

Title: 14/15 PSI - Condensed Matter-Lecture 4

Date: Nov 13, 2014 10:45 AM

URL: <http://pirsa.org/14110028>

Abstract:

HARTRE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad \hat{H}_0 = \sum_{k, \lambda} \epsilon_0(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\hat{H}_1 = \frac{1}{2} \sum_{\substack{k, l, p, q \\ \lambda, \mu}} V_{klpq} c_{k, \lambda}^\dagger c_{l, \mu}^\dagger c_{p, \lambda} c_{q, \mu}$$

HARTRE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad \hat{H}_0 = \sum_{k, \lambda} \epsilon_0(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\hat{H}_1 = \frac{1}{2} \sum_{\substack{k, k', q \\ \lambda, \lambda'}} c_{k, \lambda}^\dagger c_{k', \lambda'}^\dagger c_{k+q, \lambda} c_{k'-q, \lambda'}$$

Q. What is the best non-interacting Hamiltonian that approximates \hat{H}_0 .

HARTRE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad \hat{H}_0 = \sum_{k, \lambda} \epsilon_0(\omega) c_{k, \lambda}^\dagger c_{k, \lambda} \quad H^{\text{HF}} = \sum_{k, \lambda} \epsilon_\lambda(\omega) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\hat{H}_1 = \frac{1}{2} \sum_{\substack{k, p, q, r \\ k+p=q+r}} V(q) c_{k+q, \lambda}^\dagger c_{p+\mu, \lambda}^\dagger c_{p, \lambda} c_{q, \mu}$$

Q: What is the best non-interacting Hamiltonian \hat{H}^{HF} that approximates \hat{H}_0 .

HARTRE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad \hat{H}_0 = \sum_{k, \lambda} \epsilon_{k, \lambda} c_{k, \lambda}^\dagger c_{k, \lambda} \quad H^{\text{HF}} = \sum_{k, \lambda} \epsilon_{k, \lambda} \bar{c}_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\hat{H}_1 = \frac{1}{2} \sum_{\substack{k_1, k_2 \\ k_3, k_4}} V(q) \overbrace{c_{k_1+k_2}^\dagger c_{k_3+k_4}}^{\Delta \hat{A}} \overbrace{c_{k_1} c_{k_2}}^{\Delta \hat{B}}$$

Q: What is the best non-interacting Hamiltonian \hat{H}^{HF} that approximates \hat{H}_0 .

$$\begin{aligned} \hat{A} \hat{B} &= (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) \\ &+ \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} \\ &- \langle \hat{A} \rangle \langle \hat{B} \rangle \end{aligned}$$

$$\hat{H}_1^{\text{HF}}$$

HARTREE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H}_0 = \sum_{k,\lambda} \epsilon_{k,\lambda} c_{k,\lambda}^\dagger c_{k,\lambda}$$

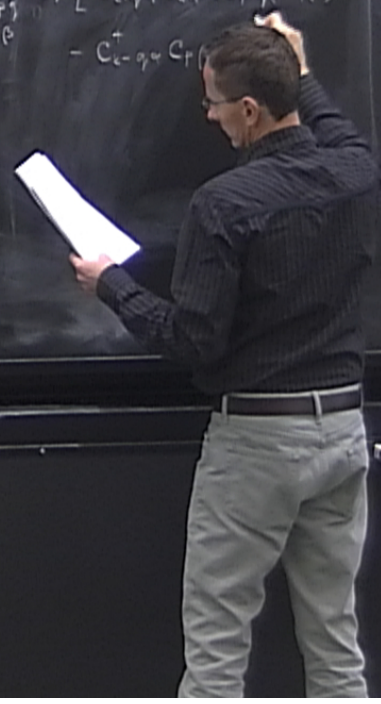
$$H^{HF} = \sum_{k,\lambda} \epsilon_{k,\lambda} c_{k,\lambda}^\dagger c_{k,\lambda}$$

$$V(q) = \frac{1}{2} \sum_{\lambda, \lambda'} \left[c_{k+q,\lambda}^\dagger c_{k,\lambda} c_{k,\lambda'}^\dagger c_{k+q,\lambda'} - c_{k,\lambda}^\dagger c_{k+q,\lambda} c_{k+q,\lambda'}^\dagger c_{k,\lambda'} \right]$$

best non-interacting HF that approximates \hat{H}_0 .

$$\hat{A}\hat{B} = (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) + \hat{A}\langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\hat{H}_1^{HF} = \frac{1}{2} \sum_{\substack{L+R \\ q}} V(q) \left[c_{k+q,\lambda}^\dagger c_{k,\lambda} \langle c_{k+q,\lambda'}^\dagger c_{k,\lambda'} \rangle + \langle c_{k+q,\lambda}^\dagger c_{k,\lambda} \rangle c_{k+q,\lambda'}^\dagger c_{k,\lambda'} - \langle \dots \rangle \right]$$



HARTRE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad \hat{H}_0 = \sum_{k, \lambda} \epsilon_{k, \lambda} c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\frac{1}{2} \sum_{\substack{\alpha, \beta, \gamma, \delta \\ \alpha \neq \beta}} V(\mathbf{q}) \begin{matrix} \alpha & \beta & \gamma & \delta \\ \boxed{c_{\alpha-\gamma}^\dagger c_{\beta-\delta}^\dagger c_{\gamma+\delta} c_{\alpha+\beta}} \end{matrix}$$

What is the best non-interacting Hamiltonian \hat{H}^{HF} that approximates \hat{H}_0 .

$$H^{HF} = \sum_{k, \lambda} \epsilon_{k, \lambda} c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\hat{A} \hat{B} = \overset{\Delta \hat{A}}{(\hat{A} - \langle \hat{A} \rangle)} \overset{\Delta \hat{B}}{(\hat{B} - \langle \hat{B} \rangle)} + \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\hat{H}_1^{HF} = \frac{1}{2} \sum_{\substack{\alpha, \beta, \gamma, \delta \\ \alpha \neq \beta}} V(\mathbf{q}) \left[c_{\alpha-\gamma}^\dagger c_{\beta-\delta}^\dagger \langle c_{\gamma+\delta}^\dagger c_{\alpha+\beta} \rangle + \langle c_{\alpha-\gamma}^\dagger c_{\beta-\delta}^\dagger \rangle c_{\gamma+\delta} c_{\alpha+\beta} - c_{\alpha-\gamma}^\dagger c_{\beta-\delta}^\dagger \langle c_{\gamma+\delta}^\dagger c_{\alpha+\beta} \rangle - \langle c_{\alpha-\gamma}^\dagger c_{\beta-\delta}^\dagger \rangle c_{\gamma+\delta} c_{\alpha+\beta} \right]$$

$$\langle c_{\gamma+\delta}^\dagger c_{\alpha+\beta} \rangle = \delta_{\alpha, \gamma} \langle c_{\beta\delta}^\dagger c_{\alpha\beta} \rangle$$

HARTRE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad \hat{H}_0 = \sum_{k, \lambda} \epsilon_0(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\hat{H}_1 = \frac{1}{2} \sum_{k, \lambda, \lambda'} V(k) c_{k, \lambda}^\dagger c_{k, \lambda'}^\dagger c_{k, \lambda'} c_{k, \lambda}$$

$$H^{HF} = \sum_{k, \lambda} \epsilon_\lambda(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$\hat{A} \hat{B} = (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) + \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\hat{H}_1^{HF} = \frac{1}{2} \sum_{k, \lambda, \lambda'} V(k) [c_{k, \lambda}^\dagger c_{k, \lambda'}^\dagger \langle c_{k, \lambda'} c_{k, \lambda} \rangle + \langle c_{k, \lambda}^\dagger c_{k, \lambda'} \rangle - c_{k, \lambda}^\dagger c_{k, \lambda'} \langle c_{k, \lambda}^\dagger c_{k, \lambda} \rangle - \langle c_{k, \lambda}^\dagger c_{k, \lambda} \rangle]$$

$$\langle c_{k, \lambda}^\dagger c_{k, \lambda'} \rangle = \delta_{\lambda, \lambda'} \langle c_{k, \lambda}^\dagger c_{k, \lambda} \rangle$$

Q: What + non-interacting
How + approximates \hat{H}_0

HARTRE-FOCK (MEAN-FIELD) APPROXIMATION

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad \hat{H}_0 = \sum_{k, \lambda} \epsilon_0(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$H^{HF} = \sum \epsilon_i(k) c_{k, i}^\dagger c_{k, i}$$

$$\hat{H}_1 = \frac{1}{2} \sum_{\substack{q, p \\ \lambda, \mu}} V(q) \overbrace{c_{k+q, \lambda}^\dagger c_{k+q, \mu}^\dagger c_{k, \mu} c_{k, \lambda}}^{\Delta B}$$

$$\hat{A} \hat{B} = \left(\begin{array}{c} \hat{A} \\ \hat{B} - \langle \hat{B} \rangle \end{array} \right) \left(\begin{array}{c} \Delta B \\ \hat{B} - \langle \hat{B} \rangle \end{array} \right)$$

$$\hat{H}_1^{HF} = \frac{1}{2} \sum_{\substack{q, p \\ \lambda, \mu}} V(q) \left[c_{k+q, \lambda}^\dagger c_{k, \lambda} \langle c_{p, \mu}^\dagger c_{p, \mu} \rangle + \langle c_{k+q, \lambda}^\dagger c_{k, \lambda} \rangle - c_{k+q, \mu}^\dagger c_{p, \mu} \langle c_{k+q, \mu}^\dagger c_{k, \mu} \rangle - \langle c_{k+q, \mu}^\dagger c_{k, \mu} \rangle \right]$$

$$\langle c_{p, \mu}^\dagger c_{p, \mu} \rangle = \delta_{\mu, \nu} \langle c_{p, \mu}^\dagger c_{p, \mu} \rangle$$

$$\langle c^\dagger c^\dagger \rangle$$

Q: What is the best non-interacting Hamiltonian \hat{H}^{HF} that approximates \hat{H}_0 .

FOCK (MEAN-FIELD) APPROXIMATION

$$= \sum_{\mathbf{k}, \lambda} \epsilon_{\mathbf{k}, \lambda} c_{\mathbf{k}, \lambda}^\dagger c_{\mathbf{k}, \lambda}$$

$$= \sum_{\mathbf{k}, \lambda} \epsilon_{\mathbf{k}, \lambda} c_{\mathbf{k}, \lambda}^\dagger c_{\mathbf{k}, \lambda}$$

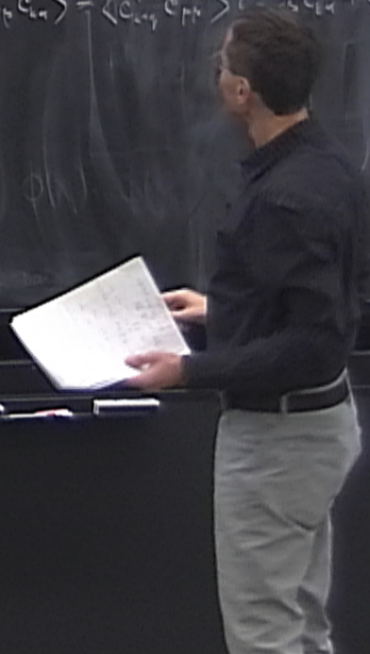
non-interacting approximates \hat{H}_0

$$\hat{H}^{\text{HF}} = \sum_{\mathbf{k}, \lambda} \epsilon_{\mathbf{k}, \lambda} c_{\mathbf{k}, \lambda}^\dagger c_{\mathbf{k}, \lambda}$$

$$\hat{A} \hat{B} = (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) + \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\hat{H}_I^{\text{HF}} = \frac{1}{2} \sum_{\substack{\mathbf{q}, \lambda \\ \mathbf{p}}} V(\mathbf{q}) \left[c_{\mathbf{k}, \lambda}^\dagger c_{\mathbf{k}-\mathbf{q}, \lambda} \langle c_{\mathbf{p}-\mathbf{q}, \lambda}^\dagger c_{\mathbf{p}, \lambda} \rangle + \langle c_{\mathbf{k}, \lambda}^\dagger c_{\mathbf{k}-\mathbf{q}, \lambda} \rangle c_{\mathbf{p}-\mathbf{q}, \lambda}^\dagger c_{\mathbf{p}, \lambda} - \langle \dots \rangle \right]$$

$$\langle c_{\mathbf{p}-\mathbf{q}, \lambda}^\dagger c_{\mathbf{p}, \lambda} \rangle = \delta_{\mathbf{q}, 0} \langle c_{\mathbf{p}, \lambda}^\dagger c_{\mathbf{p}, \lambda} \rangle$$



FOCK (MEAN-FIELD) APPROXIMATION

$$= \sum_{k, \lambda} \epsilon_0(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$H^{HF} = \sum_{k, \lambda} \epsilon_0(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

$$= \sum_{k, \lambda} \epsilon_0(k) c_{k, \lambda}^\dagger c_{k, \lambda}$$

non-interacting approximates \hat{H}_0 .

$$\hat{A} \hat{B} = (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) + \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\hat{H}_I^{HF} = \frac{1}{2} \sum_{\substack{L, P, Q \\ \uparrow \downarrow}} V(q) \left[c_{L, \uparrow}^\dagger c_{L, \downarrow} \langle c_{P, \uparrow}^\dagger c_{P, \downarrow} \rangle + \langle c_{L, \uparrow}^\dagger c_{L, \downarrow} \rangle c_{P, \uparrow}^\dagger c_{P, \downarrow} - \langle \dots \rangle \langle \dots \rangle \right]$$

$$\langle c_{P, \uparrow}^\dagger c_{P, \downarrow} \rangle = \delta_{q, 0} \langle c_{P, \uparrow}^\dagger c_{P, \downarrow} \rangle \rightarrow \text{"Direct" (Hartree)}$$

$$\langle c_{L, \uparrow}^\dagger c_{L, \downarrow} \rangle = \delta_{L, P} \delta_{\uparrow, \downarrow} \langle c_{L, \uparrow}^\dagger c_{L, \downarrow} \rangle \rightarrow \text{"Exchange" (Fock)}$$

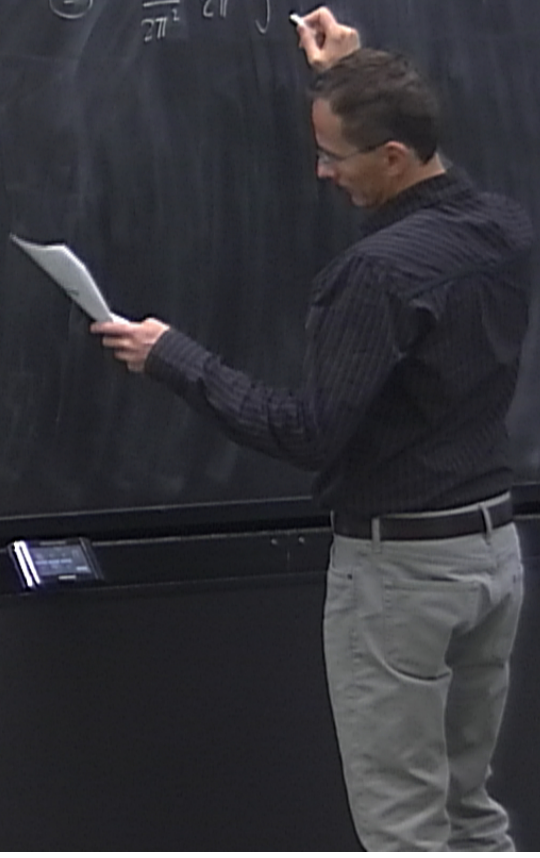
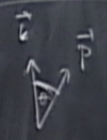
$$\hat{H}^{HF} = \sum_{\mathbf{k}\alpha} \left[\epsilon_0(\mathbf{k}) + \underbrace{V(0) \sum_{\mathbf{p}\beta} \langle c_{\mathbf{p}\beta}^\dagger c_{\mathbf{p}\beta} \rangle}_{\Sigma^{\text{Direct}} \text{ (Hartree)}} - \underbrace{\sum_{\mathbf{p}} V(\mathbf{p}-\mathbf{k}) \langle c_{\mathbf{p}\alpha}^\dagger c_{\mathbf{p}\alpha} \rangle}_{\Sigma^{\text{ex}}(\mathbf{k}) \text{ (Fock)}} \right] c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha}$$

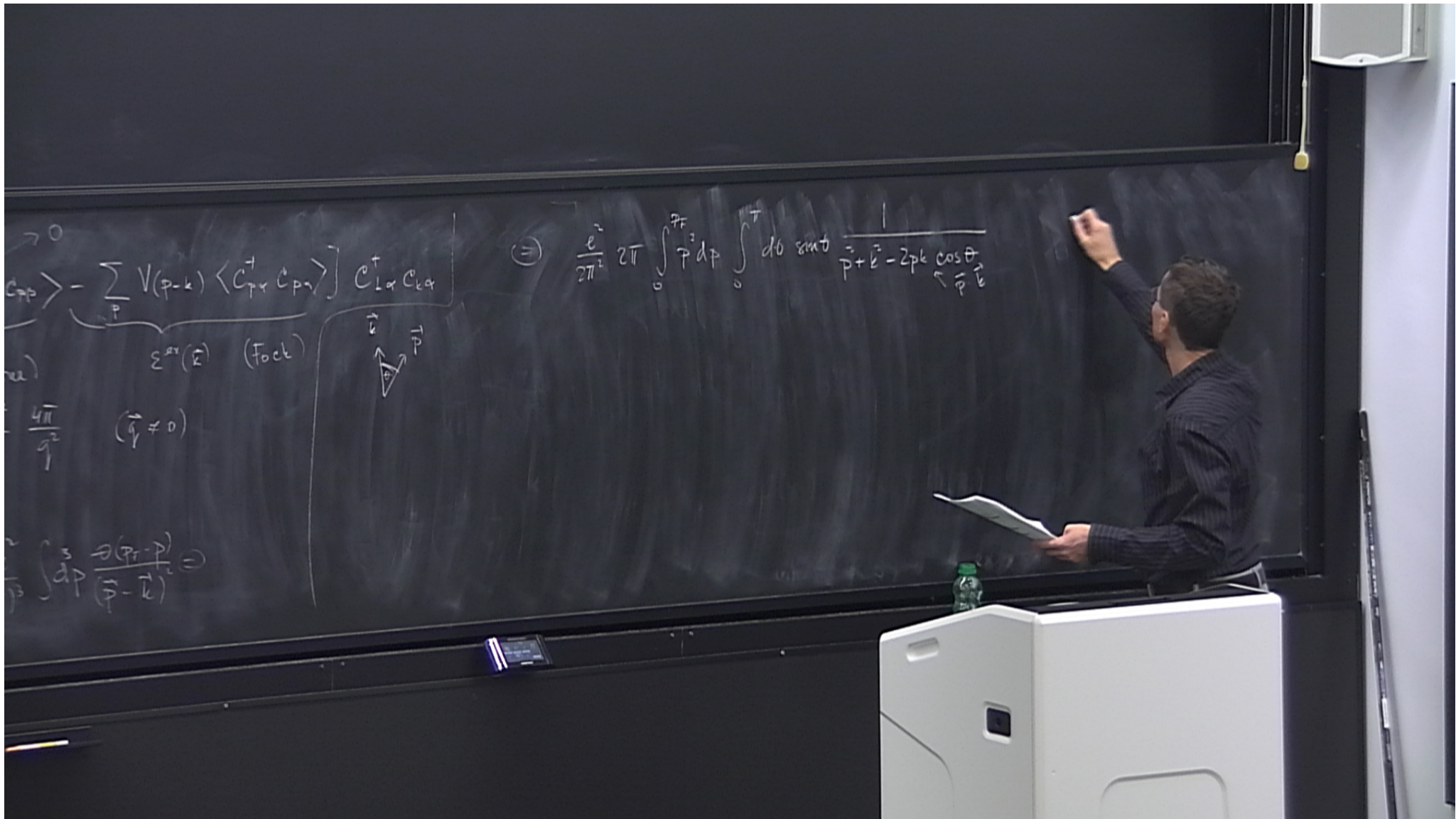
$$\Leftrightarrow \frac{e^2}{2\pi^2} 2\pi \int$$

• Coulomb interaction $V(\mathbf{q}) = \frac{e^2}{V} \frac{4\pi}{q^2} \quad (\mathbf{q} \neq 0)$

Fock term evaluation:

$$-\Sigma^{\text{ex}}(\mathbf{k}) = 4\pi \frac{e^2}{V} \sum_{\mathbf{p}} \frac{\Theta(\mathbf{p}-\mathbf{p})}{(\mathbf{p}-\mathbf{k})^2} = \frac{4\pi e^2}{(2\pi)^3} \int d\mathbf{p} \frac{\Theta(\mathbf{p}-\mathbf{p})}{(\mathbf{p}-\mathbf{k})^2} \Leftrightarrow$$





$$\langle C_{pp} \rangle = \sum_p V(p-k) \langle C_{p+k}^\dagger C_{p+k} \rangle C_{L\alpha}^\dagger C_{k\alpha}$$

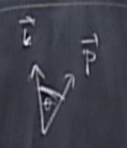
$\Sigma^{\text{ret}}(k)$ (Fock)

$\frac{4\pi}{q^2}$ ($\vec{q} \neq 0$)

$\int dp \frac{\partial(\vec{p}-\vec{p}')}{(\vec{p}-\vec{k})} = 0$

$$\Rightarrow \frac{e^2}{2\pi^2} 2\pi \int_0^{p_F} p^2 dp \int_0^\pi d\theta \sin\theta \frac{1}{p+k-2pk \cos\theta}$$

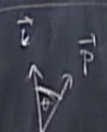
$\vec{p} + \vec{k} - 2pk \cos\theta$
 $\swarrow \quad \searrow$
 $\vec{p} \quad \vec{k}$



$$\langle C_{pp}^\dagger C_{pp} \rangle = \sum_{\vec{p}} V(\vec{p}-\vec{k}) \langle C_{p+\vec{k}}^\dagger C_{p+\vec{k}} \rangle C_{L\alpha}^\dagger C_{L\alpha}$$

(Hartree) $\Sigma^{\text{ex}}(\vec{k})$ (Fock)

$$= \frac{c^2}{V} \frac{4\pi}{q^2} \quad (\vec{q} \neq 0)$$



$$\Rightarrow \frac{c^2}{2\pi^2} 2\pi \int_0^{p_F} p^2 dp \int_0^\pi d\theta \sin\theta \frac{1}{p+k-zpk \cos\theta}$$

$$= \frac{c^2}{\pi} \int_0^{p_F} p dp \int_{-1}^1 \frac{dz}{p+k-zpk}$$

$$= \frac{c^2}{k\pi} \int_0^{p_F} dp p [\ln|k-p| - \ln|k+p|]$$

$$z = \cos\theta$$

$$\Sigma^{\text{ex}}(k) = -\frac{c^2 k_F}{\pi} \left[1 + \frac{k_F - k}{2k_F k} \ln \left| \frac{k+k_F}{k-k_F} \right| \right]$$

$$\frac{4\pi c^2}{(2\pi)^3} \int d^3p \frac{\partial(\vec{p}_F - \vec{p})}{(\vec{p} - \vec{k})^2} \Rightarrow$$



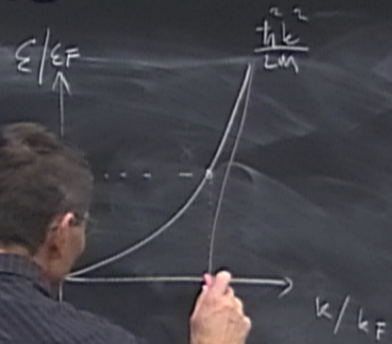
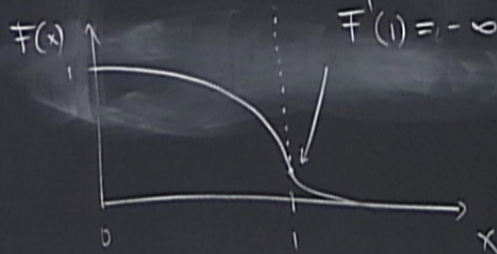
Q: What is the best non-interacting Hamiltonian \hat{H}^{HF} that approximates \hat{H}_0 .

$$+ \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

HF approx. with Coulomb potential

$$\epsilon(\vec{k}) = \epsilon_0(\vec{k}) - \frac{2e^2}{\pi} k_F F\left(\frac{k}{k_F}\right)$$

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|$$



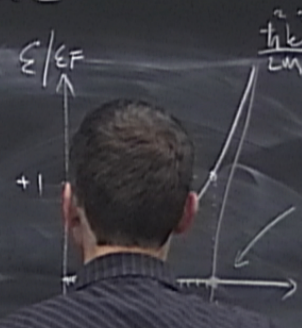
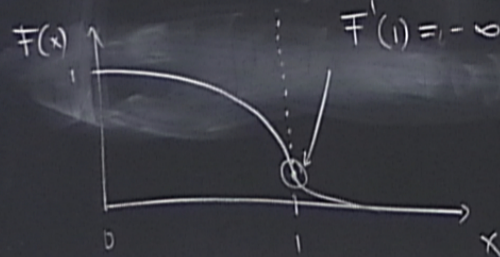
Q: What is the best non-interacting Hamiltonian \hat{H}^{HF} that approximates \hat{H}_0 .

$$+ \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

HF approx. with Coulomb potential

$$\epsilon(\vec{k}) = \epsilon_0(\vec{k}) - \frac{ze^2}{\pi} k_F F\left(\frac{k}{k_F}\right)$$

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|$$



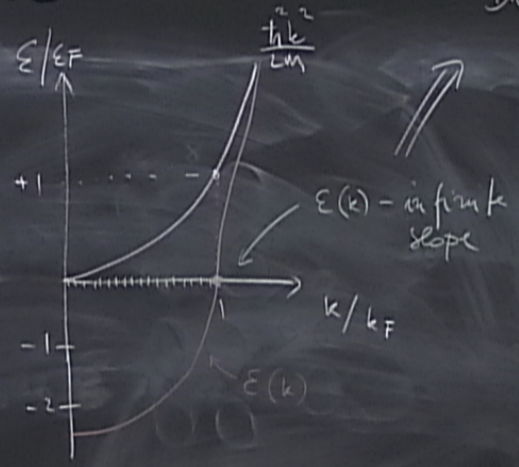
non-interacting
 at approximates \hat{H}_0

$$+ \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\langle C_{p-\sigma} C_{k\sigma} \rangle = \langle C_{p-\sigma} \delta_{p-k} \rangle \langle C_{k\sigma} C_{k\sigma} \rangle \rightarrow$$

Coulomb potential

$$k_F \left[\frac{1+x}{1-x} \right]$$



Divergent Fermi velocity $v_F = \frac{\partial E}{\partial k}$

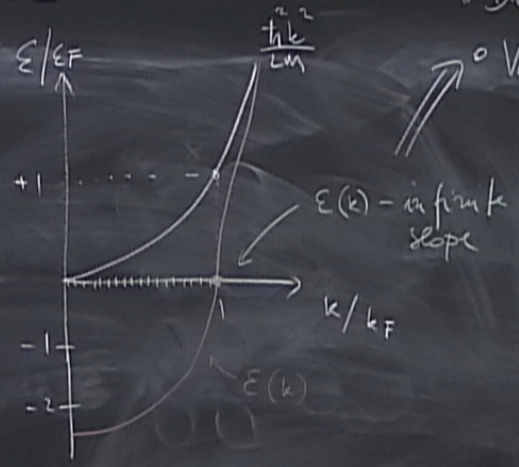
non-interacting
 at approximates \hat{H}_0

$$+ \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\langle C_{p-\eta} C_{k\eta} \rangle = \delta_{p,\eta} \delta_{k,\eta} \langle C_{k\eta} C_{k\eta} \rangle$$

Coulomb potential

$$k_F \left[\frac{1+x}{1-x} \right]$$



• Divergent Fermi velocity $v_F = \frac{\partial E}{\partial k}$!!!
 • Vanishing density of states

$$\begin{aligned}
 & \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} \\
 & - \langle \hat{A} \rangle \langle \hat{B} \rangle
 \end{aligned}
 \quad
 \langle C_{p\uparrow} C_{q\downarrow} \rangle = \langle C_{p\uparrow} C_{q\downarrow} \rangle \rightarrow \text{Exchange (Fock)}$$

SCREENING

• Divergent Fermi velocity $v_F = \frac{d\epsilon}{dk}$

↗ • Vanishing density of states

- infinite slope
 k_F

• These problems can be traced to the long-range nature of the Coulomb potential

• Co
Fock
- ϵ^{∞}

$$+ \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B}$$

$$- \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\langle C_{p\alpha} C_{q\beta} \rangle = \delta_{pq} \delta_{\alpha\beta} \langle C_{p\alpha} C_{p\alpha} \rangle \rightarrow \text{Exchange (Fock)}$$

• Divergent Fermi velocity $v_F = \frac{\partial \epsilon}{\partial k}$

↗ Vanishing density of states

• These problems can be traced to the long-range nature of the Coulomb potential

$\epsilon(k)$ - infink slope
 k/k_F



ϕ^{ext}, ϕ

SCREENING

$$\phi(\vec{r}) = \frac{1}{\epsilon(\vec{q})} \phi^{\text{ext}}(\vec{r})$$

$$\rho^{\text{ind}}(\vec{q}) = \chi(\vec{q}) \phi(\vec{q})$$

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \chi(q) = 1 - \frac{4\pi}{q}$$

$$+ \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B}$$

$$- \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\langle C_{p\uparrow} C_{k\downarrow} \rangle = \delta_{pk} \delta_{\uparrow\downarrow} \langle C_{k\downarrow} C_{k\uparrow} \rangle \rightarrow \text{Exchange (Fock)}$$

• Divergent Fermi velocity $v_F = \frac{\partial \epsilon}{\partial k}$

↗ Vanishing density of states

• These problems can be traced to the long-range nature of the Coulomb potential

$\epsilon(k)$ - infinite slope
 k/k_F



ϕ^{ext}, ϕ

SCREENING

$$\phi(\vec{r}) = \frac{1}{\epsilon(\vec{q})} \phi^{\text{ext}}(\vec{q})$$

$$\rho^{\text{ind}}(\vec{q}) = \chi(\vec{q}) \phi(\vec{q})$$

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \chi(q) = 1 - \frac{4\pi}{q} \frac{\rho^{\text{ind}}(\vec{q})}{\phi(\vec{q})}$$

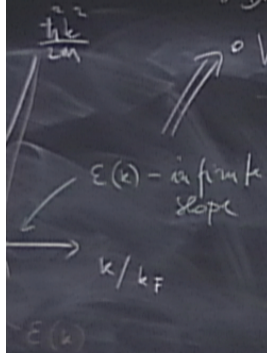
$$AB = (A - \langle \hat{A} \rangle)(B - \langle \hat{B} \rangle) + \hat{A}\langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

$$\langle C_{p-q}^\dagger C_{q\alpha} \rangle = \sum_{p_1 q_1 k} \delta_{p_1 q_1} \delta_{q_1 p} \langle C_{p_1}^\dagger C_{q_1 \alpha} \rangle \rightarrow \text{'Exchange' (Fock)}$$

• Divergent Fermi velocity $v_F = \frac{\partial \epsilon}{\partial k}$

• Vanishing density of states

• These problems can be traced to the long-range nature of the Coulomb potential

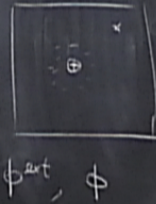


SCREENING

$$\phi(\vec{r}) = \frac{1}{\epsilon(\vec{q})} \phi^{\text{ext}}(\vec{r})$$

$$\rho^{\text{ind}}(\vec{r}) = \chi(\vec{q}) \phi(\vec{r})$$

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \chi(q) = 1 - \frac{4\pi}{q^2} \frac{\rho^{\text{ind}}(\vec{r})}{\phi(\vec{r})}$$



\hat{H}^{HF}

• Coulomb
Fock term
- $\epsilon^{\text{ext}}(\vec{r})$

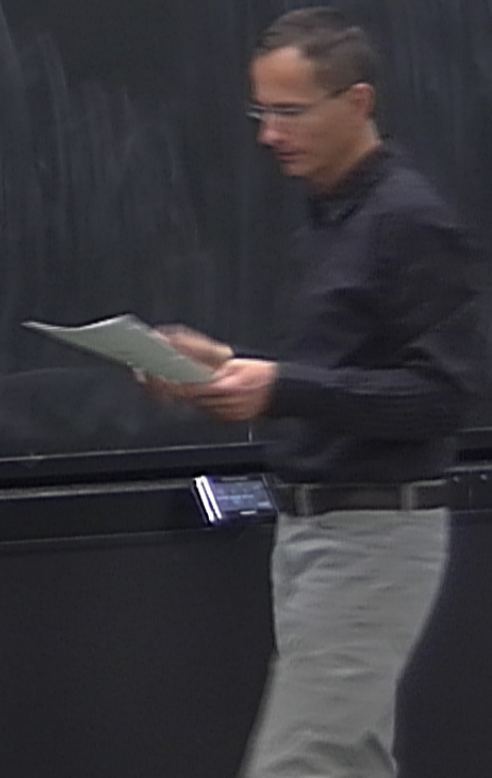
$$-\xi^{\text{ex}}(\vec{l}) = 4\pi \frac{e^2}{V} \sum_{\vec{p}} \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} = \frac{4\pi e^2}{(2\pi)^3} \int d^3p \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} \ominus$$

$$\xi^{\text{ex}}(k) = -\frac{e^2 v_F}{\pi} \left[1 + \frac{v_F}{2v_F k} \ln \left| \frac{k + v_F}{k - v_F} \right| \right]$$

Thomas-Fermi approx (semiclassical)

$$\hat{H} = \int d^3x \hat{\psi}^\dagger(\vec{x}) T(\vec{x}) \hat{\psi}(\vec{x}) \quad (\text{neglect interactions})$$

$$T(\vec{x}) = -\frac{\hbar^2 \nabla^2}{2m} - e\phi(\vec{x})$$



$$-\xi^{\text{ex}}(\vec{l}) = 4\pi \frac{e^+}{V} \sum_{\vec{p}} \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} = \frac{4\pi e^+}{(2\pi)^3} \int d^3p \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} \ominus$$

$$\xi^{\text{ex}}(k) = -\frac{e^+ v_F}{\pi} \left[1 + \frac{v_F}{2v} \ln \left| \frac{k}{k - k_F} \right| \right]$$

Thomas-Fermi approx (semiclassical)

$$\hat{H} = \int d^3x \hat{\psi}^\dagger(\vec{x}) T(\vec{x}) \hat{\psi}(\vec{x}) \quad (\text{neglect interactions})$$

$$T(\vec{x}) = -\frac{\hbar^2 \nabla^2}{2m} - e\phi(\vec{x})$$

For $\phi(\vec{x}) = \phi_0 = \text{const.}$

$$H = \sum_k$$

$$-\xi^{\text{ex}}(\vec{l}) = 4\pi \frac{e^2}{V} \sum_{\vec{p}} \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} = \frac{4\pi e^2}{(2\pi)^3} \int d^3p \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} \ominus$$

$$\xi^{\text{ex}}(\vec{k}) = -\frac{e^2 v_F}{\pi} \left[1 + \frac{v_F}{2v_{F,k}} \ln \left| \frac{v_F + k}{v_F - k} \right| \right]$$

Thomas-Fermi approx (semiclassical)

$$\hat{H} = \int d^3x \hat{\psi}^\dagger(\vec{x}) T(\vec{x}) \hat{\psi}(\vec{x}) \quad (\text{neglect interactions} \\ \& \text{ spin})$$

$$T(\vec{x}) = -\frac{\hbar^2 \nabla^2}{2m} - e\phi(\vec{x})$$

For $\phi(\vec{x}) = \phi_0 = \text{const}$

$$H = \sum_{\vec{k}} \left(\frac{\hbar^2 k^2}{2m} - e\phi_0 \right) c_{\vec{k}}^\dagger c_{\vec{k}} = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}}$$



$$-\epsilon^{\text{ex}}(\vec{l}) = 4\pi \frac{e^2}{V} \sum_{\vec{p}} \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} = \frac{4\pi e^2}{(2\pi)^3} \int d^3p \frac{\Theta(p_F - p)}{(\vec{p} - \vec{l})^2} \ominus$$

$$\epsilon^{\text{ex}}(k) = -\frac{e^2 v_F}{\pi} \left[1 + \frac{v_F}{2v_F k} \ln \left| \frac{v_F + k}{v_F - k} \right| \right]$$

Thomas-Fermi approx (semiclassical)

$$\hat{H} = \int d^3x \hat{\psi}^\dagger(\vec{x}) T(\vec{x}) \hat{\psi}(\vec{x})$$

(neglect interactions & spin)

$$T(\vec{x}) = -\frac{\hbar^2 \nabla^2}{2m} - e\phi(\vec{x})$$

For $\phi(\vec{x}) = \phi_0 = \text{const}$

$$H = \sum_{\vec{k}} \left(\frac{\hbar^2 k^2}{2m} - e\phi_0 \right) c_{\vec{k}}^\dagger c_{\vec{k}} = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}}$$

TF - for slowly varying $\phi(\vec{x})$
we can replace $\epsilon_{\vec{k}}$

$$-\Sigma^{\alpha}(\vec{k}) = 4\pi \frac{e^2}{V} \sum_{\vec{p}} \frac{\Theta(p_F - p)}{(\vec{p} - \vec{k})^2} = \frac{4\pi e^2}{(2\pi)^3} \int d^3p \frac{\Theta(p_F - p)}{(\vec{p} - \vec{k})^2} \ominus$$

$$\Sigma^{\alpha}(\vec{k}) = -\frac{e^2 k_F}{\pi} \left[1 + \frac{k_F}{2k} 2n \left| \frac{k_F}{k} \right| \right]$$

Thomas-Fermi approx (semiclassical)

$$\hat{H} = \int d^3x \hat{\psi}^{\dagger}(\vec{x}) T(\vec{x}) \hat{\psi}(\vec{x}) \quad (\text{neglect interactions \& spin})$$

$$T(\vec{x}) = -\frac{\hbar^2 \nabla^2}{2m} - e\phi(\vec{x})$$

For $\phi(\vec{x}) = \phi_0 = \text{const.}$

$$H = \sum_{\vec{k}} \left(\frac{\hbar^2 k^2}{2m} - e\phi_0 \right) c_{\vec{k}}^{\dagger} c_{\vec{k}} = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^{\dagger} c_{\vec{k}}$$

TF - for slowly varying $\phi(\vec{x})$
we can replace $(\vec{x} \leftrightarrow \vec{r})$

$$\epsilon_{\vec{k}} \rightarrow \epsilon_{\vec{k}}(\vec{r}) = \frac{\hbar^2 k^2}{2m} -$$

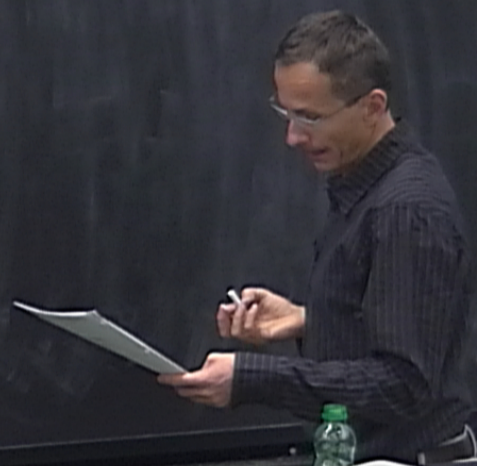
$$= \frac{4\pi e}{(2\pi)^3} \int d^3p \frac{\partial(\epsilon_F - \epsilon)}{(\vec{p} - \vec{k})^2} \ominus$$

$$\epsilon^{\text{TF}}(\vec{k}) = -\frac{e^2 k_F}{\pi} \left[1 + \frac{k_F^2}{2k_F k} \ln \left| \frac{k_F + k}{k - k_F} \right| \right]$$

approx (semiclassical)
(neglect interactions & spin)

TF - for slowly varying $\phi(\vec{x})$
we can replace $(\vec{x} \leftrightarrow \vec{r})$
 $\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r})$

$$= \sum_k \epsilon_k c_k^\dagger c_k$$



$$= \frac{4\pi e}{(2\pi)^3} \int d^3p \frac{\partial(\psi_T - \psi)}{(\vec{p} - \vec{k})^2} \Rightarrow$$

$$\epsilon^{\infty}(k) = -\frac{e^2 k_F}{\pi} \left[1 + \frac{k_F^2}{2k_F k} 2\pi \left| \frac{k_F + k}{k - k_F} \right| \right]$$

prox (semiclassical)

(neglect interactions & spin)

TF - for slowly varying $\phi(\vec{x})$
we can replace $(\vec{x} \leftrightarrow \vec{r})$

$$\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r})$$

Calculate \bar{n} density

$$\rho(\vec{r}) = -e \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle = -e \sum_{k, k'} \langle \psi_k^\dagger(\vec{r}) \psi_{k'}(\vec{r}) c_k^\dagger c_{k'} \rangle$$

$$= -e \sum_{k, k'} \psi_k^*(\vec{r}) \psi_{k'}(\vec{r}) \underbrace{\langle c_k^\dagger c_{k'} \rangle}_{\delta_{kk'} f(\epsilon_k(\vec{r}))}$$

Fermi-Dirac distribution

$$= \sum_k \epsilon_k c_k^\dagger c_k$$

$$= \frac{4\pi e}{(2\pi)^3} \int d^3p \frac{\partial(\epsilon_F - \epsilon)}{(\vec{p} - \vec{k})^2} \Theta(\epsilon_F - \epsilon)$$

$$\epsilon(k) = -\frac{\hbar^2 k^2}{2m} \left[1 + \frac{k_F^2}{2k^2} \ln \left| \frac{k+k_F}{k-k_F} \right| \right]$$

prox (semiclassical)

(neglect interactions & spin)

TF - for slowly varying $\phi(\vec{r})$
we can replace $(\vec{x} \leftrightarrow \vec{r})$

$$\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r})$$

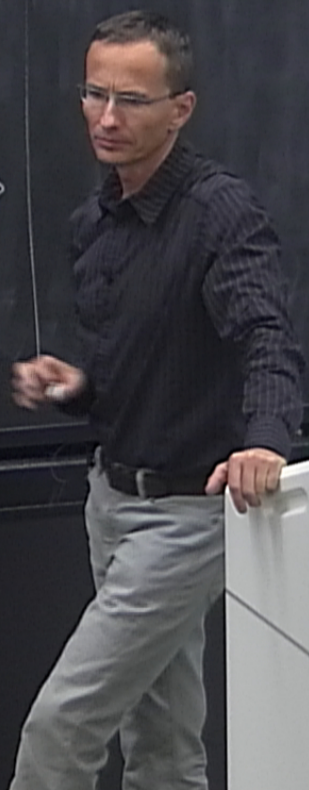
Calculate \bar{n} density

$$\rho(\vec{r}) = -e \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle = -e \sum_{k,k'} \langle \psi_k^\dagger(\vec{r}) \psi_{k'}(\vec{r}) c_k^\dagger c_{k'} \rangle$$

$$= -e \sum_{k,k'} \psi_k^*(\vec{r}) \psi_{k'}(\vec{r}) \underbrace{\langle c_k^\dagger c_{k'} \rangle}_{\delta_{kk'} f(\epsilon_k(\vec{r}))}$$

Fermi-Dirac distribution

$$= \sum_k \epsilon_k c_k^\dagger c_k$$



$$\epsilon(k) = -\frac{e k_F}{\pi} \left[1 + \frac{k_F - k}{2k_F k} \ln \left| \frac{k + k_F}{k - k_F} \right| \right]$$

\vec{r} - for slowly varying $\phi(\vec{r})$

we can replace $(\vec{x} \leftrightarrow \vec{r})$

$$\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e \phi(\vec{r})$$

calculate e^- density

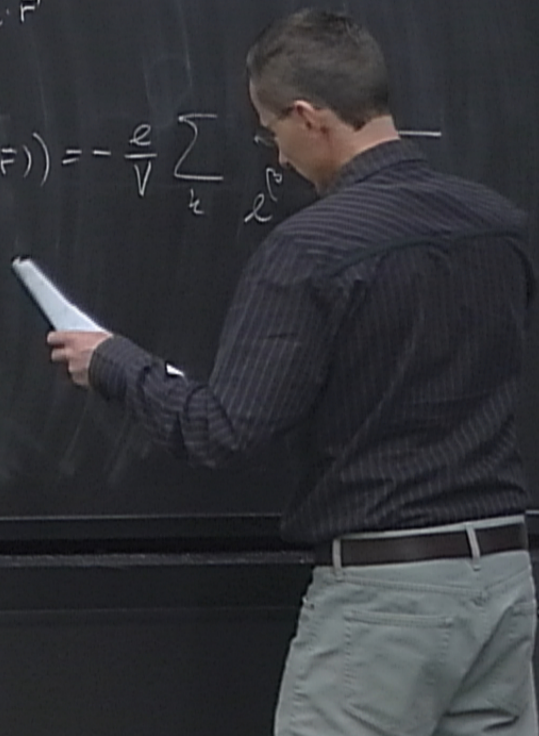
$$\langle \hat{\rho}(\vec{r}) \rangle = -e \sum_{k, l} \langle \psi_k^*(\vec{r}) \psi_l(\vec{r}) c_k^\dagger c_l \rangle$$

$$\psi_k^*(\vec{r}) \psi_l(\vec{r}) \langle c_k^\dagger c_l \rangle \xrightarrow{\text{Fermi-Dirac distribution}} \delta_{kl} f(\epsilon_k(\vec{r}))$$

$$\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f(\epsilon_k(\vec{r}))$$

$$\text{for } \psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}}$$

$$\rho(\vec{r}) = -\frac{e}{V} \sum_k f(\epsilon_k(\vec{r})) = -\frac{e}{V} \sum_k e^{i\vec{k}\cdot\vec{r}}$$



$$\epsilon(k) = -\frac{e k_F}{\pi} \left[1 + \frac{k_F - k}{2k_F k} \ln \left| \frac{k + k_F}{k - k_F} \right| \right]$$

F - for slowly varying $\phi(\vec{x})$

we can replace $(\vec{x} \leftrightarrow \vec{r})$

$$\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e \phi(\vec{r})$$

calculate e^- density

$$\langle \hat{\rho}(\vec{r}) \rangle = -e \sum_{k, l} \langle \psi_k^*(\vec{r}) \psi_l(\vec{r}) c_k^\dagger c_l \rangle$$

$$\psi_k^*(\vec{r}) \psi_l(\vec{r}) \langle c_k^\dagger c_l \rangle \xrightarrow{\text{Fermi-Dirac distribution}} \delta_{kl} f(\epsilon_k(\vec{r}))$$

$$\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f(\epsilon_k(\vec{r}))$$

$$\text{for } \psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{-i\vec{k} \cdot \vec{r}}$$

$$\beta = \frac{1}{k_B T}$$

$$\rho(\vec{r}) = -\frac{e}{V} \sum_k f(\epsilon_k(\vec{r})) = -\frac{e}{V} \sum_k \frac{1}{e^{\beta(\epsilon_k(\vec{r}) - \mu)} + 1}$$

$$\epsilon(k) = -\frac{\hbar^2 k_F^2}{2m} \left[1 + \frac{k_F - k}{2k_F k} \ln \left| \frac{k + k_F}{k - k_F} \right| \right]$$

\vec{r} - for slowly varying $\phi(\vec{x})$

we can replace $(\vec{x} \leftrightarrow \vec{r})$

$$\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r})$$

calculate \bar{n} density

$$\langle \hat{\psi}(\vec{r}) \rangle = -e \sum_{k, l} \langle \psi_k^*(\vec{r}) \psi_l(\vec{r}) c_k^\dagger c_l \rangle$$

$$\psi_k^*(\vec{r}) \psi_l(\vec{r}) \langle c_k^\dagger c_l \rangle \xrightarrow{\text{Fermi-Dirac distribution}} \delta_{kl} f(\epsilon_k(\vec{r}))$$

$$\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f(\epsilon_k(\vec{r}))$$

$$\text{for } \psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}}$$

$$\beta = \frac{1}{k_B T}$$

$$\rho(\vec{r}) = \sum_k f(\epsilon_k(\vec{r})) = -\frac{e}{V} \sum_k \frac{1}{e^{\beta(\epsilon_k(\vec{r}) - \mu)} + 1}$$

Define

n_0

$$\varepsilon(k) = -\frac{e k_F}{\pi} \left[1 + \frac{k_F - k}{2k_F k} \ln \left| \frac{k + k_F}{k - k_F} \right| \right]$$

F - for slowly varying $\phi(\vec{x})$

we can replace $(\vec{x} \rightarrow \vec{r})$

$$\varepsilon_k \rightarrow \varepsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e \phi(\vec{r})$$

calculate \bar{n} density

$$\langle \hat{\psi}(\vec{r}) \rangle = -e \sum_{k, l} \langle \psi_k^*(\vec{r}) \psi_l(\vec{r}) c_k^\dagger c_l \rangle$$

$$\psi_k^*(\vec{r}) \psi_l(\vec{r}) \langle c_k^\dagger c_l \rangle \xrightarrow{\text{Fermi-Dirac distribution}} \delta_{kl} f(\varepsilon_k(\vec{r}))$$

$$\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f(\varepsilon_k(\vec{r}))$$

$$\text{for } \psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{-i\vec{k} \cdot \vec{r}}$$

$$\beta = \frac{1}{k_B T}$$

$$\rho(\vec{r}) = -\frac{e}{V} \sum_k f(\varepsilon_k(\vec{r})) = -\frac{e}{V} \sum_k \frac{1}{e^{\beta(\varepsilon_k(\vec{r}) - \mu)} + 1}$$

Define

$$n_0(\mu) = \int \frac{d^3k}{4\pi^3} \frac{1}{e^{\beta \left[\frac{\hbar^2 k^2}{2m} - \mu \right]} + 1}$$

$$\epsilon(k) = -\frac{e k_F}{\pi} \left[1 + \frac{k_F - k}{2k_F k} \ln \left| \frac{k + k_F}{k - k_F} \right| \right]$$

\vec{r} - for slowly varying $\phi(\vec{x})$

we can replace $(\vec{x} \rightarrow \vec{r})$

$$\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e \phi(\vec{r})$$

calculate \bar{n} density

$$\langle \hat{\rho}(\vec{r}) \rangle = -e \sum_{k, l} \langle \psi_k^*(\vec{r}) \psi_l(\vec{r}) c_k^\dagger c_l \rangle$$

$$\psi_k^*(\vec{r}) \psi_l(\vec{r}) \langle c_k^\dagger c_l \rangle \xrightarrow{\delta_{kl}} f(\epsilon_k(\vec{r}))$$

Fermi-Dirac distribution

$$\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f(\epsilon_k(\vec{r}))$$

$$\text{for } \psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}}$$

$$\beta = \frac{1}{k_B T}$$

$$\rho(\vec{r}) = -\frac{e}{V} \sum_k f(\epsilon_k(\vec{r})) = -\frac{e}{V} \sum_k \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}$$

Define

$$n_0(\mu) = \int \frac{d^3k}{4\pi^3} \frac{1}{e^{\beta \left[\frac{\hbar^2 k^2}{2m} - \mu \right]} + 1}$$

F - for slowly varying $\phi(\vec{x})$
 we can replace $(\vec{x} \leftrightarrow \vec{r})$
 $\epsilon_k \rightarrow \epsilon_k(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r})$

calculate \bar{n} density

$$\langle \hat{n}(\vec{r}) \rangle = -e \sum_{k \neq l} \langle \psi_k^*(\vec{r}) \psi_l(\vec{r}) c_l^\dagger c_k \rangle$$

$$\psi_k^*(\vec{r}) \psi_l(\vec{r}) \langle c_l^\dagger c_k \rangle \xrightarrow{\delta_{kk'}} f(\epsilon_k(\vec{r}))$$

Fermi-Dirac distribution

$$\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f(\epsilon_k(\vec{r}))$$

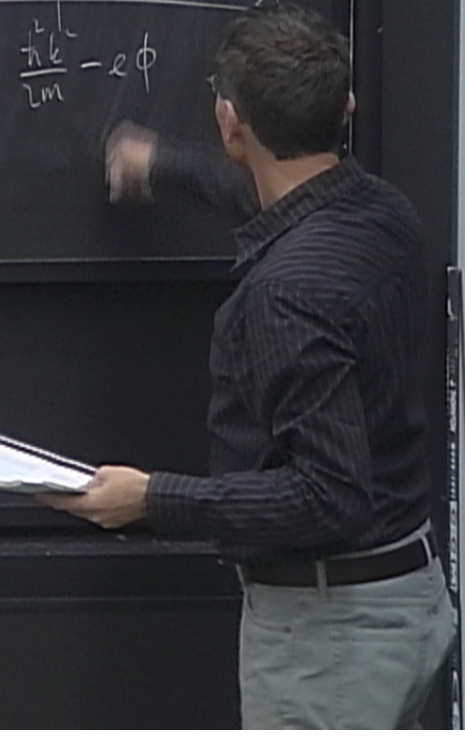
for $\psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}}$

$$\beta = \frac{1}{k_B T}$$

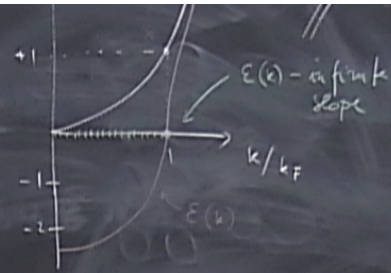
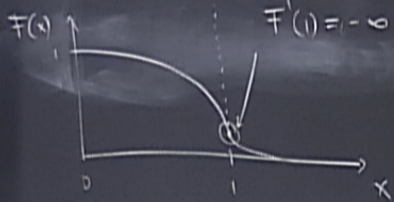
$$\rho(\vec{r}) = -\frac{e}{V} \sum_k f(\epsilon_k(\vec{r})) = -\frac{e}{V} \sum_k \frac{1}{e^{\beta(\epsilon_k(\vec{r}) - \mu)} + 1}$$

Define

$$n_0(\mu) = \int \frac{d^3k}{4\pi^3} \frac{1}{e^{\beta[\frac{\hbar^2 k^2}{2m} - \mu]} + 1}$$



$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|$$



• These problems can be traced to the long-range nature of the Coulomb potential.

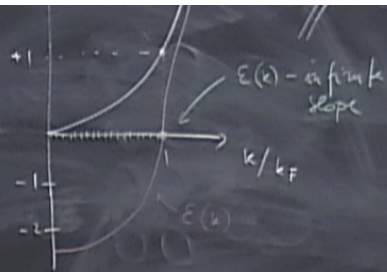
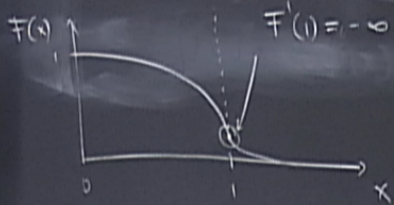


Induce charge density

$$\rho_{ind}(\vec{r}) = -e [n_0(\mu + e\phi(\vec{r})) - n_0(\mu)]$$

• As $e\phi(\vec{r})$ is small compared to μ

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|$$



• These problems can be traced to the long-range nature of the Coulomb potential.

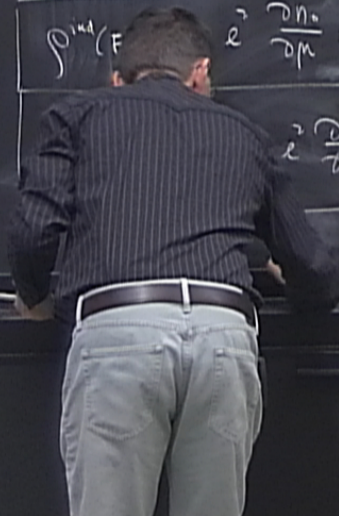


Induce charge density

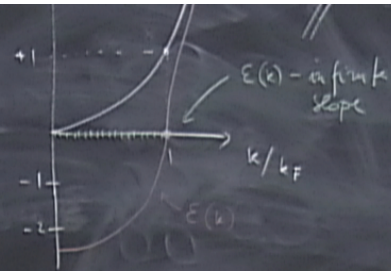
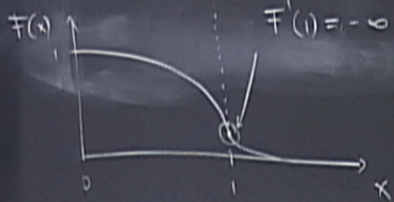
$$\rho_{\text{ind}}(\mathbf{r}) = -e [n_0(\mu + e\phi(\mathbf{r})) - n_0(\mu)]$$

• Assumption: $e\phi(\mathbf{r})$ is small compared to μ

$$\rho_{\text{ind}}(\mathbf{r}) \approx -e^2 \frac{\partial n_0}{\partial \mu} \phi(\mathbf{r})$$



$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|$$



• These problems can be traced to the long-range nature of the Coulomb potential.



Induce charge density

$$\rho_{\text{ind}}(\vec{r}) = -e [n_0(\mu + e\phi(\vec{r})) - n_0(\mu)]$$

• Assumption: $e\phi(\vec{r})$ is small compared to μ

$$\rho_{\text{ind}}(\vec{r}) = -e^2 \frac{\partial n_0}{\partial \mu} \phi(\vec{r})$$

$$\Rightarrow \chi(\vec{q}) = -e^2 \frac{\partial n_0}{\partial \mu}$$

(indep. of \vec{q})

Dielectric const

$$\epsilon(\vec{q}) = 1 + \frac{4\pi e^2}{q^2} \frac{\partial n_0}{\partial \mu}$$

k/k_F nature of the Coulomb potential

ϕ_{ext}, ϕ

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \chi(q) = 1 - \frac{4\pi}{q^2} \frac{\rho^{ext}(\vec{q})}{\phi(\vec{q})}$$

dielectric const.

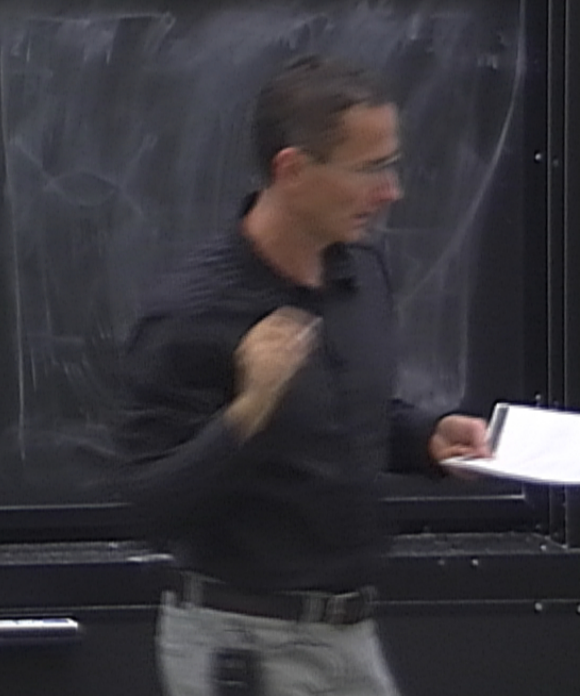
$$\epsilon(\vec{q}) = 1 + \frac{4\pi e^2}{q^2} \frac{\partial n_0}{\partial \mu}$$

finds TF wavevector

$$k_{TF}^2 = 4\pi e^2 \frac{\partial n_0}{\partial \mu}$$

$$\epsilon(\vec{q}) = 1 + \frac{k_{TF}^2}{q^2}$$

EXAMPLE: Point charge



k/k_F

nature of the Coulomb potential

ϕ^{ext}, ϕ

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \chi(q) = 1 - \frac{4\pi}{q^2} \frac{\rho^{ext}(\vec{q})}{\phi(\vec{q})}$$

dielectric const:

$$\epsilon(\vec{q}) = 1 + \frac{4\pi e^2}{q^2} \frac{\partial n_0}{\partial \mu}$$

TF wavevector

$$k_{TF}^2 = 4\pi e^2 \frac{\partial n_0}{\partial \mu}$$

$$\epsilon(\vec{q}) = 1 + \frac{k_{TF}^2}{q^2}$$

EXAMPLE: Point charge

$$\phi^{ext}(\vec{r}) = \frac{Q}{r}, \quad \phi^{ext}(\vec{q}) = \frac{4\pi Q}{q^2}$$

$$\phi(\vec{q}) = \frac{1}{\epsilon(\vec{q})} \phi^{ext}(\vec{q}) = \frac{4\pi Q}{q^2 + k_{TF}^2}$$

$$\phi(\vec{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} \frac{4\pi Q}{q^2 + k_{TF}^2} = \frac{Q}{r} e^{-r k_{TF}}$$

"Screened Coulomb" (Yukawa) potential

$$k_{TF} \leftrightarrow \frac{1}{\lambda_D}$$

$$H = \int d^3 \psi^\dagger(\vec{x}) T(\vec{x}) \psi(\vec{x}) \quad (\text{neglect interactions})$$

$$T(\vec{x}) = -\frac{\hbar^2 \nabla^2}{2m} - e\phi(\vec{x})$$

For $\phi(\vec{x}) = \phi_0 = \text{const.}$

$$H = \sum_{\vec{k}} \left(\frac{\hbar^2 k^2}{2m} - e\phi_0 \right) c_{\vec{k}}^\dagger c_{\vec{k}} = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}}$$

(neglect interactions & spin)

$$\epsilon_{\vec{k}} \rightarrow \epsilon_{\vec{k}}(\vec{r}) = \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r})$$

Calculate \bar{n} density

$$\begin{aligned} \rho(\vec{r}) &= -e \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle = -e \sum_{\vec{k}, l} \langle \psi_{\vec{k}}^\dagger(\vec{r}) \psi_{\vec{k}}(\vec{r}) c_{\vec{k}}^\dagger c_{\vec{k}} \rangle \\ &= -e \sum_{\vec{k}, l} \psi_{\vec{k}}^*(\vec{r}) \psi_{\vec{k}}(\vec{r}) \langle c_{\vec{k}}^\dagger c_{\vec{k}} \rangle \end{aligned}$$

Fermi-Dirac distribution:
 $\langle c_{\vec{k}}^\dagger c_{\vec{k}} \rangle = f(\epsilon_{\vec{k}}(\vec{r}))$

for $\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$

$$\rho(\vec{r}) = -\frac{e}{V} \sum_{\vec{k}} f(\epsilon_{\vec{k}}(\vec{r})) = -$$

Define

$$n_0(\mu) = \int \frac{d^3k}{4\pi^3} \frac{1}{e^{\beta(\frac{\hbar^2 k^2}{2m} - \mu)} + 1}$$

The Lindhard dielectric function
(aka 'random phase approx')



for $\phi(\vec{r}) = \phi_0 = \text{const.}$

$$H = \sum_{\vec{k}} \left(\frac{\hbar^2 \vec{k}^2}{2m} - e\phi_0 \right) c_{\vec{k}}^\dagger c_{\vec{k}} = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}}$$

$$\rho(\vec{r}) = -e \sum_{\vec{k}} \langle \psi(\vec{r}) | \psi(\vec{r}) \rangle = -e \sum_{\vec{k}} \langle \psi_{\vec{k}}(\vec{r}) | \psi_{\vec{k}}(\vec{r}) \rangle c_{\vec{k}}^\dagger c_{\vec{k}}$$

$$= -e \sum_{\vec{k}, \vec{k}'} \psi_{\vec{k}}^*(\vec{r}) \psi_{\vec{k}'}(\vec{r}) \underbrace{\langle c_{\vec{k}}^\dagger c_{\vec{k}'} \rangle}_{\delta_{\vec{k}, \vec{k}'} f(\epsilon_{\vec{k}}(\vec{r}))}$$

Fermi-Dirac distribution;

The Lindhard dielectric function
(aka "random phase approx.")

Assume ϕ is small, treat it as
a perturbation

$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_H + \dots$$

for $\phi(\vec{r}) = \phi_0 = \text{const.}$

$$H = \sum_{\vec{k}} \left(\frac{\hbar^2 \vec{k}^2}{2m} - e\phi_0 \right) c_{\vec{k}}^\dagger c_{\vec{k}} = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}}$$

$$\rho(\vec{r}) = -e \langle \psi(\vec{r}) \psi(\vec{r}) \rangle = -e \sum_{\vec{k}, \vec{l}} \psi_{\vec{k}}(\vec{r}) \psi_{\vec{l}}(\vec{r}) c_{\vec{k}} c_{\vec{l}}$$

$$= -e \sum_{\vec{k}, \vec{l}} \psi_{\vec{k}}^*(\vec{r}) \psi_{\vec{l}}(\vec{r}) \underbrace{\langle c_{\vec{k}}^\dagger c_{\vec{l}} \rangle}_{\delta_{\vec{k}\vec{l}} f(\epsilon_{\vec{k}}(\vec{r}))}$$

Fermi-Dirac distribution:

Define:
 $n_0(\mu) =$

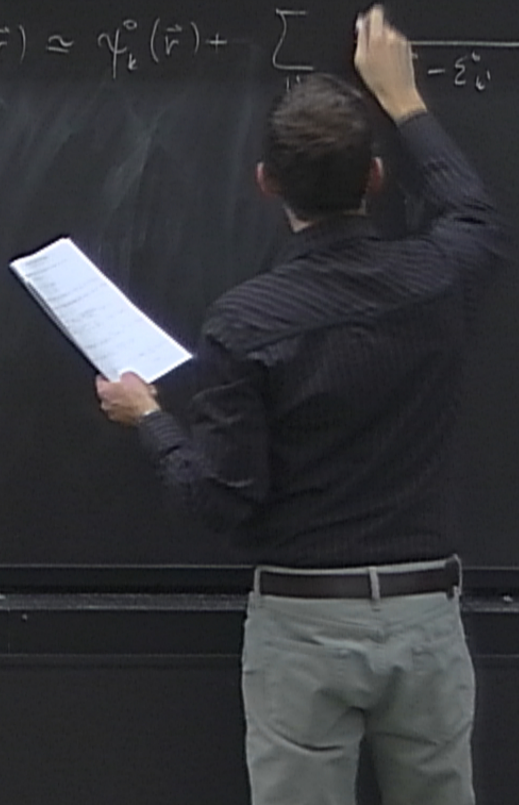
The Lindhard dielectric function
(aka "random phase approx.")

Assume $\phi(\vec{r})$ is small, treat it as a perturbation

$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - \underbrace{e\phi(\vec{r})}_{H'}$$

Want to calculate $\rho(\vec{r})$ in leading order P.t.

$$\psi_{\vec{k}}(\vec{r}) \approx \psi_{\vec{k}}^0(\vec{r}) + \sum_{\vec{l}} \frac{1}{-\epsilon_{\vec{l}}} \dots$$



For $\phi(\vec{r}) = \phi_0 = \text{const}$

$$H = \sum_{\vec{k}} \left(\frac{\hbar^2 \vec{k}^2}{2m} - e\phi_0 \right) c_{\vec{k}}^\dagger c_{\vec{k}} = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}}$$

$$\rho(\vec{r}) = - \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle = -e \sum_{\vec{k}, \vec{k}'} \langle \psi_{\vec{k}}^*(\vec{r}) \psi_{\vec{k}'}(\vec{r}) c_{\vec{k}}^\dagger c_{\vec{k}'} \rangle$$

$$= -e \sum_{\vec{k}, \vec{k}'} \psi_{\vec{k}}^*(\vec{r}) \psi_{\vec{k}'}(\vec{r}) \underbrace{\langle c_{\vec{k}}^\dagger c_{\vec{k}'} \rangle}_{\substack{\text{Fermi-Dirac} \\ \text{distribution:} \\ \delta_{\vec{k}, \vec{k}'} f(\epsilon_{\vec{k}}(\vec{r}))}}$$

Define

$$n_0(\vec{r}) = \int \frac{d^3k}{4\pi^3}$$

The Lindhard dielectric function
(aka "random phase approx")

Assume $\phi(\vec{r})$ is small, treat it
a perturbation

$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - \underbrace{e\phi(\vec{r})}_{H'}$$

Want to calculate $\rho(\vec{r})$ in
leading order P.T.

$$\psi_{\vec{k}}(\vec{r}) \approx \psi_{\vec{k}}^0(\vec{r}) + \sum_{\vec{k}'} \frac{\langle \psi_{\vec{k}'}^0 | -e\phi(\vec{r}) | \psi_{\vec{k}}^0 \rangle}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \psi_{\vec{k}'}^0(\vec{r})$$

$$\psi_{\vec{k}}^0(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}, \quad \epsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}; \quad H_0 \psi_{\vec{k}}^0 = \epsilon_{\vec{k}} \psi_{\vec{k}}^0$$

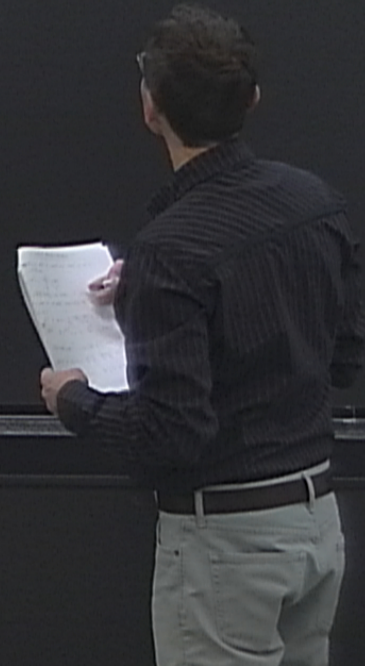
$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - \underbrace{e\phi(\vec{r})}_{H'}$$

Want to calculate $\rho(\vec{r})$ in leading order P.T.

$$\langle \psi_{\vec{k}}^0 | -e\phi(\vec{r}) | \psi_{\vec{k}'}^0 \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{k}\cdot\vec{r}} \phi(\vec{r}) e^{i\vec{k}'\cdot\vec{r}} = -\frac{e}{V} \phi(\vec{k}-\vec{k}')$$

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}^0(\vec{r}) - \frac{e}{V} \sum_{\vec{k}'} \frac{\phi(\vec{k}-\vec{k}')}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \psi_{\vec{k}'}^0(\vec{r})$$

Density $\rho(\vec{r}) = -e \sum_{\vec{k}} |\psi_{\vec{k}}(\vec{r})|^2 f_{\vec{k}} \quad f_{\vec{k}} \equiv f(\epsilon_{\vec{k}})$



$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - \underbrace{e\phi(\vec{r})}_{H'}$$

Want to calculate $\rho(\vec{r})$ in leading order P.T.

$$\langle \psi_k^0 | -e\phi(\vec{r}) | \psi_k^0 \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{k}\cdot\vec{r}} \phi(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = -\frac{e}{V} \phi(\vec{k}-\vec{k}')$$

$$\psi_k(\vec{r}) = \psi_k^0(\vec{r}) - \frac{e}{V} \sum_{k'} \frac{\phi(\vec{k}-\vec{k}')}{\epsilon_k - \epsilon_{k'}} \psi_{k'}^0(\vec{r})$$

Density $\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f_k \quad f_k \equiv f(\epsilon_k)$

$$= -e \left[\sum_k f_k |\psi_k^0|^2 - \right]$$

$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - \underbrace{e\phi(\vec{r})}_{H'}$$

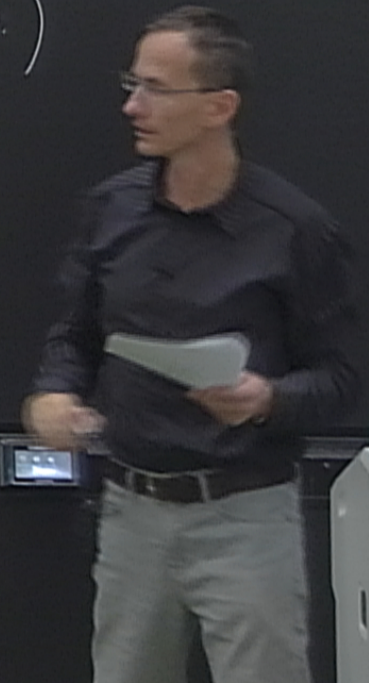
Want to calculate $\rho(\vec{r})$ in leading order P.T.

$$\langle \psi_{\vec{k}}^0 | -e\phi(\vec{r}) | \psi_{\vec{k}'}^0 \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{k}\cdot\vec{r}} \phi(\vec{r}) e^{i\vec{k}'\cdot\vec{r}} = -\frac{e}{V} \phi(\vec{k}-\vec{k}')$$

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}^0(\vec{r}) - \frac{e}{V} \sum_{\vec{k}'} \frac{\phi(\vec{k}-\vec{k}')}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \psi_{\vec{k}'}^0(\vec{r})$$

Density $\rho(\vec{r}) = -e \sum_{\vec{k}} |\psi_{\vec{k}}(\vec{r})|^2 f_{\vec{k}} \quad f_{\vec{k}} \equiv f(\epsilon_{\vec{k}})$

$$= -e \left[\underbrace{\sum_{\vec{k}} f_{\vec{k}} |\psi_{\vec{k}}^0|^2}_{\rho_0(\vec{r})} - \frac{e}{V} \sum_{\vec{k}} \left(f_{\vec{k}} \psi_{\vec{k}}^{0*} \sum_{\vec{k}'} \frac{\psi_{\vec{k}'}^0}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \phi(\vec{k}-\vec{k}') + \text{c.c.} \right) \right]$$



$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - \underbrace{e\phi(\vec{r})}_{H'}$$

Want to calculate $\rho(\vec{r})$ in leading order P.T.

$$\langle \psi_{\vec{k}}^0 | -e\phi(\vec{r}) | \psi_{\vec{k}'}^0 \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{k}\cdot\vec{r}} \phi(\vec{r}) e^{i\vec{k}'\cdot\vec{r}} = -\frac{e}{V} \phi(\vec{k}-\vec{k}')$$

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}^0(\vec{r}) - \frac{e}{V} \sum_{\vec{k}'} \frac{\phi(\vec{k}-\vec{k}')}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \psi_{\vec{k}'}^0(\vec{r})$$

Density $\rho(\vec{r}) = -e \sum_{\vec{k}} |\psi_{\vec{k}}(\vec{r})|^2 f_{\vec{k}} \quad f_{\vec{k}} \equiv f(\epsilon_{\vec{k}})$

$$= -e \left[\underbrace{\sum_{\vec{k}} f_{\vec{k}} |\psi_{\vec{k}}^0|^2}_{\rho_0(\vec{r})} - \frac{e}{V} \sum_{\vec{k}} \left(f_{\vec{k}} \psi_{\vec{k}}^{0*} \sum_{\vec{k}'} \frac{\psi_{\vec{k}'}^0}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \phi(\vec{k}-\vec{k}') + \text{c.c.} \right) \right]$$

ρ_{int}

$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - e\phi(\vec{r})$$

Want to calculate $\rho(\vec{r})$ in leading order P.T.

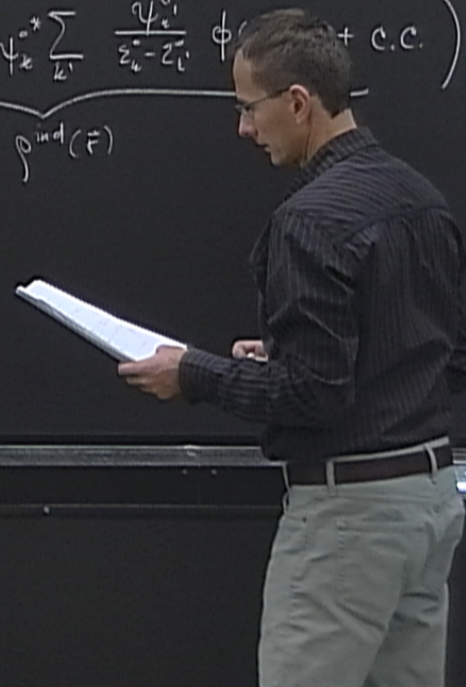
$$\langle \psi_{\vec{k}}^0 | -e\phi(\vec{r}) | \psi_{\vec{k}}^0 \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{k}\cdot\vec{r}} \phi(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = -\frac{e}{V} \phi(\vec{k}-\vec{k}')$$

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}^0(\vec{r}) - \frac{e}{V} \sum_{\vec{k}'} \frac{\phi(\vec{k}-\vec{k}')}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \psi_{\vec{k}'}^0(\vec{r})$$

Density $\rho(\vec{r}) = -e \sum_{\vec{k}} |\psi_{\vec{k}}(\vec{r})|^2 f_{\vec{k}} \quad f_{\vec{k}} \equiv f(\epsilon_{\vec{k}})$

$$= -e \left[\underbrace{\sum_{\vec{k}} f_{\vec{k}} |\psi_{\vec{k}}^0|^2}_{\rho_0(\vec{r})} - \frac{e}{V} \sum_{\vec{k}} \left(f_{\vec{k}} \psi_{\vec{k}}^{0*} \sum_{\vec{k}'} \frac{\psi_{\vec{k}'}^0}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \phi(\vec{r}) + \text{c.c.} \right) \right]$$

$$\rho_{\text{ind}}(\vec{r}) = -\frac{e^2}{V} \sum_{\vec{k}, \vec{k}'} \left[f_{\vec{k}} \frac{e^{i\vec{r}\cdot(\vec{k}-\vec{k}')}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \phi(\vec{r}-\vec{k}') + \text{c.c.} \right]$$



$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - e\phi(\vec{r}) \underbrace{H_1}$$

Want to calculate $\rho(\vec{r})$ in leading order P.T.

$$\langle \psi_{\vec{k}}^0 | -e\phi(\vec{r}) | \psi_{\vec{k}}^0 \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{k}\cdot\vec{r}} \phi(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = -\frac{e}{V} \phi(\vec{k}-\vec{k}')$$

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}^0(\vec{r}) - \frac{e}{V} \sum_{\vec{k}'} \frac{\phi(\vec{k}-\vec{k}')}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \psi_{\vec{k}'}^0(\vec{r})$$

Density $\rho(\vec{r}) = -e \sum_{\vec{k}} |\psi_{\vec{k}}(\vec{r})|^2 f_{\vec{k}} \quad f_{\vec{k}} \equiv f(\epsilon_{\vec{k}})$

$$= -e \left[\underbrace{\sum_{\vec{k}} f_{\vec{k}} |\psi_{\vec{k}}^0|^2}_{\rho_0(\vec{r})} - \frac{e}{V} \sum_{\vec{k}} \left(f_{\vec{k}} \psi_{\vec{k}}^{0*} \sum_{\vec{k}'} \frac{\psi_{\vec{k}'}^0}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \phi(\vec{k}-\vec{k}') + \text{c.c.} \right) \right]$$

$$\rho_{\text{ind}}(\vec{r}) = -\frac{e^2}{V} \sum_{\vec{k}, \vec{k}'} \left[f_{\vec{k}} \frac{e^{i\vec{r}\cdot(\vec{k}-\vec{k}')}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \phi(\vec{k}-\vec{k}') + \text{c.c.} \right] \Rightarrow \rho_{\text{ind}}(\vec{r}) = -\frac{e^2}{V} \sum_{\vec{q}} e^{i\vec{r}\cdot\vec{q}} \left(\sum_{\vec{k}} \frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}-\vec{q}}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}-\vec{q}}} \right)$$

Subst. $\vec{k}, \vec{k}' \rightarrow \vec{k} + \frac{1}{2}\vec{q}, \vec{k} - \frac{1}{2}\vec{q}$

$$H = \underbrace{-\frac{\hbar^2 \nabla^2}{2m}}_{H_0} - \underbrace{e\phi(\vec{r})}_{H'}$$

Want to calculate $\rho(\vec{r})$ in leading order P.T.

$$\langle \psi_{k'}^0 | -e\phi(\vec{r}) | \psi_k^0 \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{k}'\cdot\vec{r}} \phi(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = -\frac{e}{V} \phi(\vec{k}-\vec{k}')$$

$$\psi_k(\vec{r}) = \psi_k^0(\vec{r}) - \frac{e}{V} \sum_{k'} \frac{\phi(\vec{k}-\vec{k}')}{\epsilon_k - \epsilon_{k'}} \psi_{k'}^0(\vec{r})$$

Density $\rho(\vec{r}) = -e \sum_k |\psi_k(\vec{r})|^2 f_k \quad f_k \equiv f(\epsilon_k)$

$$= -e \left[\underbrace{\sum_k f_k |\psi_k^0|^2}_{\rho_0(\vec{r})} - \frac{e}{V} \sum_k \left(f_k \psi_k^0 \sum_{k'} \frac{\psi_{k'}^0}{\epsilon_k - \epsilon_{k'}} \phi(\vec{k}-\vec{k}') + \text{c.c.} \right) \right]$$

$$\rho_{\text{ind}}^{\text{ind}}(\vec{r}) = -\frac{e^2}{V} \sum_{k, k'} \left[f_k \frac{e^{i\vec{r}\cdot(\vec{k}-\vec{k}')}}{\epsilon_k - \epsilon_{k'}} \phi(\vec{k}-\vec{k}') + \text{c.c.} \right] \Rightarrow \rho_{\text{ind}}^{\text{ind}}(\vec{r}) = -\frac{e^2}{V} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} \left(\sum_k \frac{f_k}{\epsilon_k - \epsilon_{k+\vec{q}}} \right) \chi(\vec{q})$$

Subst. $\vec{k}, \vec{k}' \rightarrow \vec{k} + \frac{1}{2}\vec{q}, \vec{k} - \frac{1}{2}\vec{q}$

$$\langle \vec{e}_i | -\phi(\vec{r}) | \psi_{\vec{e}_i} \rangle = -\frac{e}{V} \int d^3r e^{-i\vec{e}_i \cdot \vec{r}} \phi(\vec{r}) e^{i\vec{e}_i \cdot \vec{r}} = -\frac{e}{V} \phi(\vec{e}_i - \vec{e}_i')$$

$$\psi_{\vec{e}_i}(\vec{r}) = \psi_{\vec{e}_i}^0(\vec{r}) - \frac{e}{V} \sum_{\vec{e}_i'} \frac{\phi(\vec{e}_i - \vec{e}_i')}{\epsilon_{\vec{e}_i} - \epsilon_{\vec{e}_i'}} \psi_{\vec{e}_i'}^0(\vec{r})$$

$$f_{\vec{e}_i} \equiv f(\epsilon_{\vec{e}_i})$$

$$\underbrace{\sum_{\vec{e}_i} \left(f_{\vec{e}_i} \psi_{\vec{e}_i}^* \sum_{\vec{e}_i'} \frac{\psi_{\vec{e}_i'}^0}{\epsilon_{\vec{e}_i} - \epsilon_{\vec{e}_i'}} \phi(\vec{e}_i - \vec{e}_i') + \text{c.c.} \right)}_{\rho^{\text{ind}}(\vec{r})}$$

$$\left. \text{c.} \right\} \Rightarrow \rho^{\text{ind}}(\vec{r}) = -\frac{e}{V} \sum_{\vec{q}} e^{i\vec{r} \cdot \vec{q}} \underbrace{\left(\sum_{\vec{k}} \frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}-\vec{q}}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}-\vec{q}}} \right)}_{\chi(\vec{q})} \phi(\vec{q})$$

$$\boxed{\text{Lindhard}} \quad \chi(\vec{q}) = -\frac{e^2}{V} \sum_{\vec{k}} \frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}-\vec{q}}}{\hbar^2 \vec{k} \cdot \vec{q} / m}$$