

I.D. #
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Subject Physics 560
Course Section
Instructor
Date

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Lecture 8:

1.) Review

Last class, we showed that for the 1D TBM, the DOS diverges at $\epsilon = \pm 2t$. What is special about these energies. $\Sigma(k) = -2t \cos k = \pm 2t$ at $0, \pi$.
 At $k = 0, \pi$ $\partial \Sigma / \partial k = 2t \sin k = 0 \Rightarrow$ The band is flat at these points. Recall $D(\epsilon) \sim 1/|d\epsilon/dk| \rightarrow \infty$.

2.) Geometric Phases:

Wannier states are defined as

$$W_n(R, r) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k} \cdot R} e^{i\phi(\vec{k})} \psi_{n\vec{k}}(\vec{r})$$

Is $\phi(k)$ determinable? arbitrary phase

$$i\hbar |\dot{\psi}\rangle = H_{\lambda(t)} |\psi(t)\rangle$$

where H depends on a series of parameters $\lambda \in (\lambda_1(t), \lambda_2(t), \dots, \lambda_n(t))$ slowly varying w.r.t. t .

$$\text{Let } |\psi(t)\rangle = e^{i\hbar \int_0^t dt' E_{\lambda(t')} } e^{i\phi(t)} |\psi_{\lambda}(t)\rangle$$

$$\Rightarrow i\hbar |\dot{\psi}\rangle = \left(\epsilon_{\lambda}(t) - \hbar \frac{\partial \phi}{\partial t} + i\hbar \frac{\partial}{\partial t} \right) |\psi_{\lambda}(t)\rangle = \epsilon_{\lambda} |\psi_{\lambda}(t)\rangle.$$

cancel these terms.

$$\Rightarrow \frac{\partial \phi}{\partial t} = i\lambda \cdot \langle \psi_{\lambda} | \frac{\partial}{\partial \lambda} | \psi_{\lambda} \rangle.$$

$$\Rightarrow \phi(t) - \phi(0) = \int_{\lambda(0)}^{\lambda(t)} d\vec{\lambda} \cdot \vec{R}_{\lambda}$$

$$R_{\lambda} \equiv i \langle \psi_{\lambda} | \frac{\partial}{\partial \lambda} | \psi_{\lambda} \rangle.$$

if $\lambda = k$ then $i \frac{\partial}{\partial k} \Rightarrow X_{\alpha}$ the position.

R_{λ} is the Berry phase. If ψ_{λ} is periodic \Rightarrow

$$\Gamma = \oint d\lambda \cdot \vec{R}_{\lambda}.$$

3.) Interactions:

In general $H = P^2/2m + V_{el} + V_{ions} + V_{int}$.

We want to look at V_{el} .

a.) $V_{el}(r) = e^2 \int dr' \frac{n(r')}{|r-r'|}$ Hartree approx.

b.) Hartree-Fock: Evaluate energy with a single state determinant. Consider just 2 e's. $|\psi(r)\rangle = \frac{1}{\sqrt{2}} (\phi_1(r_1)\phi_2(r_2) - \phi_2(r_1)\phi_1(r_2))$

$$|\psi(r)\rangle = \text{det} \begin{vmatrix} \phi_1(r_1) & \phi_2(r_1) \\ \phi_1(r_2) & \phi_2(r_2) \end{vmatrix}$$

$$|\psi\rangle = \frac{1}{\sqrt{n!}} \sum_P \phi_1(r_1) \dots \phi_n(r_n) (-1)^P$$

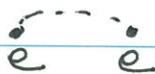
$P \triangleq$ Permutations.

for a general 2-body interaction $g(\vec{r}_1, \vec{r}_2)$.

$$\langle g \rangle = \int dr_1 dr_2 \psi^*(r_1, r_2) g(r_1, r_2) \psi(r_1, r_2)$$

Expanding out, we see there are 2 kinds of terms.

$$U_{\phi_1 \phi_2} = \int dr_1 dr_2 \overbrace{|\phi_1(r_1)|^2}^{n(r_1)} \frac{e^2}{|r_1 - r_2|} \overbrace{|\phi_2(r_2)|^2}^{n(r_2)}$$

This is the direct interaction. 

Exchange interaction:

$$J_{\phi_1 \phi_2} = - \int \phi_1^*(r_2) \phi_2^*(r_1) \frac{e^2}{|r_1 - r_2|} \phi_1(r_1) \phi_2(r_2)$$

This term cannot be written as a density-density int. Notice the - sign. This comes about from interchanging particles 1, 2.

If you interchange two electrons, their spins must be equal. $\langle \sigma_1 | \sigma_2 \rangle = \delta_{\sigma_1, \sigma_2}$

$$J_{\lambda, \nu} = \int dr_1 dr_2 \phi_\lambda^*(r_2) \phi_\nu^*(r_1) \left| \frac{e^2}{|r_1 - r_2|} \right| \phi_\lambda(r_1) \phi_\nu(r_2)$$

$$\Rightarrow E = \langle H \rangle = \langle K.E. \rangle + \frac{1}{2} \sum_{\lambda, \nu} U_{\lambda, \nu} - J_{\lambda, \nu}$$

The 1-body part is: $H_1 = -\frac{\hbar^2}{2m} \sum_i \nabla_{r_i}^2 + \hat{V}_{ion}(r)$

$$\langle H_1 \rangle = \sum_\lambda \int dr \frac{-\hbar^2}{2m} \phi_\lambda^*(r) \nabla_r^2 \phi_\lambda(r) + \phi_\lambda^*(r) V_{ion}(r) \phi_\lambda(r).$$

step 1: $\Rightarrow E_{HF} = \langle H_1 \rangle + \frac{1}{2} \sum_{\lambda, \nu} U_{\lambda\nu} - J_{\lambda\nu}.$

Step 2: $\frac{\delta E_{HF}}{\delta \phi_\nu^*} = \epsilon_\nu \frac{\delta}{\delta \phi_\nu^*} \int dr' |\phi_\nu(r')|^2.$

Lagrange multiplier. Now plug in E_{HF} and do the variation.

$$\frac{1}{2} \frac{\delta \sum_{\lambda, \nu} U_{\lambda, \nu}}{\delta \phi_\nu^*} = \sum_\lambda \int n_\lambda \phi_\lambda \frac{e^2}{|r_1 - r_2|} dr_1 dr_2 \phi_\nu(r_2)$$

$$\frac{1}{2} \frac{\delta \sum_{\lambda, \nu} J_{\lambda, \nu}}{\delta \phi_\nu^*} = \sum_\lambda \phi_\lambda^*(r') \phi_\nu(r') \frac{e^2}{|r - r'|} \phi_\lambda(r)$$

Varying $\langle H_1 \rangle$, we find that

$$\left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_{ion}(r) + \sum_\lambda \int dr' \frac{e^2}{|r - r'|} n_\lambda \phi_\lambda(r') \right] \phi_\nu(r) - \sum_\lambda \int dr' \phi_\lambda^*(r') \phi_\nu(r') \frac{e^2}{|r - r'|} \phi_\lambda(r) = \epsilon_\nu \phi_\nu(r)$$

Now multiply by $\phi_\nu^*(r)$ and integrate over r .

$$\Rightarrow \epsilon_\nu = \langle \nu | \hat{H}_1 | \nu \rangle + \sum_\lambda U_{\nu\lambda} - J_{\nu\lambda}.$$

$$\Rightarrow E_{HF} = \sum_v \epsilon_v - \frac{1}{2} \sum_{\lambda, \nu} U_{\lambda, \nu} - J_{\lambda, \nu}$$

What happens when we add an extra particle?

$$\begin{aligned} \delta E_{HF} &= E_{HF}^{N+1} - E_{HF}^N = \langle N+1 | \hat{H}_1 | N \rangle + \sum_{\lambda} U_{N+1, \lambda} - J_{N+1, \lambda} \\ &= E_{N+1} \end{aligned}$$

This is known as Koopmans' theorem. The HF energies are the energies either to add or subtract a particle.

4.) Jellium Model:

consider the int. e⁻s with a neutralizing background.

$$V_{ion}(r) = -Z \sum_i \frac{e^2}{|r-R_i^0|} = -e^2 n_e \int \frac{dR}{|r-R|}$$

The H.F. equations are

$$\begin{aligned} \epsilon_v \phi_v(r) &= \left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_{ion}(r) + e^2 \sum_{\lambda} \int d r' n_{\lambda}(r') \frac{1}{|r-r'|} \right] \phi_v(r) \\ &\quad - e^2 \sum_{\lambda} \int d r' \frac{\phi_v(r') \phi_{\lambda}^*(r') \phi_{\lambda}(r)}{|r-r'|} \end{aligned}$$

What are the eigenstates? Let's see if p.w.s work

$$\phi_v(r) = \frac{e^{i p \cdot r / \hbar}}{\sqrt{V}}$$

$$\sum_{p'} \int d^3r' \phi_p(r) \phi_{p'}^*(r') \phi_{p'}(r) \frac{1}{|r-r'|} ; \text{Note } \sum_p \rightarrow V \int \frac{d^3p}{(2\pi\hbar)^3}$$

$$= V \int \frac{d^3p'}{(2\pi\hbar)^3} \int d^3r' \frac{e^{i\vec{p}\cdot r/\hbar}}{V} \frac{e^{-i\vec{p}'\cdot r'/\hbar}}{V} \frac{e^{i\vec{p}'\cdot r/\hbar}}{V} \frac{1}{|r-r'|} e^{i\vec{p}'\cdot r'/\hbar} e^{-i\vec{p}\cdot r/\hbar}$$

Let $x = r' - r$.

$$= \int \frac{d^3p'}{(2\pi\hbar)^3} e^{i(\vec{p}-\vec{p}')\cdot x/\hbar} \frac{e^{i\vec{p}\cdot r/\hbar}}{V}$$

$$= \int \frac{d^3p'}{(2\pi\hbar)^3} dx e^{i(\vec{p}-\vec{p}')\cdot x/\hbar} \phi_p(r)$$

⇒ Plane-waves work. What are the energies?

Note: $\sum_{\vec{k}} n_{\vec{k}} |\phi_{\vec{k}}(r)|^2 \equiv n_e$ electron density.

$$E_p \phi_p(r) = \left[\frac{p^2}{2m} + V_{ion}(r) + e^2 n_e \int d^3r' \frac{1}{|r-r'|} \right] \phi_p(r)$$

$$- e^2 \int \frac{d^3p'}{(2\pi\hbar)^3} dx \frac{e^{i(\vec{p}-\vec{p}')\cdot x/\hbar}}{|\vec{x}|} \phi_p(r)$$

$$\rightarrow -e^2 n_e \int d^3r' \frac{1}{|r-r'|} + e^2 n_e \int \frac{d^3r'}{|r-r'|} = 0$$

⇒ V_{ion} cancels out the direct term.

$$\Rightarrow E_p = \frac{p^2}{2m} - e^2 \int \frac{d^3p'}{(2\pi\hbar)^3} dx \frac{e^{i(\vec{p}-\vec{p}')\cdot x/\hbar}}{|\vec{x}|}$$

$$= \frac{p^2}{2m} + E_{exch}(p)$$

$$\begin{aligned} \Rightarrow \epsilon_{\text{exch}}(P) &= -e^2 \int \frac{d^3 p'}{(2\pi\hbar)^3} dx \frac{e^{i(P-p') \cdot X/\hbar}}{|X|} \\ &= -e^2 \int \frac{d^3 p'}{(2\pi\hbar)^3} \frac{4\pi\hbar^2}{|P-p'|^2} \\ &= \frac{-e^2}{(2\pi\hbar)^3} 4\pi\hbar^2 \int_0^{P_F} \int_{-1}^1 \frac{p'^2 dp' d(\cos\theta)}{P^2 + p'^2 - 2Pp'\cos\theta} \\ &= \frac{e^2}{\pi\hbar} \int_0^{P_F} \frac{dp'}{2Pp'} p'^2 \ln \left| \frac{P^2 + p'^2 - 2Pp'x}{-1} \right| \\ &= \frac{e^2}{\pi\hbar} \int_0^{P_F} \frac{p'^2 dp'}{2Pp'} \frac{\ln(P^2 + p'^2 - 2Pp')}{(P^2 + p'^2 + 2Pp')} \\ &= \frac{e^2}{\pi\hbar P} \int_0^{P_F} p' [\ln|P-p'| - \ln|P+p'|] dp' \end{aligned}$$

use $\int x \ln(x+a) = \frac{(x^2 - a^2)}{2} \ln(x+a) - \frac{1}{4}(x-a)^2$

$$\Rightarrow \epsilon_{\text{exch}}(P) = \frac{-e^2 P_F}{\pi\hbar} \left(1 + \frac{(P_F^2 - P^2)}{2PP_F} \ln \left| \frac{P+P_F}{P-P_F} \right| \right)$$

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

$$\begin{aligned} \Rightarrow \epsilon_{\text{exch}}(P) &= \frac{-e^2 P_F}{\pi\hbar} \left[1 + \frac{P_F^2 (1 - (P/P_F)^2)}{2PP_F} \ln \left| \frac{1+x}{1-x} \right| \right] \\ &= \frac{-e^2 P_F \cdot 2}{\pi\hbar} \left[\frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right| \right] \\ &= \frac{-2e^2 P_F}{\pi\hbar} F(x) \end{aligned}$$

$$\Rightarrow \frac{E(P)}{E_F} = X^2 - \left(\frac{2e^2 P_F}{\pi \hbar} \right) \frac{2m}{P_F^2} F(X).$$

$$= X^2 - \frac{4e^2 m}{\hbar^2} \frac{\hbar}{P_F} F(X)$$

but $v_F = 1.92 \hbar / P_F$
and $a_0 = \hbar^2 / m e^2$.

$$= X^2 - \frac{4}{\pi a_0} \frac{v_F}{1.92} F(X)$$

$$= X^2 - 0.663 r_D F(X).$$

$$F(x=0) = \frac{1}{2} + \frac{(1-x^2)}{4} \Big|_{x=0} \quad \text{Use L'Hospital's rule}$$

$$F(x=0) = \frac{1}{2} + \frac{(1-x^2)}{4} \left[\frac{1}{1+x} + \frac{1}{1-x} \right]_{x=0} = 1$$

$$F(x=1) = \frac{1}{2}.$$

Estimate the bandwidth: $\Delta = E(1) - E(0)$.

$$\Delta = 2E_F [1 - 0.331 r_D + 0.663 r_D] = (1 + 0.331 r_D) E_F > E_F$$

