Computational Study of Strongly Correlated Systems

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Introduction

- What are Strongly Correlated Systems and why study them?

Many intersting physical phenomenon in solids appear due to strong correlations such as

- Metal Insulator Transitions
- Magnetism
- Superconductivity
- Quantum Hall Effect

Non-interactive models cannot explain these phenomenon

How do we explain these phenomenon?

Many Body Problem

Microscopically solids are complicated many body systems described by the Hamiltonian

$$\hat{H}_{solid} = \underbrace{\left[-\frac{\hbar^2}{2M}\sum_{\alpha=1}^{K}\nabla_\alpha^2 + \frac{e^2}{4\pi\epsilon_0}\frac{1}{2}\sum_{\alpha,\beta}^{\alpha\neq\beta}\frac{Z_\alpha Z_\beta}{|\vec{R}_\alpha - \vec{R}_\beta|}\right]}_{\hat{H}_{ion}} + \underbrace{\left[\frac{e^2}{4\pi\epsilon_0}\sum_{i,\alpha}\frac{Z_\alpha}{|\vec{R}_\alpha - \vec{r}_i|}\right]}_{\hat{H}_{el-ion}}$$
$$+ \underbrace{\left[-\frac{\hbar^2}{2m_e}\sum_{i=1}^{N}\nabla_i^2 + \frac{e^2}{4\pi\epsilon_0}\frac{1}{2}\sum_{i,j}^{i\neq j}\frac{1}{|\vec{r}_i - \vec{r}_j|}\right]}_{\hat{H}_{el}}$$

The Hamiltonian is quite complicated and we need to make some appproximations. One of the most cruical approximations is the Born-Oppenheimer Approximation

As $m_{el} << m_{ion}$ the motions of the electrons are much faster compared to ions.

$$\Psi_{solid}(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N; \vec{R}_1, \vec{R}_2, ..., \vec{R}_K) \xrightarrow{BOA} \Phi_{el}(\{\vec{R}_i\}, \vec{r}_1, \vec{r}_2, ..., \vec{r}_N)\Phi_{ion}(\vec{R}_1, \vec{R}_2, ..., \vec{R}_K)$$

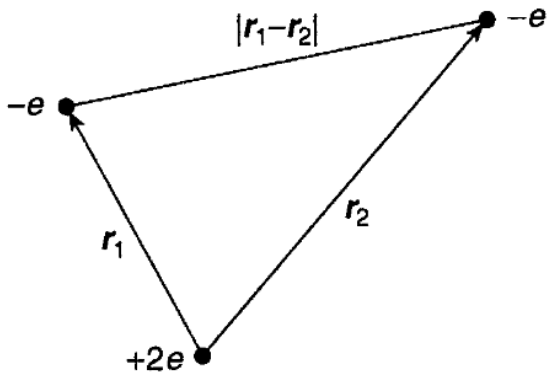
Conclusion of BOA

- Motion of ions are independent of that of the electrons
- Motion of the electrons depend on the motion of the ions parameterically.

Let us now concentrate on the electronic problem.
For simplicity let us consider general atomic Hamiltonian (in atomic units)

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N}\frac{Z}{r_i} + \frac{1}{2}\sum_{ij}^{i\neq j}\frac{1}{|\vec{r}_i - \vec{r}_j|}$$

If not for the electron-electron interation term this would have been exactly solvable



Trial Wavefunctions

Product Wavefunctions — Hartree Method

Slater Determinantal Type — Hartree-Fock Method

Use Variational Principle
Find Ground State

Hartree Method - Helium Atom

Trial Wavefunction $\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \phi(\vec{r}_1)\alpha(s_1)\phi(\vec{r}_2)\beta(s_2)$

Expanding the Wavefuction in a Basis $\phi(r) = \sum_{q=1}^{M} C_q \chi_q(r)$

Minimizing the Energy w.r.t. expansion coefficients $\{C_q\}$ gives Hartree equation*

$$\boxed{\sum_q \left(h_{pq} + \sum_{mn} C_m^\star C_n Q_{pmqn} \right) C_q = E' \sum_q S_{pq} C_q}$$

$$S_{pq} = \int \chi_p^\star(r)\chi_q(r) d^3\vec{r} \quad h_{pq} = \int \chi_p^\star(r) h(r) \chi_q(r) d^3\vec{r}$$

$$Q_{pmqn} = \int \chi_p^\star(r_1)\chi_m^\star(r_2) \frac{1}{r_{12}} \chi_q(r_1)\chi_n(r_2) d^3\vec{r}_1 d^3\vec{r}_2$$

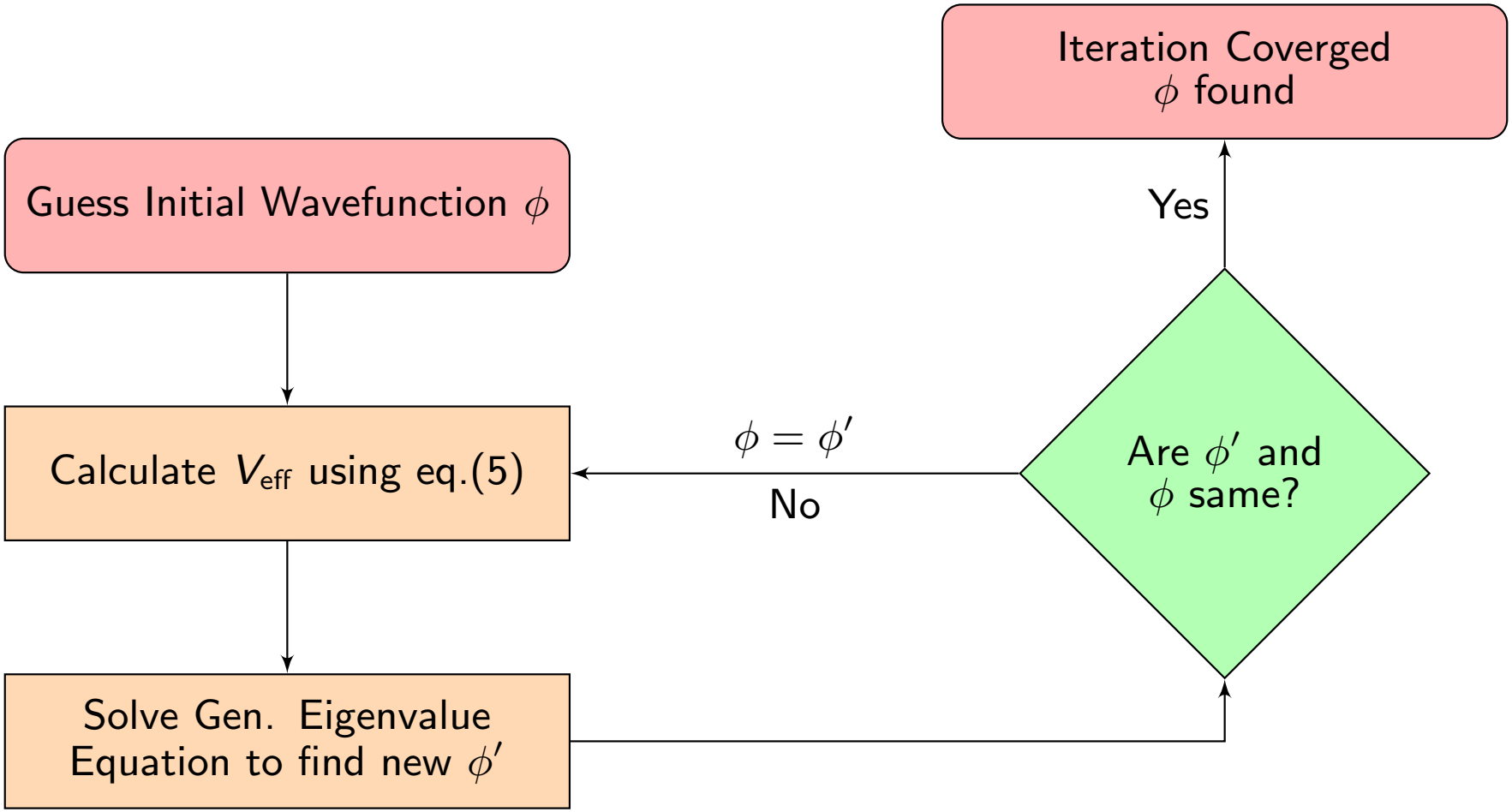
Now with $\chi_p(r) = e^{-a_p r^2}$ Gaussian Type Orbitals (GTO)

$$S_{pq} = \left(\frac{\pi}{a_p + a_q} \right)^{3/2} \quad H_{pq} = \frac{3 a_p a_q \pi^{3/2}}{(a_p + a_q)^{5/2}} - \frac{4\pi}{a_p + a_q}$$

$$Q_{pmqn} = \frac{2\pi^{5/2}}{(a_p + a_q)(a_m + a_n)\sqrt{a_p + a_q + a_m + a_n}}$$

Self Consistent Field Algorithm

$$\sum_q \left(h_{pq} + \sum_{mn} C_m^\star C_n Q_{pmqn} \right) C_q = E' \sum_q S_{pq} C_q$$



Hartree-Fock Method

Let us consider N electrons described by a set of quantum numbers $\{a_i, \text{for } i = 1, 2, ..N\}$

The electronic wavefunction is given by the Slater Determinant

$$\Psi_a(\vec{x}_1, \vec{x}_2.., \vec{x}_N) = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \phi_{a_1}(\vec{x}_1)\phi_{a_2}(\vec{x}_2)...\phi_{a_N}(\vec{x}_N)$$

If we write the Hamiltonian in a form

$$\hat{H} = \sum_i \hat{h}(\vec{x}_i) + \frac{1}{2} \sum_{i \neq j} \hat{g}(\vec{x}_i, \vec{x}_j)$$

For finding the ground state with the constraint that different spin orbitals are orthogonal to each other we need to minimize the action

$$A[\phi_1, \phi_2, ..\phi_N] = \sum_k \left\langle \phi_k \middle| \hat{h} + \frac{1}{2}(\hat{J} - \hat{K}) \middle| \phi_k \right\rangle - \sum_{kl} \Lambda_{kl} \Big(\langle \phi_k | \phi_l \rangle - \delta_{kl} \Big)$$

Doing this we obtain

$$\hat{F}\phi_k = \epsilon_k \phi_k \quad \forall k = 1, 2, ..N$$

Where $\hat{F} = \hat{h} + \hat{J} - \hat{K}$, $\hat{J}$ is called direct integral while $\hat{K}$ is called the exchange integral

Hartree-Fock-Roothan equations

Expanding the wavefunctions in a basis (in general non-orthogonal) as

$$\phi_k(r) = \sum_{q=1}^{M} C_q^k \chi_q(r)$$

We arrive at the Hartree-Fock-Roothan equations given by

$$\boxed{\sum_m (h_{nm} + G_{nm}^k) C_m^k = \epsilon_k \sum_m S_{nm} C_m^k}$$

$$S_{nm} = \langle n|m\rangle = \int \phi_n^\star(\vec{x})\phi_m(\vec{x})\, d\vec{x}$$

$$h_{nm} = \langle n|\hat{h}|m\rangle = \int \phi_n^\star(\vec{x})\hat{h}(\vec{x})\phi_m(\vec{x})\, d\vec{x}$$

$$g_{klmn} = \langle kl|\hat{g}|mn\rangle = \int \phi_k^\star(\vec{x}_1)\phi_l^\star(\vec{x}_2)\hat{g}(\vec{x}_1,\vec{x}_2)\phi_m(\vec{x}_1)\phi_n(\vec{x}_2)\, d\vec{x}_1 d\vec{x}_2$$

and

$$G_{nm}^k = \sum_l \sum_{pq} C_{pl}^\star C_{ql} (g_{npmq} - g_{npqm}\delta_{\sigma_k\sigma_l})$$

Hartree-Fock-Roothan equations - Simulation

We have used Gaussian Type Orbitals (GTO) as basis functions

$$\chi_q(r) = e^{-a_q r^2}$$

For the case of Helium atoms the optimized basis set is given by

$$a_1 = 13.0073,\ a_2 = 1.962079,\ a_3 = 0.444529,\ a_4 = 0.1219492$$

With the matrix elements given by

$$S_{pq} = \left(\frac{\pi}{a_p + a_q}\right)^{3/2}$$

$$H_{pq} = \frac{3a_p a_q \pi^{3/2}}{(a_p + a_q)^{5/2}} - \frac{4\pi}{a_p + a_q}$$

$$Q_{pmqn} = \frac{2\pi^{5/2}}{(a_p + a_q)(a_m + a_n)\sqrt{a_p + a_q + a_m + a_n}}$$

Results - Helium Atom

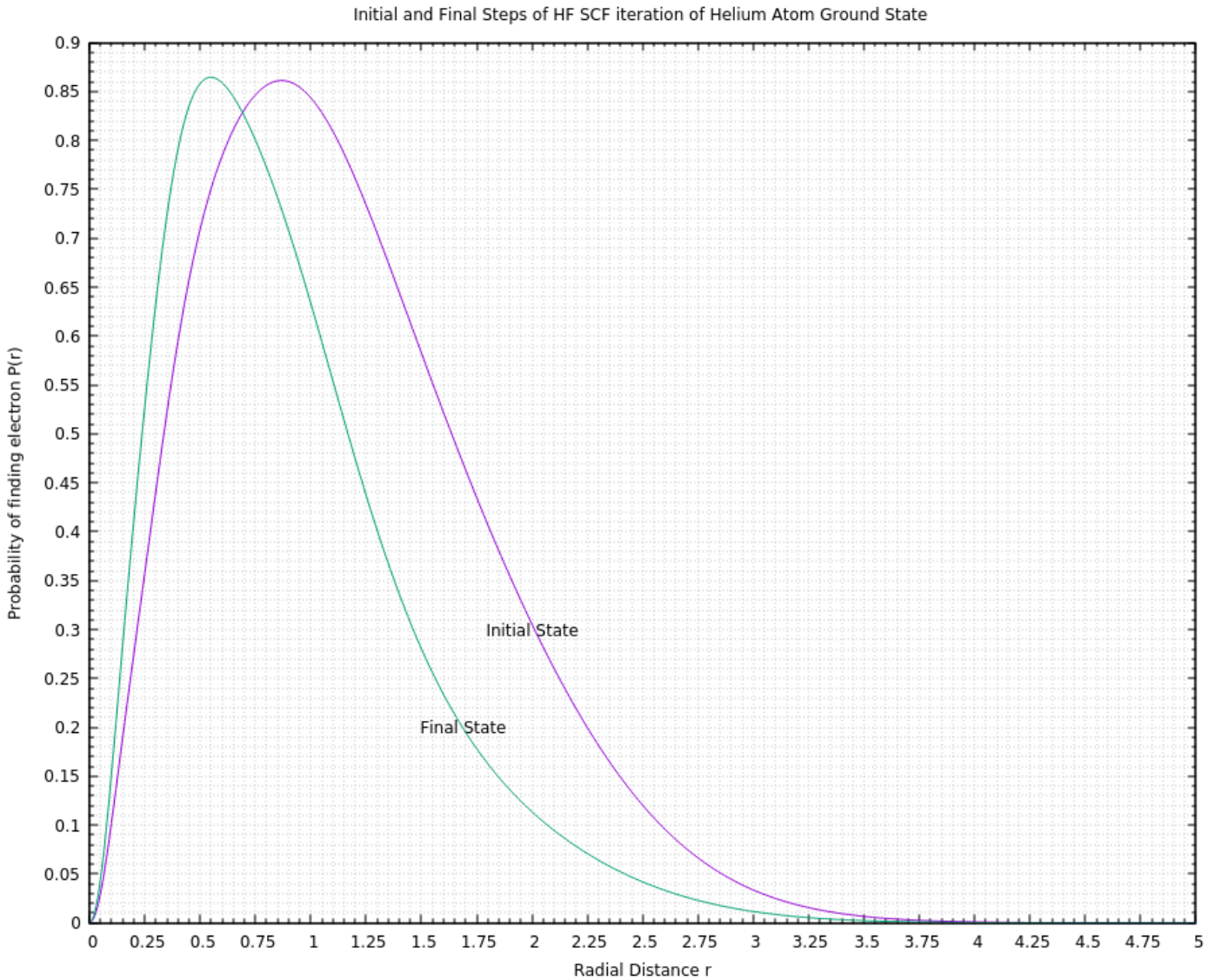
For Helium Atom we choose the quantum numbers for ground state as

$$k_1 = \left(n = 1, l = 0, s = \tfrac{1}{2}, m_s = +\tfrac{1}{2}\right) \; ; \; k_2 = \left(n = 1, l = 0, s = \tfrac{1}{2}, m_s = -\tfrac{1}{2}\right)$$

Ground State Energy of Heium Atom

Method	Energy(Ha)
HF	-2.85
EXPT	-2.90

Results - Ground State Wavefunctions



HF applied to Solids

Metals	Insulators
$\rho(\epsilon_F) \neq 0$	$\rho(\epsilon_F) = 0$

Prediction of Band Theory

- Odd number of conduction electrons $\Longrightarrow$ Metals
- Even number of conduction electrons $\Longrightarrow$ Insulators

But materials such as $\mathrm{CaCuO_2}, \mathrm{NiO}$ do not follow this classification

So we need to bring interaction between electrons into the picture.
Let us now see if we can apply the Hartree-Fock treatment to solids

A very minimal kind of interaction can be dealt with using the *Hubbard Model*

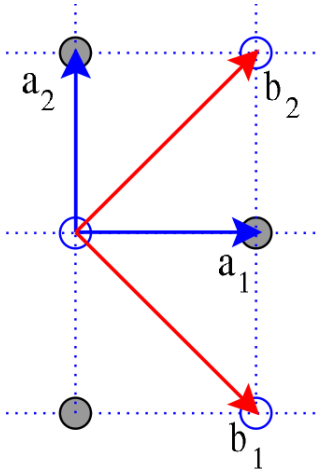
The One band Hubbard Model is defined by the following model Hamiltonian

$$\hat{H} = \sum_{ij,\sigma}^{i \neq j} t_{ij}(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + \frac{U}{2} \sum_{i\sigma} \hat{n}_{i\sigma} \hat{n}_{i\bar{\sigma}}$$

The first part is due to the hopping of the electron from one lattice site to its nearest neighbour lattice site while the second part represents the interaction between electrons at the same site.

Hartree Fock on Hubbard Model

Consider a 2D bipartite lattice, Deviation from Mean $= \delta\hat{n}_{i\alpha\sigma} = \hat{n}_{i\alpha\sigma} - \langle\hat{n}_{i\alpha\sigma}\rangle$



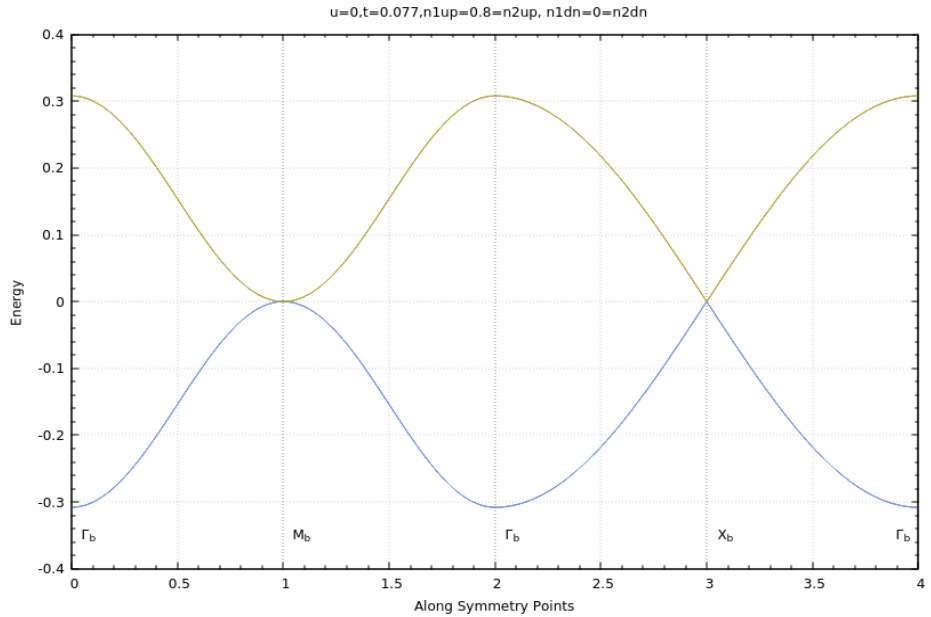
$$H_{\vec{k}\sigma} = \begin{bmatrix} u\langle n_{1\bar{\sigma}}\rangle & t\gamma_{\vec{k}} \\ t\gamma^{\star}_{\vec{k}} & u\langle n_{2\bar{\sigma}}\rangle \end{bmatrix}$$

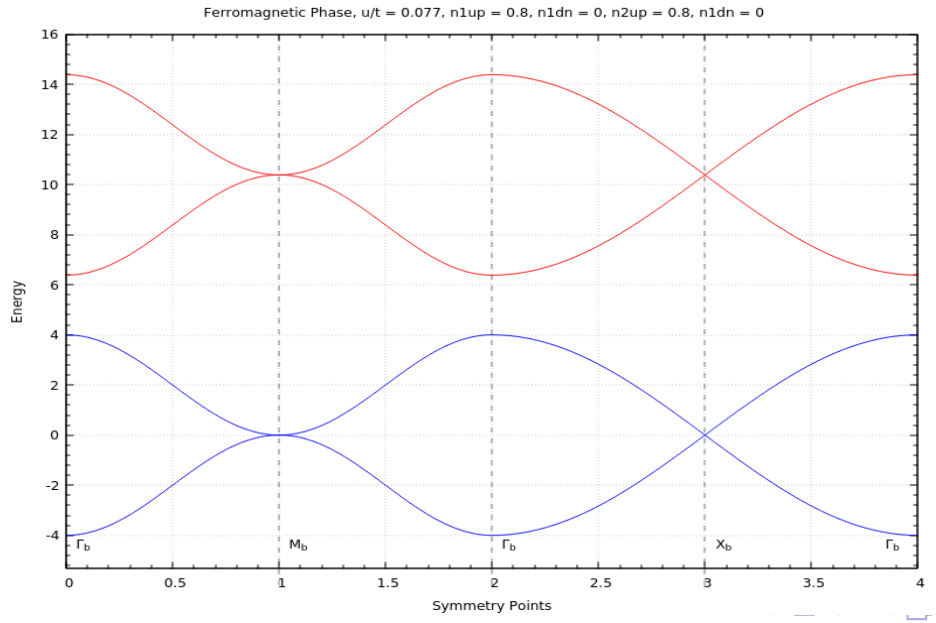
Solve for the eigenvalues and eigenvectors of this Hamiltonian numerically then

$$\rho(\epsilon) = \frac{1}{N}\sum_{j\vec{k}\sigma}\delta\Big[\epsilon - \epsilon_{j\sigma}(\vec{k})\Big] \qquad \int_{-\infty}^{\infty} d\epsilon\ \rho(\epsilon)\ \frac{1}{e^{\beta(\epsilon-\mu)}+1} = n_e$$

$$\langle n_{\alpha\sigma}\rangle_{GS} = \frac{1}{N}\sum_{\vec{k},j=1,2}|A^{j}_{\alpha\sigma}(\vec{k})|^2\frac{1}{e^{\beta(\epsilon-\mu)}+1} \qquad f_{FD}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1}$$

Results, $n_{1\uparrow} = n_{2\uparrow} = 0.8, n_{1\downarrow} = n_{2\downarrow} = 0$ FM configuration





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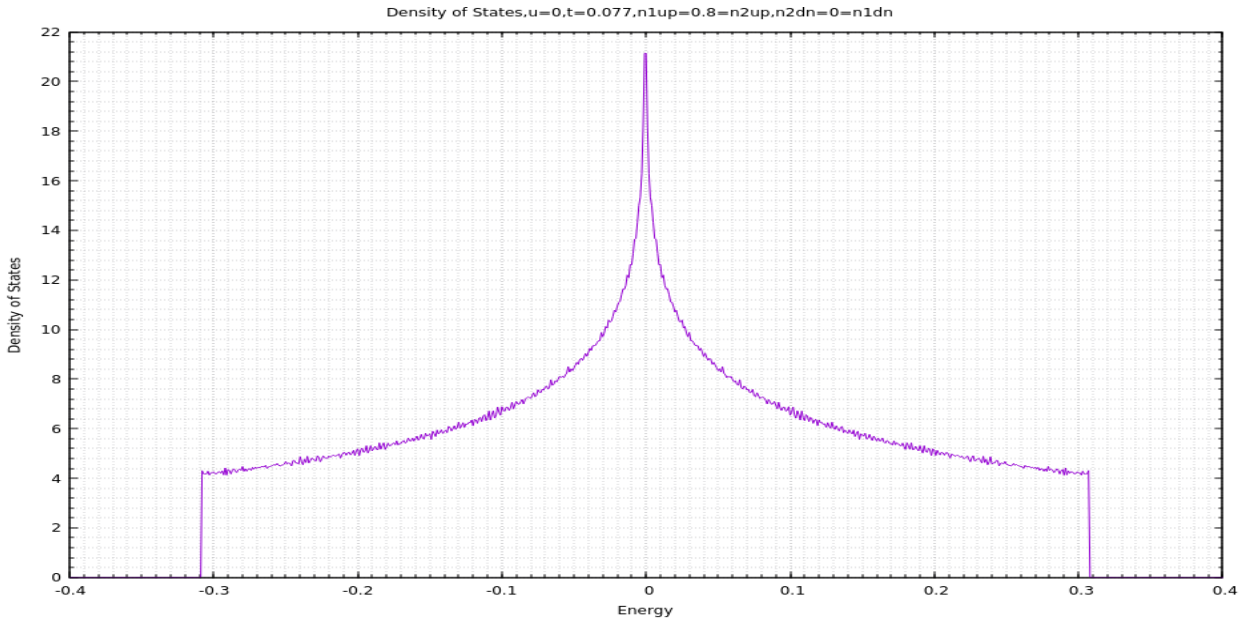
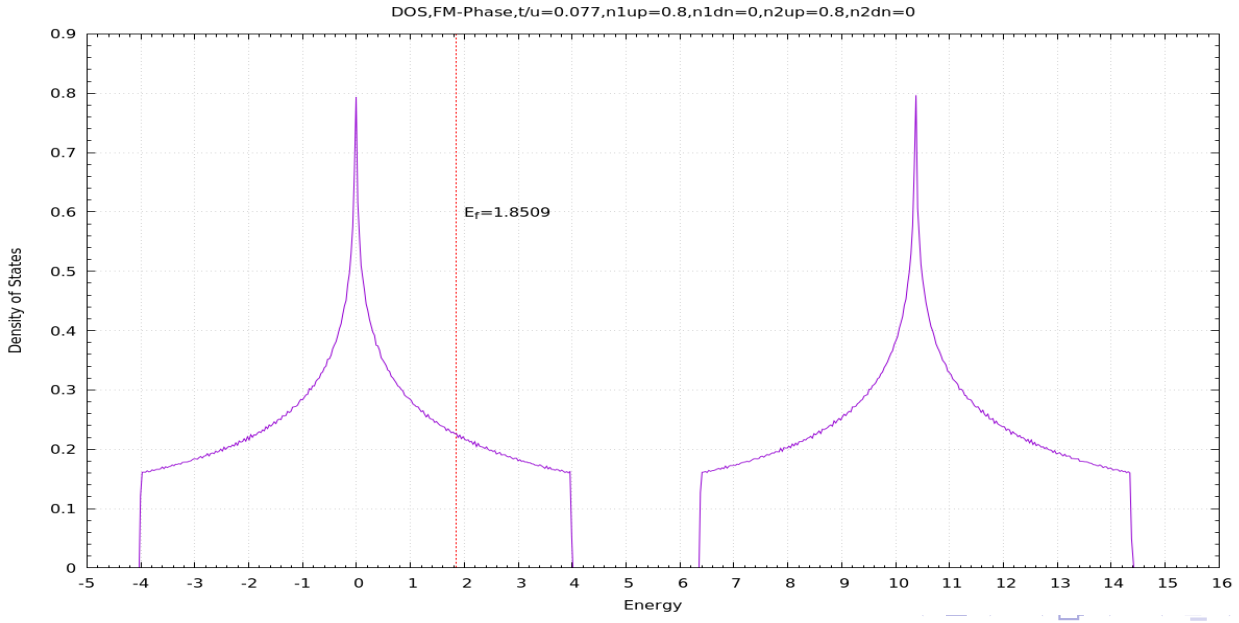
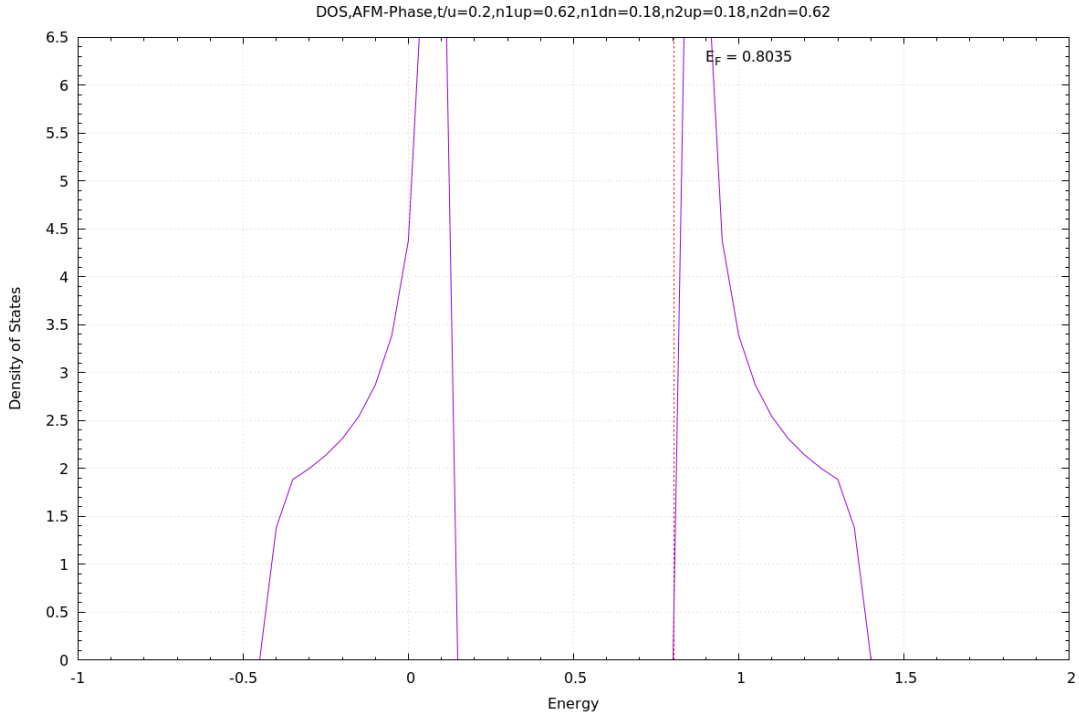
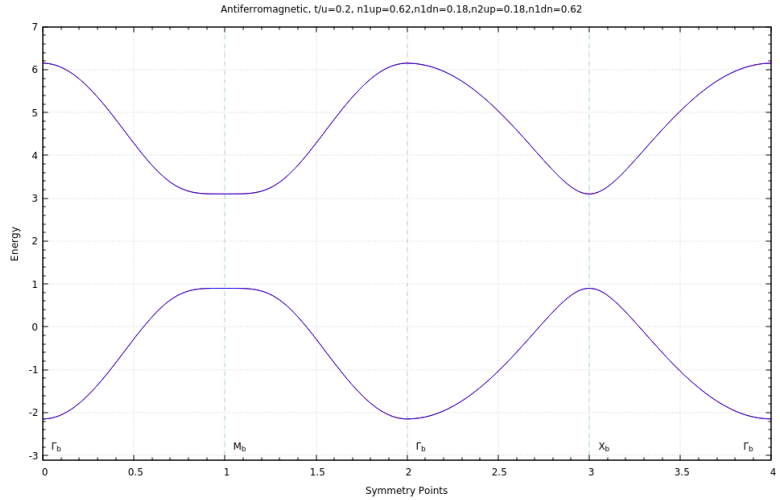





DOS,AFM-Phase,t/u=0.2,n1up=0.62,n1dn=0.18,n2up=0.18,n2dn=0.62
E_F = 0.8035
Density of States
Energy


Antiferromagnetic, t/u=0.2, n1up=0.62,n1dn=0.18,n2up=0.18,n1dn=0.62
Energy
Symmetry Points

Hubbard Model $\rightarrow$ Heisenberg Model

The different properties such as conductivity and magnetization are dependent on the hopping parameter t_{ij} and interaction parameter U

In the strong coupling limit i.e. $U >> t$, $\hat{H}_0 = \frac{U}{2} \sum_{i\sigma} \hat{n}_{i\sigma} \hat{n}_{i\bar{\sigma}}$
Perturbation $\hat{H}_1 = \sum_{ij,\sigma}^{i \neq j} t_{ij} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma})$

$$E_{0\alpha}^{(2)} = -\frac{1}{U} \left\langle 0\alpha \middle| \hat{H}_1^2 \middle| 0\alpha \right\rangle$$

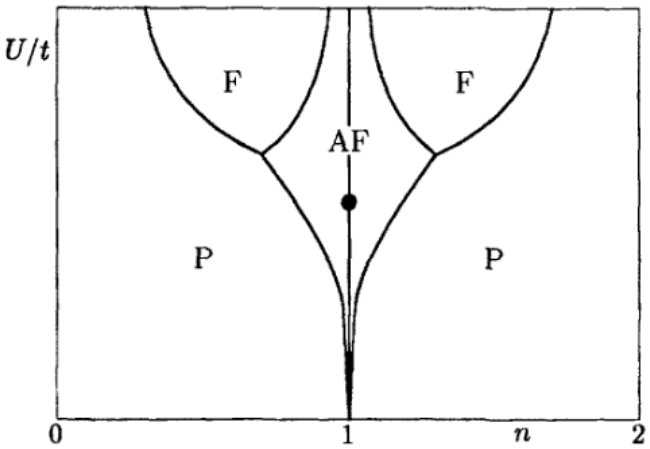
Expanding this and changing from creation annihilation operators to spin operators using the definitions

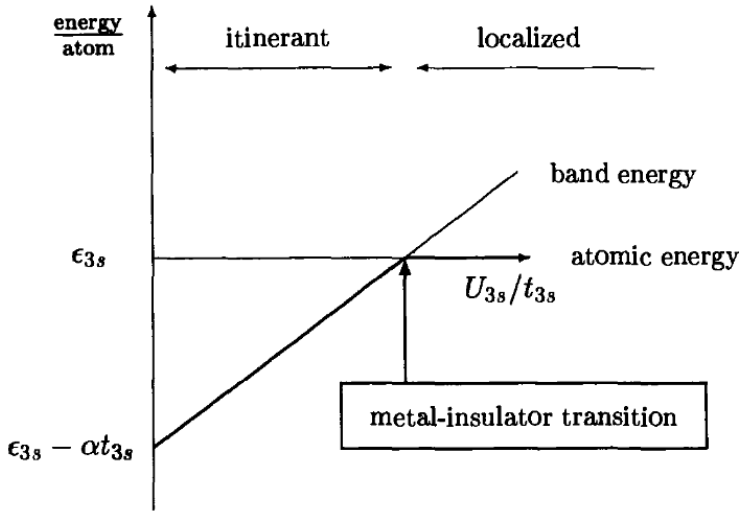
$$S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) \quad S_i^+ = c_{i\uparrow}^{\dagger} c_{i\downarrow} \quad S_i^- = c_{i\downarrow}^{\dagger} c_{i\uparrow}$$

We have an effective Hamiltonian of the form $\hat{H}_{eff} = \sum_{ij} J \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j$ where $J = \frac{4t^2}{U}$

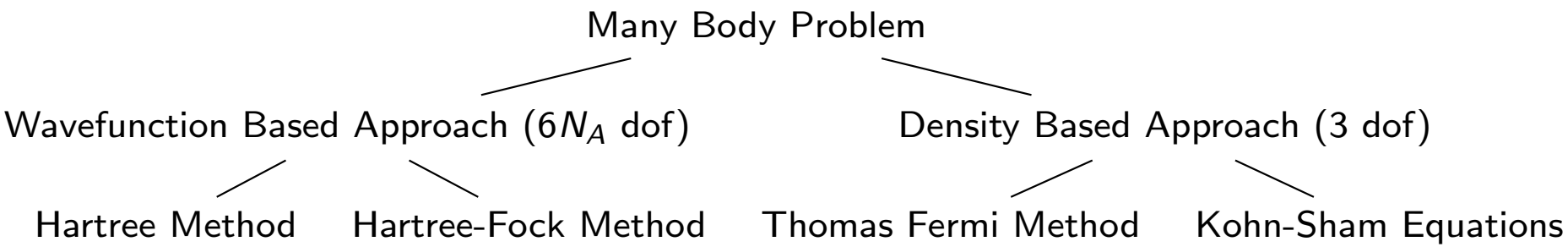
Conclusion-Success of Hubbard Model

- **Mott Insulators** : They are different from band insulators and arise because of the onsite coulomb repulsion splits the DOS in two parts
- **Heisenberg Antiferromagnet** : At half filling in the strong coupling limit the Hubbard Model is converted into an antiferromagnetic Heisenberg model.





Different Approaches to Many body Physics



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I am also very thankful to my friends who were always available for discussion.

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