)} \tag{3.39}$$

By making an analytic continuation from $\omega \to i\omega$

$$\det \left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v^{\alpha'}_{ji} v^\alpha_{ij} \frac{f_i - f_j}{\Delta_{ij} + i\omega} \right] = \frac{\prod_\nu \left(\Omega^2_\nu + \omega^2\right)}{\prod'_{ij} \left(\Delta^2_{ij} + \omega^2\right)} \tag{3.40}$$

PSPA: Path integral approach for finding dynamical fluctuation

Let us consider the exact many body propagator derived earlier.

$$U = \int \mathcal{D}[\xi] \exp\left[-\frac{1}{2}\sum_{\alpha}\int_0^\beta d\tau \chi_\alpha \xi_\alpha^2(\tau)\right] \mathrm{T}\exp\left[-\int_0^\beta d\tau \left(K - \sum_\alpha \chi_\alpha \xi_\alpha(\tau) V_\alpha\right)\right] \tag{3.41}$$

Here instead of a saddle point approximation, let's take a Fourier decomposition of the auxiliary field $\xi(\tau)$ in terms of Matsubara frequencies $\omega_r = 2\pi r/\beta$ as

$$\xi(\tau = n\epsilon) = \sum_{r=-(N-1)/2}^{(N-1)/2} \sigma_r e^{i\omega_r \tau} \tag{3.42}$$

We have assumed here $\sigma_{-r} = \sigma_r^*$ to keep $\xi(\tau)$ real . The path integral can now be written in terms of σ_r as (for the sake of simplicity only one separable term is kept):

$$U = \int \mathcal{D}[\sigma] \exp\left(-\frac{1}{2}\chi\beta\sum_r |\sigma_r|^2\right) \mathbf{T}\exp\left[-\int_0^\beta d\tau \left(K - \chi\sigma_0 V - \chi\sum_{r\neq 0}\sigma_r e^{i\omega_r\tau} V\right)\right] \tag{3.43}$$

The functional integral can now be split into τ-dependent and independent parts as

$$H_\sigma = h_0 + h_1, \quad h_0 = K - \chi\sigma_0 V, \quad h_1 = -\chi\sum_{r\neq 0}\sigma_r e^{i\omega_r\tau} V \tag{3.44}$$

so that with $h_1(\tau) = e^{\tau h_0} h_1 e^{-\tau h_0}$,

$$\mathbf{T}\exp\left[-\int_0^\beta d\tau \left(K - \chi\sigma_0 V - \chi\sum_{r\neq 0}\sigma_r e^{i\omega_r\tau} V\right)\right] = e^{-\beta h_0}\mathrm{T}\exp\left[\int_0^\beta d\tau h_1(\tau)\right] \equiv e^{-\beta h_0}\mathcal{U}_\sigma \tag{3.45}$$

Now the complete many -body propagator can be written as

$$U = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} e^{-\beta h_0} \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta\sum_{r>0}|\sigma_r|^2\right) u_\sigma \tag{3.46}$$

This propagator is the Gaussian weighted average of one-body evolutions $e^{-\beta h_0}$ corresponding to a static field σ_0 along with a correction factor contributed by time-dependent fluctuations of $\xi(\tau)$ around σ_0. For $\sigma_r = 0$, SPA result is recovered.

Partition Function and thermodynamics of PSPA propagator

The partition function of the grand-canonical ensemble, using 3.46 ($\mu = 0$) is given by

$$Z = \text{Tr } U = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} \text{Tr } e^{-\beta h_0} \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} |\sigma_r|^2\right) \frac{\text{Tr } e^{-\beta h_0} u_\sigma}{\text{Tr } e^{-\beta h_0}}$$

$$\implies Z = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}x\beta\sigma_0^2} \zeta_0 \zeta_0' \equiv \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\beta F_0(\beta;\sigma_0)} \tag{3.47}$$

Where,

$$\zeta_0 = \text{Tr}\, e^{-\beta h_0} = \prod_i \left[1 + e^{-\beta\epsilon_i(\sigma_0)}\right] \tag{3.48}$$

$$\zeta_0{}' = \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} |\sigma_r|^2\right) \langle \mathcal{U}_\sigma \rangle_0 \tag{3.49}$$

The further calculations are performed in the eigenbasis of h_0. ζ_0 gives the partition function for static part h_0 while $\zeta_0{}'$ describes the time-dependent fluctuations about σ_0. For SPA, since $\sigma_r = 0 \forall r \neq 0$; $\zeta_0{}' = 1$. To evaluate $\zeta_0{}'$, we have to evaluate $\langle \mathcal{U}_\sigma \rangle_0$. We use the interaction picture $V(\tau) = e^{\tau h_0} V e^{-\tau h_0}$ and keep up to second order [12]

$$\begin{aligned} \log \langle \mathcal{U}_\sigma \rangle_0 \approx & \chi \sum_{r\neq 0} \sigma_r \int_0^\beta d\tau e^{i\omega_r \tau} \langle V(\tau) \rangle_c \\ & + \frac{1}{2}\chi^2 \sum_{rs\neq 0} \sigma_r \sigma_s \int_0^\beta d\tau d\tau' e^{i\omega_r \tau} e^{i\omega_s \tau'} \left[\langle \text{T} V(\tau) V(\tau') \rangle_c - \langle V(\tau) \rangle_c \langle V(\tau') \rangle_c\right] \end{aligned} \tag{3.50}$$

The integrations of $\langle V(\tau) \rangle_c$ vanishes and only connected diagrams are taken for evaluating four fermion operators. Using Wick's theorem, [13]

$$\langle \text{T} V(\tau) V(\tau') \rangle_c = -\sum_{ij} v_{ij} v_{ij} g_i^0(\tau' - \tau)\, g_j^0(\tau - \tau') \tag{3.51}$$

where the unperturbed temperature Green's function g_i^0 is given by

$$g_i^0(\tau - \tau') = -\left\langle a_i(\tau) a_i^\dagger(\tau') \right\rangle_0 = \frac{1}{\beta} \sum_{k=-\infty}^{\infty} \frac{e^{-i\nu_k(\tau - \tau')}}{i\nu_k - \epsilon_i} \tag{3.52}$$

The Green's function can be calculated as:

$$\int_0^\beta d\tau d\tau' e^{i\omega_r\tau} e^{i\omega_s\tau'} \left\langle \mathrm{T}V(\tau)V(\tau')\right\rangle_c = -\delta_{r,-s}\sum_{ij} v_{ij}v_{ji}\sum_{k=-\infty}^{\infty}\frac{1}{i\nu_k-\epsilon_i}\frac{1}{i\nu_k-(\epsilon_j-i\omega_r)} \tag{3.53}$$

The sum over k is performed using Matsubara technique.

$$S=\sum_{k=-\infty}^{\infty}\frac{1}{i\nu_k-\epsilon_i}\frac{1}{i\nu_k-(\epsilon_j-i\omega_r)}=\frac{1}{2\pi i}\oint_C dz\frac{-\beta}{e^{\beta z}+1}\frac{1}{z-\epsilon_i}\frac{1}{z-(\epsilon_j-i\omega_r)} \tag{3.54}$$

This contour integral along a large circle is given by the two poles $z=\epsilon_i,\epsilon_j-i\omega_r$ and the sum evaluates to

$$S=-\beta\left(\frac{1}{e^{\beta\epsilon_i}+1}\frac{1}{\epsilon_i-\epsilon_j+i\omega_r}+\frac{1}{e^{\beta\epsilon_j}+1}\frac{1}{\epsilon_j-\epsilon_i-i\omega_r}\right)=-\beta\left(\frac{f_i-f_j}{\Delta_{ij}+i\omega_r}\right) \tag{3.55}$$

Therefore the double integral 3.53 reduces to

$$\int_0^\beta d\tau d\tau' e^{i\omega_r\tau} e^{i\omega_s\tau'} \left\langle \mathrm{T}V(\tau)V(\tau')\right\rangle_c = -\beta\delta_{r,-s}\sum_{ij} v_{ij}v_{ji}\frac{f_i-f_j}{\Delta_{ij}+i\omega_r} \tag{3.56}$$

Therefore from 3.50, $\langle\mathcal{U}_\sigma\rangle_0$ can be determined as

$$\log\langle\mathcal{U}_\sigma\rangle_0=-\frac{1}{2}\chi^2\beta\sum_{r>0}|\sigma_r|^2\sum_{ij}v_{ij}v_{ji}\frac{f_i-f_j}{\Delta_{ij}+i\omega_r}=-\chi\beta\sum_{r\neq0}|\sigma_r|^2a_r \tag{3.57}$$

$$\implies \langle\mathcal{U}_\sigma\rangle_0=\exp\left(-\chi\beta\sum_{r>0}a_r\left|\sigma_r\right|^2\right) \tag{3.58}$$

Now from 3.49,

$$\zeta_0{}'=\int\mathcal{D}'[\sigma]\exp\left(-\chi\beta(1+a_r)\sum_{r>0}\left|\sigma_r\right|^2\right) \tag{3.59}$$

If $(1+a_r)>0$ for each r, then the integral for $\zeta_0{}'$ is Gaussian, so that

$$\zeta_0'=\prod_{r>0}(1+a_r)^{-1} \tag{3.60}$$

If we restore the presence of several separable terms, then the expression for $\langle\mathcal{U}_\sigma\rangle_0$ is

$$\langle\mathcal{U}_\sigma\rangle_0=\exp\left(-\chi\beta\sum_r\sum_{\alpha\gamma}\sigma_r^{\alpha*}a_r^{\alpha\gamma}\sigma_r^\gamma\right) \tag{3.61}$$

where each $\chi_\alpha = \chi$

$$a_r^{\alpha\gamma}(\sigma_0) = \chi \sum_{ij} v_{ij}^{\alpha} v_{ji}^{\gamma} \frac{(f_i - f_j)}{\Delta_{ij} + i\omega_r} \quad \text{and } \zeta_0' = \prod_{r>0} \det(1 + a_r)^{-1} \tag{3.62}$$

From 3.40 and 3.62

$$\zeta_0' = \prod_{r>0} (1 + a_r)^{-1} = \prod_{r>0} \frac{\prod_{ij}' (\omega_r^2 + \Delta_{ij}^2)}{\prod_{\nu} (\omega_r^2 + \Omega_\nu^2)} = \frac{\prod_{ij}' \frac{1}{\Delta_{ij}} \sinh \frac{\beta\Delta_{ij}}{2}}{\prod_{\nu} \frac{1}{\Omega_r} \sinh \frac{\beta\Omega_\nu}{2}} \tag{3.63}$$

where the infinite product representation of $\sinh x = x \prod_{r>0} (1 + x^2/\pi^2 r^2)$ is used. Now the effective free energy of a specific configuration is given by

$$F_0(\beta; \sigma_0) = \frac{1}{2}\chi\sigma_0^2 - \frac{1}{\beta}\log\zeta_0 - \frac{1}{\beta}\log\zeta_0' \tag{3.64}$$

The complete PSPA partition function is given by

$$Z^{(\mathrm{PSPA})} = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}x\beta\sigma_0^2} \prod_i \left(1 + e^{-\beta\epsilon_i(\sigma_0)}\right) \frac{\prod_{ij}' \frac{1}{\Delta_{ij}} \sinh \frac{\beta\Delta_{ij}}{2}}{\prod_{\nu} \frac{1}{\Omega_\nu} \sinh \frac{\beta\Omega_\nu}{2}} \tag{3.65}$$

Validity of PSPA results

As already revealed through equations 3.40 and 3.62, the idea of perturbed static path approximation at second order is deeply intertwined with Random Phase Approximation. In fact the roots obtained in the determinant equation 3.40 can be shown as the small RPA oscillation frequency about σ_0. The critical assumption in PSPA formalism is about the convergence of the Gaussian integrals in 3.60, which is true only if $1 + a_r > 0$, i.e. $-\Omega_\nu^2 < \omega_r^2$ for all r and ν. However, the RPA frequencies are real for most of the favorable configurations in free energy landscape.

At T=0, the condition requires all the RPA frequencies to be real, which in turn is decided by the SPA free energy landscape around the configuration. For finite temperature however, the formalism holds till the largest imaginary part of Ω is less than $\omega_1 = 2\pi T$, beyond which the PSPA method breaks down.

Chapter 4

Implementation and Results

We have tested the method mostly on small 1-D Fermi-Hubbard systems at half-filling. In this chapter we are going to present how the method is implemented in practice, the instructive features of Random Phase Approximation on a two-site lattice, comparison of SPA, PSPA and ED results; and finally the results from an implementation of Metropolis algorithm using PSPA.

Algorithm

These are the general steps used for obtaining PSPA result for a many body Hamiltonian with two body interaction. Specifics of Hubbard model as implemented in the project has been mentioned whenever possible as example

1. Suppose the given Hamiltonian is $\hat{H} = \sum_{ij} h_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} u_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$. Then diagonalize the interaction part $u_{\alpha\beta}$ to express given potential as a sum of separable potentials, like $\chi V = \sum_\alpha \chi_\alpha V_\alpha^2$.

   For Hubbard Model, it has been explained in chapter 2 how the interaction term can be effectively expressed in terms of spin operators as

   $$\mathcal{H} = \mathcal{H}_{\mathcal{TB}} - \frac{U}{4} \sum_i \sigma_{zi}^2 + \mu N \tag{4.1}$$

   For further computations and calculations, we assume a discrete auxiliary field Hubbard Stratonovich transformation for Hubbard model, which means the auxiliary field can take values either ± 1 at each site.

2. Construct the static path Hamiltonian and separable potentials in a suitable basis using equation 2.14.

$$H_{spa} = K - \sum_{\alpha} \chi_{\alpha} \xi_{\alpha 0} V_{\alpha} + \frac{1}{2} \sum_{\alpha} \chi_{\alpha} \xi_{\alpha 0}^2$$

We use position basis for the SPA Hamiltonian of Hubbard model

$$H_{spa} = H_0 - \frac{U}{2} \sum_{i} m_i \sigma_{zi} + \frac{U}{4} \sum_{i} m_i^2 \tag{4.2}$$

3. Diagonalize H_{spa}. Calculate the chemical potential from the eigenvalues at the given temperature and filling. Use the diagonalizing matrix (u) to transform all the potentials ($v^{\alpha} \rightarrow u^{\dagger} v^{\alpha} u$) to the eigenbasis of H_{spa}.

4. For a given value of ω, construct the $q \times q$ matrix, the determinant of which gives RPA frequencies as root. We will call this matrix "pseudoRPA matrix" (pRPA) hereafter. The (α, α') element of the matrix is given by

$$pRPA_{\alpha,\alpha'}(\omega) = \delta_{\alpha\alpha'} + \chi_{\alpha} \sum_{ij} v_{ji}^{\alpha'} v_{ij}^{\alpha} \frac{f_i - f_j}{e_i - e_j + \omega} \tag{4.3}$$

5. To evaluate the PSPA free energy, we need to find all the roots and poles of det(pRPA)(ω). Since the roots and poles are symmetric about 0, we need to scan only the positive part. We note that only possible poles are Δ_{ij}'s. Therefore check det(pRPA)($\omega = \Delta_{ij} + \delta$). if the return value is very large (greater than a threshold), then store the corresponding Δ_{ij} as pole.

6. It has been observed that the pole and roots of the function occur alternately. Therefore to find the roots, use Golden section search[14] to find the minimum of |det(pRPA)(ω)| between every poles. Store as root if |minimum value| $<$ tolerance, else the root is not real; so discard the RPA calculation.

7. If number of poles (Δ_{ij}) = number of roots (Ω_{ν}), then use the values in 3.64 to obtain the PSPA free energy.

RPA on a two site system

Let's consider a two site Hubbard model with $t = 1, U = 5$. Let's choose the real space basis as $\{1\uparrow, 2\uparrow, 1\downarrow, 2\downarrow\}$. Since we have chosen discrete auxiliary fields, there are two unique auxiliary field configurations: $\{+1, +1\}$ (Ferromagnetic) or $\{+1, -1\}$ (Antiferromagnetic) and the SPA Hamiltonian is given by

$$H_{spa} = H_{TB} - \frac{U}{2}\left(\sigma_{z1}m_1 + \sigma_{z2}m_2\right) + \frac{U}{2} \tag{4.4}$$

After absorbing the constant shift $U/2$ in μ, we are going to focus on the behavior of SPA Hamiltonian in the different auxiliary field background.

Ferromagnetic Background

For auxiliary field {+1,+1}, the diagonalizing matrix is

$$u = \begin{pmatrix} 0.707107 & -0.707107 & 0. & 0. \\ 0.707107 & 0.707107 & 0. & 0. \\ 0. & 0. & 0.707107 & -0.707107 \\ 0. & 0. & 0.707107 & 0.707107 \end{pmatrix} \tag{4.5}$$

As expected the lowest eigenstates are in spin-$\uparrow$ sector, with the ground state being $\frac{1}{\sqrt{2}}\left(|1\uparrow\rangle + |2\uparrow\rangle\right)$ (bonding), and the second lowest being $\frac{1}{\sqrt{2}}\left(|1\uparrow\rangle - |2\uparrow\rangle\right)$ (anti-bonding). The spin-$\downarrow$ sector is higher in energy and has a similar structure. Now the effects of separable potentials $\{\sigma_{z1}, \sigma_{z2}\}$ is to be studied. In the same basis arrangement, the separated potentials are given by

$$\sigma_{z1} = \begin{pmatrix} 1 & 0 & 0. & 0. \\ 0 & 0 & 0. & 0. \\ 0. & 0. & -1 & 0 \\ 0. & 0. & 0 & 0 \end{pmatrix}, \quad \sigma_{z2} = \begin{pmatrix} 0 & 0 & 0. & 0. \\ 0 & 1 & 0. & 0. \\ 0. & 0. & 0 & 0 \\ 0. & 0. & 0 & -1 \end{pmatrix}, \tag{4.6}$$

After basis transformation to the SPA eigenstate, the potentials in the energy eigenbasis $\{a_0, a_1, a_2, a_3\}$ are

$$\tilde{\sigma}_{z1} = u^\dagger \sigma_{z1} u = \begin{pmatrix} 0.5 & -0.5 & 0. & 0. \\ -0.5 & 0.5 & 0. & 0. \\ 0. & 0. & -0.5 & 0.5 \\ 0. & 0. & 0.5 & -0.5 \end{pmatrix}, \quad \tilde{\sigma}_{z2} = \begin{pmatrix} 0.5 & 0.5 & 0. & 0. \\ 0.5 & 0.5 & 0. & 0. \\ 0. & 0. & -0.5 & -0.5 \\ 0. & 0. & -0.5 & -0.5 \end{pmatrix} \tag{4.7}$$

Equations 4.7 describe the possible quantum fluctuations in the system. Two HF states, orthonormal under the action of H_{HF} can have non-zero matrix element under the action of $V_\alpha (= \sigma_{zi})$. In this case σ_{zi} couples $|e_1\rangle$ to $|e_2\rangle$; and $|e_3\rangle$ to $|e_4\rangle$, and vice-versa; which implies that only $|e_1\rangle \leftrightarrow |e_2\rangle$ transition can occur.

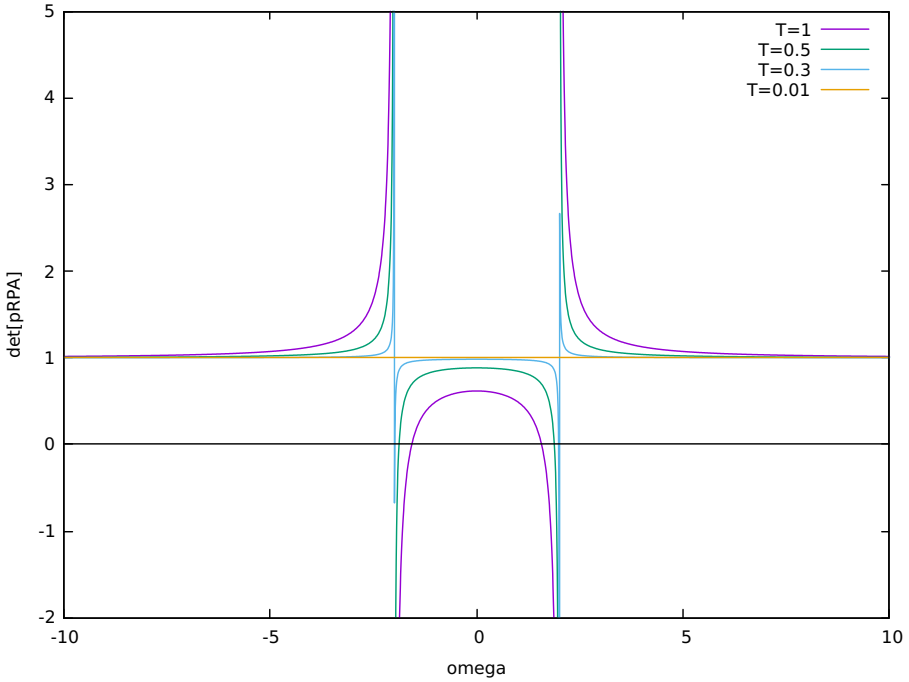
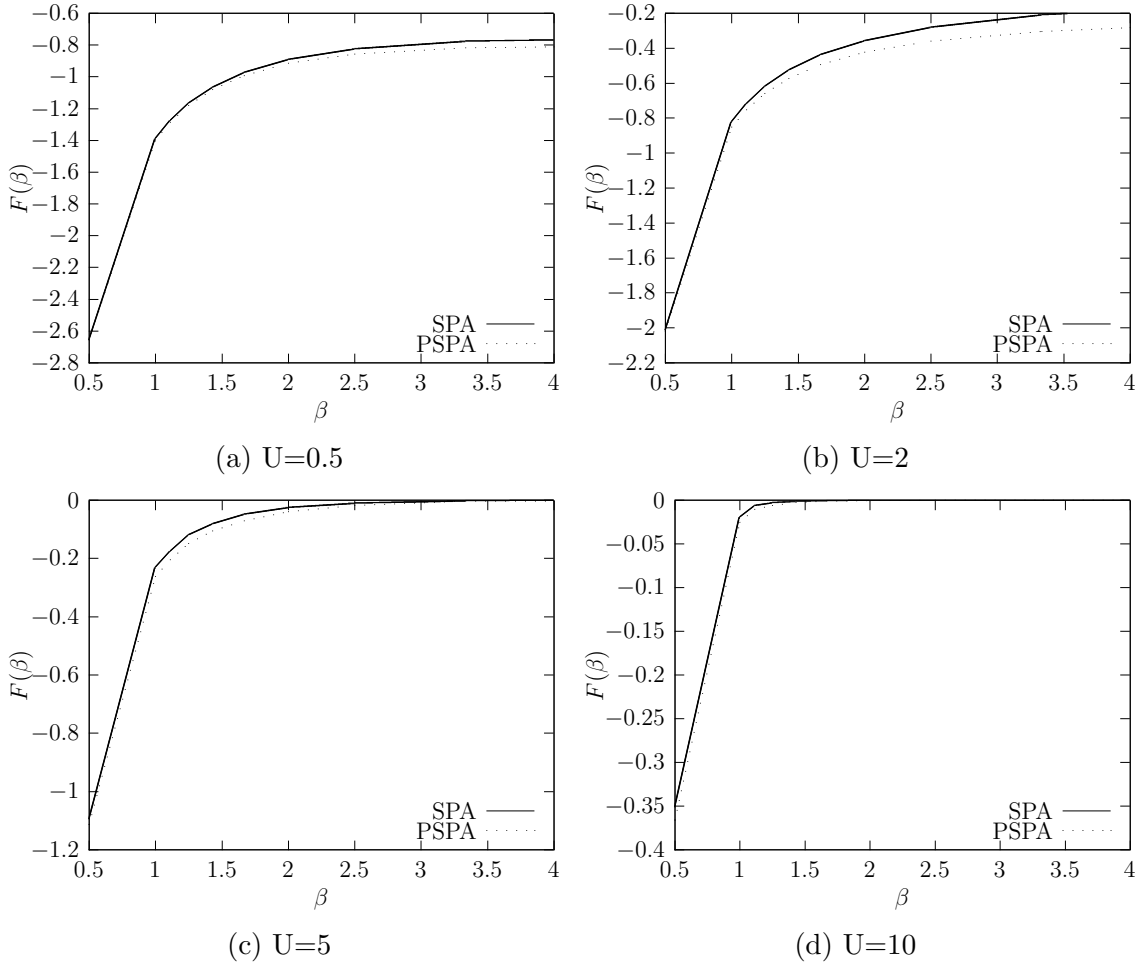


Figure 4.1: Determination of RPA frequency for $t = 1, U = 5, m_1 = m_2 = 1$

Figure-4.1 shows the determination of RPA frequencies Ω_ν as roots of and Δ_{ij} as poles from the plot of $\det[\text{pRPA}(\omega)]$. As expected, the poles occur at $\pm(E_1 - E_0)$; and as $T \to 0$ the roots keep getting closer to the poles, till it becomes constant at 1.

At $T \approx 0$, $f(e_1) = f(e_2) = 1$, so no excitations are possible at low temperature, hence no corrections. In practice, at low temperature, the pseudoRPA matrix elements become $\delta_{\alpha\alpha'} + \chi_\alpha \sum_{ij} v_{ji}^{\alpha'} v_{ij}^{\alpha} \frac{f_i - f_j}{e_i - e_j + \omega} \equiv \delta_{\alpha\alpha'}$ (Identitiy) Therefore at $T = 0$ the determinant becomes constant at 1, resulting in no solution. As temperature increases, $f(e_1) \neq f(e_2)$ allows the transition to take place and a real RPA root develops, with the poles at $\Delta = \pm(E_1 - E_0)$; which signifies the $|a_0\rangle \leftrightarrow |a_1\rangle$ transition.



(a) U=0.5

(b) U=2

(c) U=5

(d) U=10

Figure 4.2: SPA vs PSPA free energy for ferromagnetic auxiliary fields

From 4.2, we see PSPA is different in an intermediate range of temperature high enough that the Fermi-Dirac distribution allows quantum fluctuation between levels below μ, but low enough for the PSPA contribution to stay relevant.

Antiferromagnetic Background

For auxiliary field {+1,-1}, the states are doubly degenerate at $\{-\epsilon, \epsilon\}$, and the structure of the diagonalizing matrix is

$$u = \begin{pmatrix} 0 & y & -x & 0 \\ 0 & x & y & 0 \\ x & 0 & 0 & -y \\ y & 0 & 0 & x \end{pmatrix} \quad \text{such that as U} \to \infty; x \to 0. \tag{4.8}$$

Accordingly the general structure of $V_i = \sigma_{zi}$ is given by

$$V_\alpha = \begin{pmatrix} v_{11} & 0 & 0 & v_{14} \\ 0 & v_{22} & v_{23} & 0 \\ 0 & v_{32} & v_{11} & 0 \\ v_{41} & 0 & 0 & v_{22} \end{pmatrix} \tag{4.9}$$

With the knowledge of each V_α, the pRPA matrix determinant can be calculated as

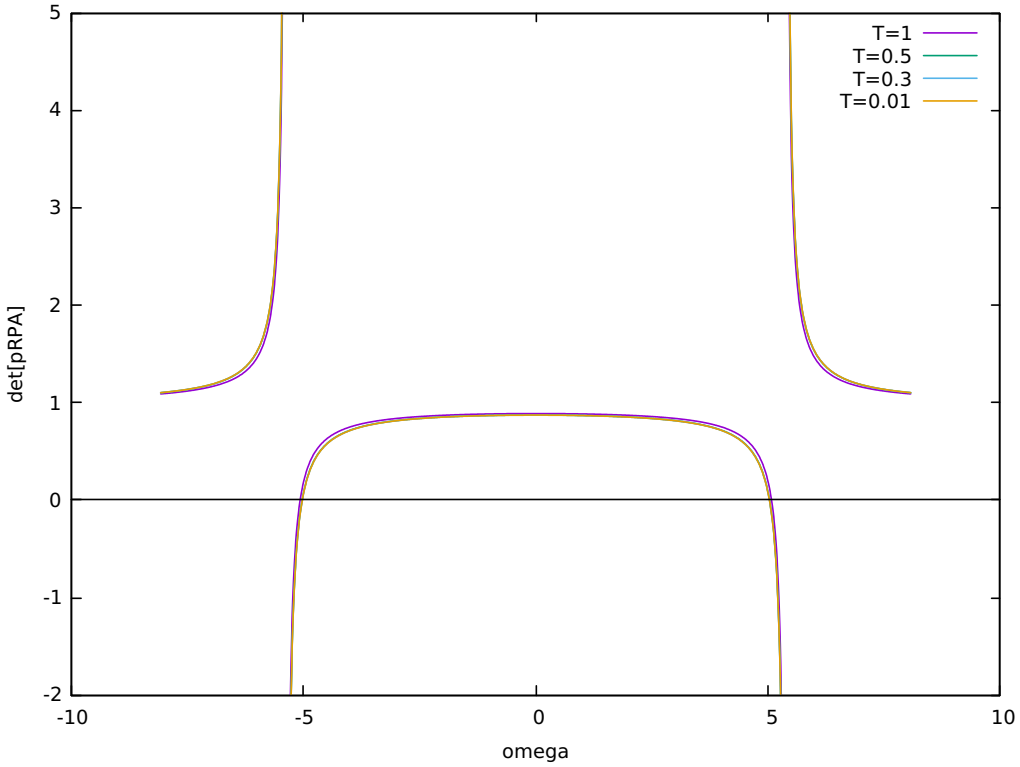
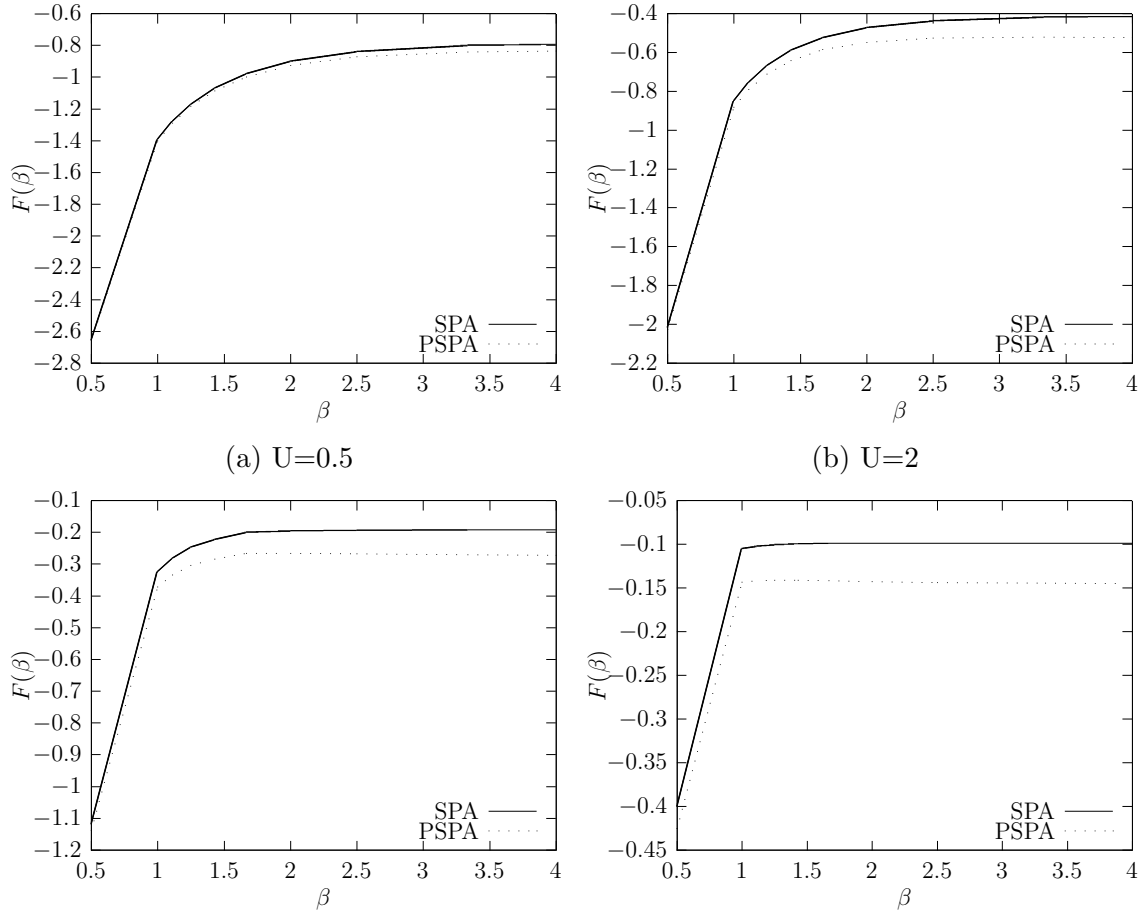


Figure 4.3: Determination of RPA frequency for $t = 1, U = 5, m_1 = 1, m_2 = -1$

Here the transition between $|a_1\rangle \leftrightarrow |a_4\rangle$ and $|a_2\rangle \leftrightarrow |a_3\rangle$ is made possible at all temperature because of the nonzero matrix element. The poles of det[[pRPA]] for $U = 5$ indeed occur at $\pm 5.38(2\epsilon)$. From figure-4.3 it is clear that RPA frequencies are nearly stable at all temperature. Moreover this transition signifies a transition to $\{|1\downarrow\rangle, |2\uparrow\rangle\}$ from $\{|1\uparrow\rangle, |2\downarrow\rangle\}$ can be treated like a two-spin flip.



(a) U=0.5 (b) U=2

(c) U=5 (d) U=10

Figure 4.4: SPA vs PSPA free energy for antiferromagnetic auxiliary fields

From 4.4, we see that even in low temperature, RPA correction still holds and the PSPA free energy lies lower than SPA free energy and obviously below SPA free energy of ferromagnetic auxiliary field.

Comparison of SPA, PSPA and ED results

So far we have observed that correlated states with PSPA correction have lower free energy than SPA states. For small number of sites, the Hubbard Hamiltonian can be exactly diagonalized, so both SPA and PSPA can be compared against exact results. However for one-dimensional system with high U, SPA result is expected to deviate more from exact result (because of "strong correlation"). SPA or PSPA free energy can be calculated as $-\frac{1}{\beta}\log Z$, where Z_{pspa} is given by equation-3.65 as

$$Z^{(\mathrm{PSPA})} = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}x\beta\sigma_0^2} \prod_i \left(1 + e^{-\beta\epsilon_i(\sigma_0)}\right) \frac{\prod'_{ij} \frac{1}{\Delta_{ij}} \sinh\frac{\beta\Delta_{ij}}{2}}{\prod_\nu \frac{1}{\Omega_\nu} \sinh\frac{\beta\Omega_\nu}{2}} \tag{4.10}$$

SPA as a limiting case of PSPA

We note that $\lim_{x\to 0} \frac{\sinh(x)}{x} = 1$, so at high temperature

$$\lim_{\beta\to 0} \frac{\prod'_{ij} \frac{1}{\Delta_{ij}} \sinh\frac{\beta\Delta_{ij}}{2}}{\prod_\nu \frac{1}{\Omega_\nu} \sinh\frac{\beta\Omega_\nu}{2}} = 1 \qquad \because \text{ (\# of roots = \# of poles)} \tag{4.11}$$

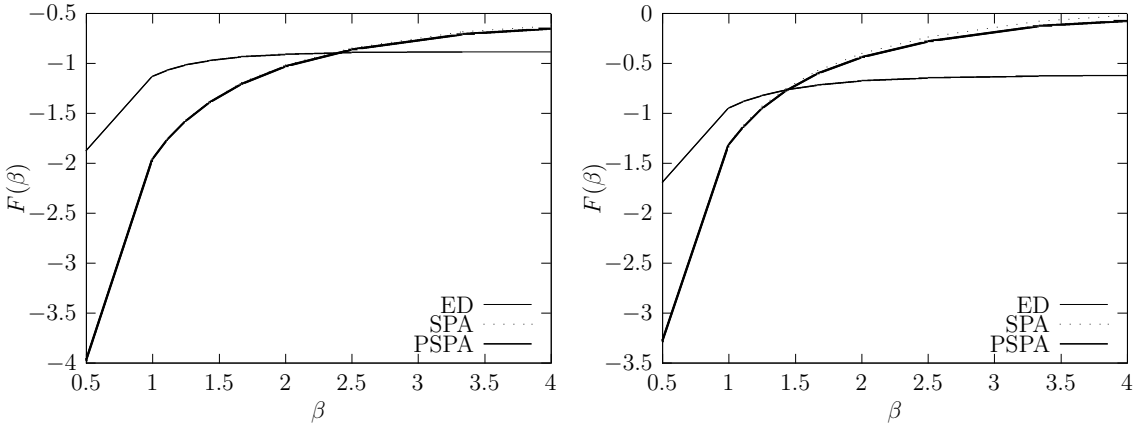
So at high temperature, Z^{PSPA} reduces to Z^{SPA} as

$$Z^{\mathrm{SPA}} = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}x\beta\sigma_0^2} \prod_i \left(1 + e^{-\beta\epsilon_i(\sigma_0)}\right) \tag{4.12}$$

The other natural limit is reducing the interaction in the system. The entire premise of PSPA is to account for correlation caused by residual interaction, so for a nearly free system of particles, it should reduce to SPA results. To determine the RPA frequencies as $u_{ijkl} \to 0$, let's consider the generalized RPA equation 3.34:

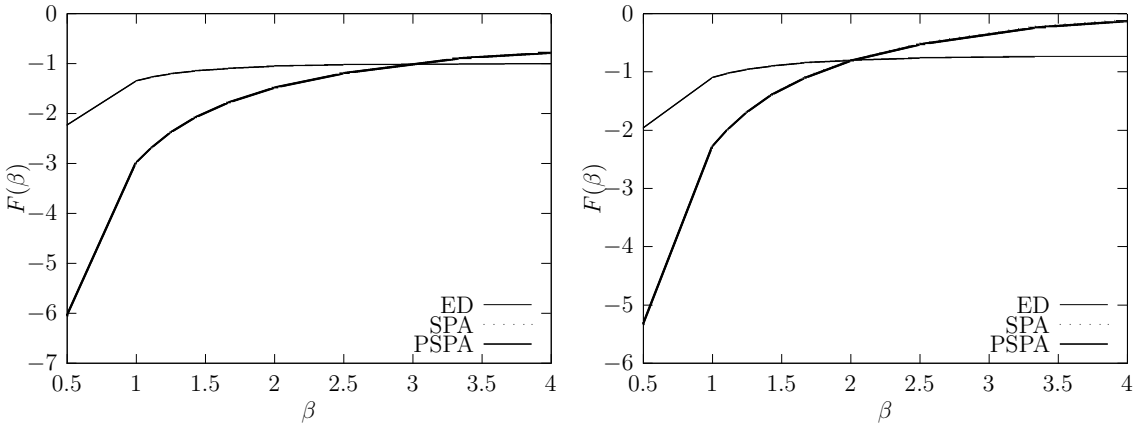
$$-\Delta_{ij}\xi^\nu_{ij} + \sum_{k,l} u_{iljk} \left(f_k - f_l\right) \xi^\nu_{kl} = \Omega_\nu \xi^\nu_{ij} \tag{4.13}$$

Clearly as $u_{ijkl} \to 0$, $\Omega_\nu \approx \Delta_{ij}$, so $\lim_{u_{ijkl}\to 0} \zeta_0{}' = 1$, therefore Z^{PSPA} reduces to Z^{SPA}.

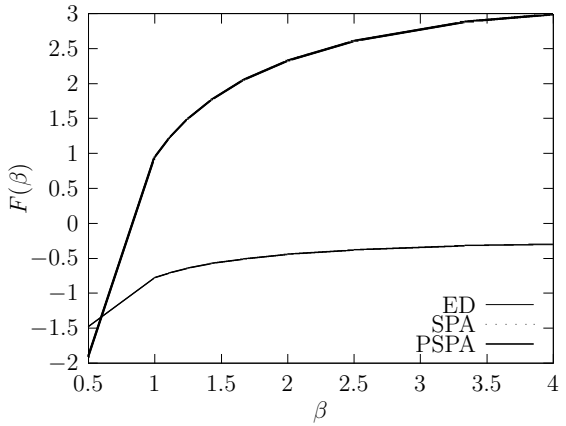


(a) U=0.5 (b) U=2

Figure 4.5: Comparison of SPA, PSPA and ED free energy for L=2



(a) U=0.5 (b) U=2



(c) U=10

Figure 4.6: Comparison of SPA, PSPA and ED free energy for L=4

PSPA correction as a function of system parameter

As seen in Figures 4.5 and 4.6, exact solution significantly deviates from SPA or PSPA energies, which is encountered many times in strongly correlated systems. So we are going to focus on correction offered by PSPA formalism is, which is $\alpha \ln(\zeta')$.

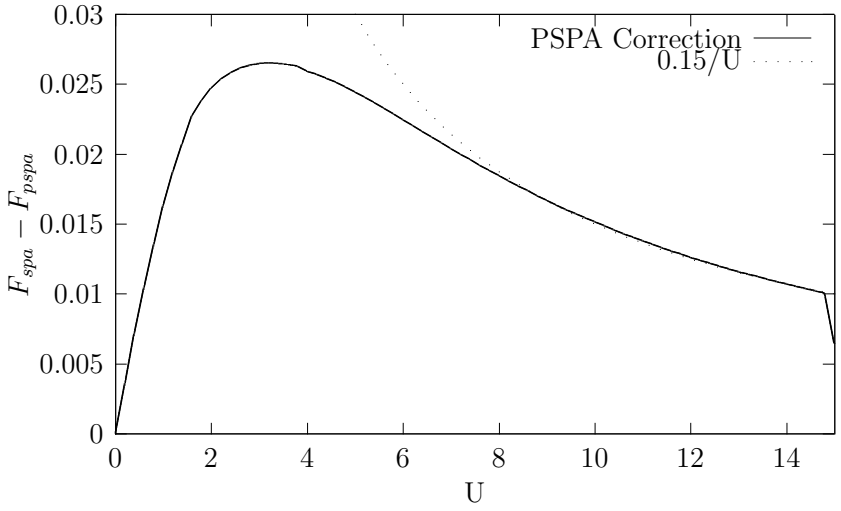


Figure 4.7: PSPA correction to SPA ground state energy for L=4

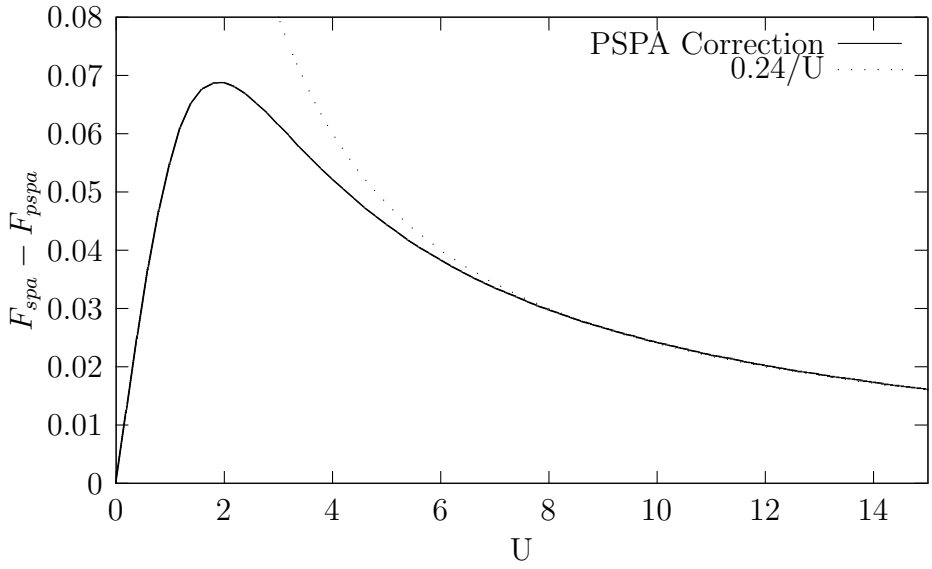


Figure 4.8: PSPA correction to SPA ground state energy for L=2

For non-interacting or nearly non interacting systems (i.e. for $U \approx 0$), SPA result itself is exact, so the correction is non-existent. On the other hand, for systems with very large U, charge fluctuations are again heavily suppressed, therefore the correction diminishes after a suitable U as $\sim 4t^2/U$[15] . This indicates that current PSPA correction is not sufficient for describing the physics at high U.

Chapter 5

Outlook

In this project, we started with a mean-field like path-integral based approach to solve many-body problems. Then after exploring Random Phase Approximation from an equation of motion approach, we found that the path integral based approach can be used to compute order-by-order correction to the "static-path" or mean field Hamiltonian. For a second order correction, the correction to the the mean field partition function for a given state was found to be proportional to generalized RPA frequency for the given state. In the limits of weak interaction or high temperature, PSPA partition function is found to coincide with SPA partition function.

We have studied the variation of the correction in different states and with different parameters. We have found that PSPA correction does introduce correction to the ground state, but it may not be sufficient for exact solution, especially at high U.

The future goals are to parallelize the algorithm for searching the RPA frequencies, which has been found to be the slowest step in the calculation. It will help us probe larger systems and 2-D systems. Moreover now we are interested in adapting the Metropolis algorithm while using the PSPA free energy for acceptance probability, and to see how if affects variations of quantities of interest like spin structure factor etc with temperature.

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