

APPROXIMATION

- a.k.a "MEAN-FIELD" approximation
- Useful in many situations when we have an intractable 4-fermion term in the Hamiltonian, see e.g. the Coulomb interaction term
- The idea: Approximate the full $H = H_0 + H_1$ by the "best possible" Hamiltonian $H_{HF} = \sum_{k,\alpha} \epsilon_{\alpha}^{HF}(\vec{k}) c_{k\alpha}^+$ (1)

(I) Heuristic approach,

Consider: $H_0 = \sum_{k\alpha} \epsilon_0(k) c_{k\alpha}^+ c_{k\alpha}$ (2)

$$H_1 = \frac{1}{2} \sum_{\substack{k p q \\ \alpha \beta}} V(\vec{q}) c_{k+\vec{q}\alpha}^+ c_{p-\vec{q}\beta}^+ c_{p\beta} c_{k\alpha}$$

- Next, "decouple" H_1 using the operator identity

$$\hat{A} \hat{B} = \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle + (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) \quad \text{← } \begin{matrix} \text{"fluctuation" around "mean field"} \\ \text{- assume small, neglect.} \end{matrix} \quad (3)$$

$$H_1^{HF} = \frac{1}{2} \sum_{\substack{k p q \\ \alpha \beta}} V(\vec{q}) \left[c_{k+\vec{q}\alpha}^+ c_{k\alpha} \langle c_{p-\vec{q}\beta}^+ c_{p\beta} \rangle + \langle c_{k+\vec{q}\alpha}^+ c_{k\alpha} \rangle c_{p-\vec{q}\beta}^+ c_{p\beta} - \langle \cdot \rangle \langle \cdot \rangle - c_{k+\vec{q}\alpha}^+ c_{p\beta} \langle c_{p-\vec{q}\beta}^+ c_{k\alpha} \rangle - \langle c_{k+\vec{q}\alpha}^+ c_{p\beta} \rangle c_{p-\vec{q}\beta}^+ c_{k\alpha} + \langle \cdot \rangle \langle \cdot \rangle \right]$$

$$\langle c_{p-\vec{q}\beta}^+ c_{p\beta} \rangle = \delta_{q=0} \langle c_{kp}^+ c_{kp} \rangle \quad \text{"direct" (Hartree)} \quad (4)$$

$$\langle c_{p-\vec{q}\beta}^+ c_{k\alpha} \rangle = \delta_{kp} \delta_{p-q=k} \langle c_{k\alpha}^+ c_{k\alpha} \rangle \quad \text{"exchange" (Fock)} \quad (5)$$

- The mean-field (Hartree-Fock) Hamiltonian thus takes the form

$$\left[\hat{H}^{MF} = \sum_{k\alpha} \left[\varepsilon_0(\vec{k}) + \underbrace{V(0) \sum_{\vec{p}\beta} \langle c_{\vec{p}\beta}^+ c_{\vec{p}\beta} \rangle}_{E_{\text{Hartree}}} - \underbrace{\sum_{\vec{p}} V(\vec{p}-\vec{k}) \langle c_{\vec{p}\alpha}^+ c_{\vec{p}\alpha} \rangle}_{E_{\text{exch}}(\vec{k})} \right] c_{k\alpha}^+ c_{k\alpha} \right] \quad (6)$$

E_{Hartree} (Hartree) $E_{\text{exch}}(\vec{k})$ (Fock)

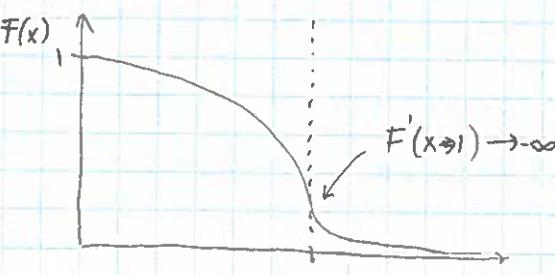
- Now let's work this out for the Coulomb interaction

$$V(q) = \frac{e^2}{V} \frac{4\pi}{q^2} \quad (\text{no Hartree term as } q \neq 0)$$

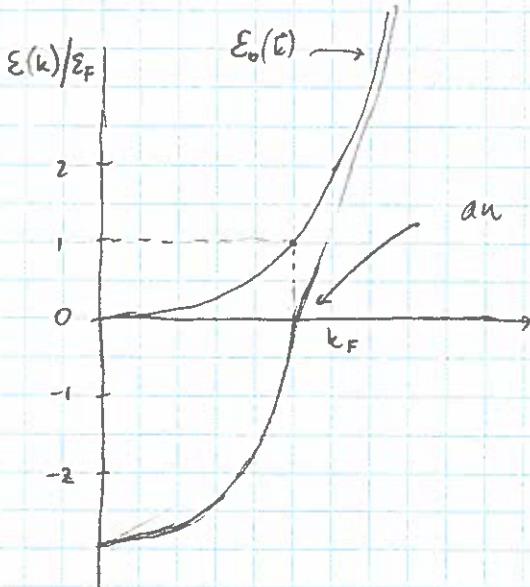
$$\begin{aligned} -E_{\text{exch}}(\vec{k}) &= \frac{4\pi e^2}{V} \sum_{\vec{p}} \frac{\Theta(p_F - p)}{(\vec{p} - \vec{k})^2} = 4\pi e^2 \int \frac{dp^3}{(2\pi)^3} \frac{\Theta(p_F - p)}{(\vec{p} - \vec{k})^2} \\ &= \frac{e^2}{2\pi^2} \cdot 2\pi \int_0^{p_F} p^2 dp \int_0^\pi d\theta \sin\theta \frac{1}{p^2 - 2pk \cos\theta + k^2} \quad z = \cos\theta \\ &= \frac{e^2}{\pi} \int_0^{p_F} p^2 dp \int_{-1}^1 \frac{dz}{p^2 + k^2 - 2pkz} \\ &= \frac{e^2}{\pi} \int_0^{k_F} dp p \left[\ln|k-p| - \ln|k+p| \right] \\ &= \frac{e^2 k_F}{\pi} \left[1 + \frac{k_F^2 - k^2}{2k_F k} \ln \left| \frac{k+k_F}{k-k_F} \right| \right] \end{aligned} \quad (7)$$

- Hence we have

$$\left[\hat{H}^{MF} = \sum_{k\alpha} \varepsilon(\vec{k}) c_{k\alpha}^+ c_{k\alpha}, \quad \varepsilon(\vec{k}) = \varepsilon_0(\vec{k}) - \frac{2e^2}{\pi} k_F F\left(\frac{k}{k_F}\right), \quad F(x) = \frac{1}{2} + \frac{(-x)^2}{4x} \ln \left| \frac{1+x}{1-x} \right| \right] \quad (8)$$



- With free-electron dispersion $\epsilon_0(\vec{k}) = \frac{\hbar^2 k^2}{2m}$ we have



- See HWK 1, prob 3
for more discussion on this.

(II) Hartree-Fock as a variational bound

The idea is to find the best possible $\epsilon(\vec{k})$ in H^{HF} through variational principle.

→ look for $\epsilon(\vec{k}) = \epsilon_0(\vec{k}) + \varepsilon_{\text{atk}}$ with ε_{atk} variational parameter, such that

$\langle H \rangle_{HF}$ is minimized

↑ expectation value with respect to
the ground state of H^{HF}
(the Fermi sphere)

$$\langle H_0 \rangle_{HF} = \sum_{k\alpha} \epsilon_0(\vec{k}) \langle c_{k\alpha}^+ c_{k\alpha} \rangle_{HF} = \sum_{k\alpha} \epsilon_0(\vec{k}) n_{k\alpha} \quad (9)$$

$$\begin{aligned} \langle H_1 \rangle_{HF} &= \frac{1}{2} \sum_{\substack{k+p,q \\ q=p}} V(q) \left[\langle c_{k+q,\alpha}^+ c_{k\alpha} \rangle_{HF} \langle c_{p-q,p}^+ c_{p\beta} \rangle_{HF} - \langle c_{k+q,\alpha}^+ c_{p\beta} \rangle_{HF} \langle c_{p-q,p}^+ c_{k\alpha} \rangle_{HF} \right] \\ &= \frac{1}{2} \sum_{\substack{k+p,q \\ q=p}} V(q) \left[\delta_{q=0} n_{k\alpha} n_{p\alpha} - \delta_{k+q=p} \delta_{q=p} \delta_{p-q=k} n_{k\alpha} n_{p\beta} \right] \\ &= \frac{1}{2} \left[V(0) \left(\sum_{k\alpha} n_{k\alpha} \right)^2 - \sum_{k+p\alpha} V(k-p) n_{k\alpha} n_{p\alpha} \right] \end{aligned} \quad (10)$$

- Now we wish to minimize $\langle H \rangle_{HF}$ with respect to $\epsilon_{k\alpha}$:

$$0 = \frac{\partial \langle H \rangle_{HF}}{\partial \epsilon_{q\lambda}} = \sum_{q'\lambda'} \frac{\partial \langle H \rangle_{HF}}{\partial n_{q\lambda'}} \frac{\partial n_{q\lambda'}}{\partial \epsilon_{q\lambda}} \quad (11)$$

$$\rightarrow \sum_{k\alpha} \left[\epsilon_0(k) + V(0) \sum_{p\beta} n_{p\beta} - \sum_p V(\vec{k}-\vec{p}) n_{p\alpha} \right] \frac{\partial n_{k\alpha}}{\partial \epsilon_{q\lambda}} = 0 \quad (12)$$

- To solve this consider $[H_{HF} = \sum_{k\alpha} (\epsilon_0(k) + \epsilon_{k\alpha}) C_{k\alpha}^+ C_{k\alpha}]$

$$\frac{\partial \langle H_{HF} \rangle_{HF}}{\partial \epsilon_{q\lambda}} = n_{q\lambda} + \sum_{k\alpha} \left[\underbrace{\epsilon_0(k) + \epsilon_{k\alpha}}_{\sim} \right] \frac{\partial n_{k\alpha}}{\partial \epsilon_{q\lambda}} \quad (13)$$

Subtract (13) from (12):

$$\sum_{k\alpha} \left[-\epsilon_{k\alpha} + V(0) \sum_{p\beta} n_{p\beta} - \sum_p V(\vec{k}-\vec{p}) n_{p\alpha} \right] \frac{\partial n_{k\alpha}}{\partial \epsilon_{q\lambda}} = n_{q\lambda} - \frac{\partial \langle H_{HF} \rangle_{HF}}{\partial \epsilon_{q\lambda}} \quad (14)$$

Solution is

$$\begin{cases} \epsilon_{k\alpha} = V(0) \sum_{p\beta} n_{p\beta} - \sum_p V(\vec{k}-\vec{p}) n_{p\alpha} \\ n_{q\lambda} = \frac{\partial \langle H_{HF} \rangle_{HF}}{\partial \epsilon_{q\lambda}} = \langle C_{q\lambda}^+ C_{q\lambda} \rangle_{HF} \end{cases} \quad (15)$$

- This is the same result obtained by the heuristic approach.
- Connection between (I) and (II): Note that assuming variational Hamiltonian $H^{HF} = \sum_{k\alpha} \epsilon(k) C_{k\alpha}^+ C_{k\alpha}$ automatically guarantees that the expectation value of the fluctuation term in eq. (3) exactly vanishes!