Mean Field Theory

- a.k.a. Hartree - Fock Methods

Reduce the many-body problem to the problem of a single particle moving in an effective mean field generated by all of the other particles.

Fundamental approximation in condensed matter and nuclear physics.

We will consider nonrelativistic mean field methods.

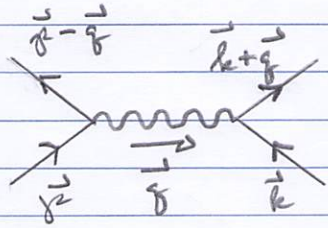
- Particles interact through an instantaneous potential:

$$V(\vec{x}-\vec{x}') = \sum_{\vec{q}} e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}\,\tilde{V}(\vec{q})$$

In the language of Second Quantization,

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

$$= \sum_{\vec{p}} \frac{p^2}{2m}\,\hat{a}^\dagger_{\vec{p}}\,\hat{a}_{\vec{p}} + \frac{1}{2}\sum_{\vec{k}\vec{p}\vec{q}} \tilde{V}(\vec{q})\,\hat{a}^\dagger_{\vec{p}-\vec{q}}\,\hat{a}^\dagger_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{k}}\,\hat{a}_{\vec{p}}$$



In the MEAN FIELD APPROXIMATION, the correction to the ground state energy is found by taking the vacuum (i.e., ground state) expectation value of $\hat{V}$:

$$E_0 \longrightarrow E_0 + \langle 0|\hat{V}|0\rangle$$

How do we calculate $\langle 0|\hat{v}|0\rangle$?

Wick's Theorem tells us how:

$$\langle 0|\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{k}}\,\hat{a}_{\vec{p}}|0\rangle$$

$$= \langle 0| :\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{k}}\,\hat{a}_{\vec{p}}: \; + \; :\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}^{\dagger}_{\vec{k}+\vec{q}}:\,\overbrace{\hat{a}_{\vec{k}}\,\hat{a}_{\vec{p}}}$$

$$+ \overbrace{\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}^{\dagger}_{\vec{k}+\vec{q}}}\,:\hat{a}_{\vec{k}}\,\hat{a}_{\vec{p}}: \; - \; \overbrace{\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}_{\vec{k}}}\,:\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{p}}:$$

$$+ \overbrace{\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}_{\vec{p}}}\,:\hat{a}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{k}}: \; + \; \overbrace{\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{k}}}\,:\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}_{\vec{p}}:$$

$$- \overbrace{\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{p}}}\,:\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}_{\vec{k}}: \; + \; \overbrace{\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}^{\dagger}_{\vec{k}+\vec{q}}}\,\overbrace{\hat{a}_{\vec{k}}\,\hat{a}_{\vec{p}}}$$

$$- \overbrace{\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}_{\vec{k}}}\,\overbrace{\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{p}}} \; + \; \overbrace{\hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}_{\vec{p}}}\,\overbrace{\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\,\hat{a}_{\vec{k}}}|0\rangle$$

The sign changes are present because we are dealing with Fermions.

All of the terms left with a normal ordering of operators will not contribute to the VEV.

So, we are left with

The mean field approximation corresponds to replacing pairs of operators with averages.

1

$$\langle 0|\hat{v}|0\rangle = \frac{1}{2}\sum_{\vec{k},\vec{p},\vec{q}} \tilde{V}(\vec{q})\left\{\langle \hat{a}^{\dagger}_{\vec{p}-\vec{q}}\,\hat{a}^{\dagger}_{\vec{k}+\vec{q}}\rangle\langle \hat{a}_{\vec{k}}\,\hat{a}_{\vec{p}}\rangle\right.$$

2

$$+ \langle \hat{a}^{\dagger}_{\vec{p}-\vec{q}} \, \hat{a}_{\vec{p}} \rangle \langle \hat{a}^{\dagger}_{\vec{k}+\vec{q}} \, \hat{a}_{\vec{k}} \rangle$$

3

$$- \langle \hat{a}^{\dagger}_{\vec{p}-\vec{q}} \, \hat{a}_{\vec{k}} \rangle \langle \hat{a}^{\dagger}_{\vec{k}+\vec{q}} \, \hat{a}_{\vec{p}} \rangle \Big\}$$

1 = Condensate Term $\equiv$ C

2 = Hartree Term $\equiv$ H

3 = Fock Term $\equiv$ F

Let's look at

$\langle 0 | \hat{a}^{\dagger}_{\vec{p}-\vec{q}} \, \hat{a}_{\vec{p}} | 0 \rangle = 0$ unless $\vec{q} = 0$

$$H = \frac{1}{2} \sum_{\vec{k}\vec{p}\vec{q}} \tilde{V}(\vec{q}) \langle \hat{a}^{\dagger}_{\vec{p}-\vec{q}} \, \hat{a}_{\vec{p}} \rangle \langle \hat{a}^{\dagger}_{\vec{k}+\vec{q}} \, \hat{a}_{\vec{k}} \rangle$$

H for Hartree, not Hamiltonian

$$= \frac{1}{2} \sum_{\vec{k}\vec{p}} \underbrace{\tilde{V}(\vec{0})} \langle \hat{a}^{\dagger}_{\vec{p}} \, \hat{a}_{\vec{p}} \rangle \langle \hat{a}^{\dagger}_{\vec{k}} \, \hat{a}_{\vec{k}} \rangle$$

$\vec{q} = 0$ corresponds to infinite wavelength – i.e., a constant

IN POSITION SPACE

$$= \frac{1}{2} \tilde{V}(0) \sum_{\vec{k}\vec{p}\vec{q}}$$

$$\times \frac{1}{V^2} \int d^3x \, d^3x' \, d^3y \, d^3y' \, \langle \hat{\psi}^{\dagger}(\vec{x}) \, \hat{\psi}(\vec{x}') \rangle \langle \hat{\psi}^{\dagger}(\vec{y}) \, \hat{\psi}(\vec{y}') \rangle$$

$$\times \, e^{i(\vec{p}-\vec{q})\cdot\vec{x}} \, e^{-i\vec{p}\cdot\vec{x}'} \, e^{i(\vec{k}+\vec{q})\cdot\vec{y}} \, e^{-i\vec{k}\cdot\vec{y}'}$$

$\sum_{\vec{p}} e^{i\vec{p}\cdot(\vec{x}-\vec{x}')}$

$= \delta^{(3)}(\vec{x}-\vec{x}')$

...

$$= \frac{1}{2} \tilde{V}(0) \sum_{\vec{q}} \int d^3x \, d^3y \, \langle \hat{\psi}^{\dagger}(\vec{x}) \hat{\psi}(\vec{x}) \rangle \langle \hat{\psi}^{\dagger}(\vec{y}) \hat{\psi}(\vec{y}) \rangle e^{-i\vec{q}\cdot(\vec{x}-\vec{y})}$$

What we expect classically from two interacting charge distributions. ④

$$= \frac{1}{2}\int d^3x\, d^3y\, V(\vec{x}-\vec{y}) \underbrace{\langle \hat{\psi}^+(\vec{x})\hat{\psi}(\vec{x})\rangle}_{\substack{\text{charge distribution}\\ \rho(x)}} \underbrace{\langle \hat{\psi}^+(\vec{y})\hat{\psi}(\vec{y})\rangle}_{\substack{\text{charge distribution}\\ \rho(y)}}$$

Now consider

$$F = -\frac{1}{2}\sum_{\vec{k}\vec{p}\vec{q}} \tilde{V}(\vec{q}) \langle \hat{a}^+_{\vec{p}-\vec{q}}\hat{a}_{\vec{k}}\rangle \langle \hat{a}^+_{\vec{k}+\vec{q}}\hat{a}_{\vec{p}}\rangle$$

$$= -\frac{1}{2}\sum_{\vec{k}\vec{p}\vec{q}} \tilde{V}(\vec{q})$$

$$\times \frac{1}{V^2}\int d^3x\, d^3x'\, d^3y\, d^3y' \langle \hat{\psi}^+(\vec{x})\hat{\psi}(\vec{x}')\rangle \langle \hat{\psi}^+(\vec{y})\hat{\psi}(\vec{y}')\rangle$$

$$\times e^{i(\vec{p}-\vec{q})\cdot\vec{x}}\, e^{-i\vec{k}\cdot\vec{x}'}\, e^{i(\vec{k}+\vec{q})\cdot\vec{y}}\, e^{-i\vec{p}\cdot\vec{y}'}$$

$$= -\frac{1}{2}\sum_{\vec{q}} \tilde{V}(\vec{q})$$

$$\times \int d^3x\, d^3y \langle \hat{\psi}^+(\vec{x})\hat{\psi}(\vec{y})\rangle \langle \hat{\psi}^+(\vec{y})\hat{\psi}(\vec{x})\rangle e^{-i\vec{q}\cdot(\vec{x}-\vec{y})}$$

$$= -\frac{1}{2}\int d^3x\, d^3y \underbrace{\langle \hat{\psi}^+(\vec{x})\hat{\psi}(\vec{y})\rangle}_{\text{correlation function}} \langle \hat{\psi}^+(\vec{y})\hat{\psi}(\vec{x})\rangle V(\vec{x}-\vec{y})$$

Exchange Energy

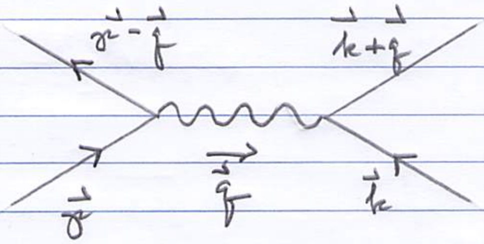
- bosons like to be spatially clumped
- fermions like the opposite

correlation functions — expectation value of having a particle at y given a particle at x

Diagrammatic Analysis

Remember our original diagram for

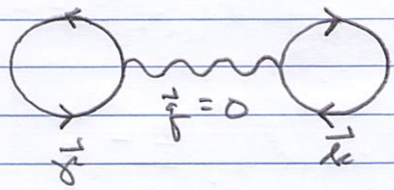
$$\hat{V} = \frac{1}{2}\sum_{\vec{k}\vec{p}\vec{q}} \tilde{V}(\vec{q})\, \hat{a}^\dagger_{\vec{p}-\vec{q}}\, \hat{a}^\dagger_{\vec{k}+\vec{q}}\, \hat{a}_{\vec{k}}\, \hat{a}_{\vec{p}}$$



The diagrams that correspond to VEV have no external lines – there are no particles in the initial and final state.

For the Hartree term, we contract $\langle \hat{a}^\dagger_{\vec{p}-\vec{q}}\, \hat{a}_{\vec{p}} \rangle$ and $\langle \hat{a}^\dagger_{\vec{k}+\vec{q}}\, \hat{a}_{\vec{k}} \rangle$.

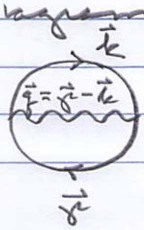
Diagrammatically, this corresponds to the graph



"TADPOLE" DIAGRAM

For the Fock term, we contract $\langle \hat{a}^\dagger_{\vec{p}-\vec{q}}\, \hat{a}_{\vec{k}} \rangle$ and $\langle \hat{a}^\dagger_{\vec{k}+\vec{q}}\, \hat{a}_{\vec{p}} \rangle$.

Diagrammatically,



"OYSTER" DIAGRAM

The Hartree-Fock Ground State Energy of a Metal

$$\langle \Psi_0 | \hat{H} | \Psi_0 \rangle = \langle \Psi_0 | \hat{H}_0 | \Psi_0 \rangle + \langle \Psi_0 | \hat{V} | \Psi_0 \rangle$$

$$\langle \Psi_0 | \hat{H}_0 | \Psi_0 \rangle = \langle \Psi_0 | \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} \hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} | \Psi_0 \rangle$$

The sum over $\vec{k}$ will go up to $\vec{k}_F$, the Fermi momentum:

$$2\int_{|\vec{k}| < k_F} \frac{d^3k}{(2\pi)^3}$$

$$N = 2V \frac{1}{(2\pi)^3} 4\pi \int_0^{k_F} k^2 dk = \frac{V}{\pi^2} \frac{1}{3} k_F^3$$

$$\varepsilon_F = \frac{k_F^2}{2m_e}$$

$$E = 2V \frac{1}{(2\pi)^3} 4\pi \int_0^{k_F} \frac{k^2}{2m_e} k^2 dk = \frac{V}{\pi^2} \frac{1}{5} \frac{k_F^5}{2m_e}$$

$$\varepsilon = E/N = \frac{3}{5} \frac{k_F^2}{2m_e} = \frac{3}{5} \varepsilon_F$$

Then

$$\langle \Psi_0 | \hat{H}_0 | \Psi_0 \rangle = \langle \Psi_0 | \sum_{\vec{k}\sigma} \varepsilon \hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} | \Psi_0 \rangle = \varepsilon \langle \Psi_0 | \sum_{\vec{k}\sigma} \hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} | \Psi_0 \rangle$$

$$= \varepsilon \langle \Psi_0 | \hat{N} | \Psi_0 \rangle = \varepsilon N$$

$$|\Psi_0\rangle = \prod_{\sigma} \prod_{\substack{\vec{k} \\ |\vec{k}| \le k_F}} \hat{a}^{+}_{\vec{k}\sigma} |0\rangle = | 1_{\vec{k}_1\uparrow} 1_{\vec{k}_1\downarrow} 1_{\vec{k}_2\uparrow} 1_{\vec{k}_2\downarrow} \ldots \underbrace{1_{\vec{k}_N\uparrow} 1_{\vec{k}_N\downarrow}}_{1_{\vec{k}_F\uparrow} 1_{\vec{k}_F\downarrow}} \rangle$$

$$E_0 = \varepsilon N = \frac{3}{5} N \varepsilon_F = N \frac{Z_1 Z_2}{r_s^2} E_{Rydberg}$$

volume / electron

$\frac{1}{n} = \frac{4\pi}{3} r^3$

$$r_s \equiv \left(\underbrace{V / \tfrac{4\pi}{3} N}_{} \right)^{1/3} / a_B = r / a_B$$

average distance per particle

We're going to adopt the JELLIUM MODEL where the ions are assumed to provide a uniform positive background, which cancels with the uniform electron distribution in the Hartree term, which is therefore 0.

Now for

standard first order perturbation theory correction

$$\Delta E^{(F)} = \langle \Psi_0 | \hat{V} | \Psi_0 \rangle$$

$$= -\frac{1}{2} \sum_{\vec{k} \vec{q}' \vec{q}} \tilde{V}(\vec{q}) \langle \hat{a}^\dagger_{\vec{q}'-\vec{q}} \hat{a}_{\vec{k}} \rangle \langle \hat{a}^\dagger_{\vec{k}+\vec{q}} \hat{a}_{\vec{q}'} \rangle$$

$$= -\frac{1}{2} \sum_{\vec{k} \vec{q}'} \tilde{V}(\vec{q}' - \vec{k}) \langle \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}} \rangle \langle \hat{a}^\dagger_{\vec{q}'} \hat{a}_{\vec{q}'} \rangle$$

$$= 2 \sum_{|\vec{q}'| < q_F} \frac{1}{2} \left\{ - \sum_{|\vec{k}| < q_F} \tilde{V}(\vec{q}' - \vec{k}) \right\}$$

for spins

$$F(x) = 1 + \frac{1-x^2}{2x} \ln \left| \frac{1+x}{1-x} \right|$$

$$= 2 \sum_{|\vec{q}'| < q_F} \frac{1}{2} \left\{ - \sum_{|\vec{k}| < q_F} \frac{e^2}{V \epsilon_0 |\vec{q}' - \vec{k}|^2} \right\}$$

Let's look at

$$\sum_{|\vec{k}| < q_F} \frac{-e^2}{V \epsilon_0 |\vec{q}' - \vec{k}|^2} = \frac{-e^2 V}{V \epsilon_0} \int_{|\vec{k}| < q_F} \frac{d^3 k}{(2\pi)^3} \frac{1}{|\vec{q}' - \vec{k}|^2} = \frac{-q_F}{\pi} \left(\frac{e^2}{4\pi\epsilon_0} \right) F\left(\frac{q'}{q_F} \right)$$

$|\vec{q}'|$

Then

$$\Delta E^{(F)} = 2 \sum_{|\vec{k}|<k_F} \frac{1}{2} \left\{ -\frac{k_F}{\pi} \left(\frac{e^2}{4\pi\epsilon_0} \right) F\left(\frac{k}{k_F} \right) \right\}$$

$$= -V \frac{k_F}{\pi} \left(\frac{e^2}{4\pi\epsilon_0} \right) \int_{|\vec{k}|<k_F} \frac{d^3k}{(2\pi)^3} F\left(\frac{k}{k_F} \right)$$

$$= -\frac{3Nk_F}{2\pi} \left(\frac{e^2}{4\pi\epsilon_0} \right) \underbrace{\int_0^1 dx\, x^2 F(x)}_{1/2}$$

with $x \equiv \frac{k}{k_F}$

$$= -\frac{3Nk_F}{4\pi} \left(\frac{e^2}{4\pi\epsilon_0} \right)$$

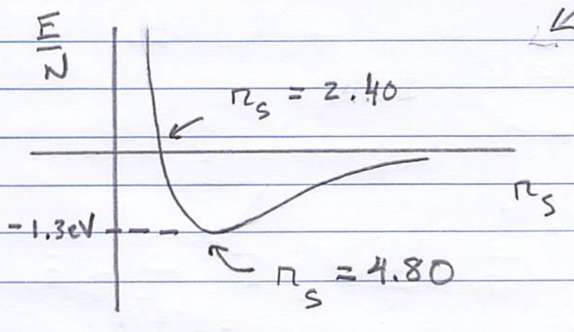
Then

$$\frac{\Delta E^{(F)}}{N} = -\frac{3k_F}{4\pi} \left(\frac{e^2}{4\pi\epsilon_0} \right) = -\frac{0.916}{r_s} \; \frac{\text{Rydbergs}}{\text{electron}}$$

Finally

$$\frac{E}{N} = \left(\frac{2.2}{r_s^2} - \frac{0.916}{r_s} \right) \frac{\text{Rydbergs}}{\text{electron}}$$

There exists a stable minimum!



Observed

	Li	Na	K
r_s	3.22	3.96	4.86