

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

Receiving or giving aid in a final examination is a cause for dismissal from the University.

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## Lecture 7:

### 1.) TBM revisited

a.)

I gave you a handout on Q.M. I will now re-derive the TBM using an approach that utilizes bra-ket notation more explicitly. Let  $|n\rangle$  represent a state vector located at site  $n$ . All of these states are orthonormal:  $\langle n|m\rangle = \delta_{n,m}$ . Our Hamiltonian is

$$H = -t \sum_n |n\rangle \langle n+1| + |n+1\rangle \langle n| + E_0 |n\rangle \langle n|$$

In general the wave function is a linear superposition

$$|\psi\rangle = \sum_n c_n |n\rangle.$$

Since the system is periodic, we suspect the  $c_n$ 's are  $e^{ikna}$ . We will show this explicitly. We need to compute

$$H|\psi\rangle = E|\psi\rangle.$$

$$\langle n | H | \psi \rangle = E \langle n | \psi \rangle$$

$$\Rightarrow \langle n | \psi \rangle = \langle n | \sum_m C_m | m \rangle = \sum_m C_m \underbrace{\langle n | m \rangle}_{\delta_{nm}} = C_n$$

$$\begin{aligned} \Rightarrow EC_n &= \langle n | (-t \sum_m | m \rangle \langle m+1 | + | m+1 \rangle \langle m | + E_0 | m \rangle \langle m |) \sum_l C_l | l \rangle \\ &= -t \sum_{m,l} \delta_{nm} \delta_{m+1,l} C_l - t \sum_{m,l} C_l \delta_{n,m+1} \delta_{m,l} + E_0 \sum_{m,l} \delta_{nm} \delta_{ml} C_l \end{aligned}$$

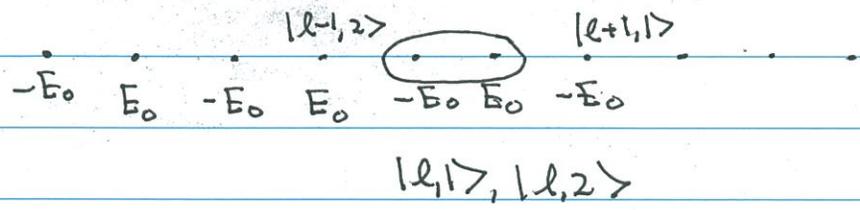
$$\Rightarrow EC_n = -t C_{n+1} - t C_{n-1} + E_0 C_n$$

This is the key eq. in the TB M. It says sites  $n \pm 1, n$  are all connected. So what's the solution? The only solution is  $C_n = e^{ikna}$ .

$$\Rightarrow E e^{ikna} = -t e^{ik(n-1)a} - t e^{ik(n+1)a} + E_0 e^{ikna}$$

$$\Rightarrow E = -2t \cos ka + E_0$$

b) 2-sites/cell.



In each cell, we have two sites and hence two states.

$$\begin{aligned} H &= E_0 \left( \sum_x |l,1\rangle \langle l,2| - |l,2\rangle \langle l,2| \right) \\ &- t \sum_x (|l,1\rangle \langle l,2| + |l,1\rangle \langle l-1,2|) - t \sum_x (|l,2\rangle \langle l,1| + |l,2\rangle \langle l+1,1|) \end{aligned}$$

Fourier transform:  $|l, n\rangle = \sum_q e^{-iqla}$

here  $a \rightarrow 2a$  in the original problem. Making the substitution,

$$H = E_0 \sum_q |q, 1\rangle \langle q, 1| - |q, 2\rangle \langle q, 2|$$

$$- t \sum_q (1 + e^{-iq}) |q, 1\rangle \langle q, 2| - t \sum_q (1 + e^{iq}) |q, 2\rangle \langle q, 1|$$

Now here's the new step

$$|\psi\rangle = \sum_q C_1^q |q, 1\rangle + C_2^q |q, 2\rangle.$$

$$\langle q, 1 | \psi \rangle = C_1^q.$$

$$\Rightarrow E C_1^q = E_0 C_1^q - t(1 + e^{iq}) C_2^q$$

$$E C_2^q = -E_0 C_2^q - t(1 + e^{-iq}) C_1^q$$

$$\begin{pmatrix} E_0 - E & -t(1 + e^{iq}) \\ -t(1 + e^{-iq}) & -E_0 - E \end{pmatrix} \begin{pmatrix} C_1^q \\ C_2^q \end{pmatrix} = 0.$$

$$(E_0 - E)(E_0 + E) + t^2 |1 + e^{iq}|^2 = 0$$

$$\Rightarrow E = \pm \sqrt{E_0^2 + 4t^2 \cos^2 qa}$$

← band halved.

This is the same answer as before

## 2.) Density of states

$$D(\epsilon) = 2 \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \delta(\epsilon - \epsilon(k))$$

We now evaluate this directly with a little help from Dirac.

$$\lim_{\Gamma \rightarrow 0} \frac{\Gamma}{\pi} \frac{1}{\epsilon - \epsilon(k) - i\Gamma} = \delta(\epsilon - \epsilon(k))$$

$\lim_{\Gamma \rightarrow 0} \frac{\Gamma}{(\epsilon - \epsilon(k))^2 + \Gamma^2}$  is the standard representation of the  $\delta$ -fcn.

We use  $\epsilon(k) = -2t \cos ka$ .

$$\Rightarrow D(\epsilon) = \frac{2}{2\pi^2} \int_{-\pi/a}^{\pi/a} \lim_{\Gamma \rightarrow 0} \frac{\Gamma}{\epsilon + 2t \cos k - i\Gamma} dk$$

$$= \frac{1}{\pi^2} \lim_{\Gamma \rightarrow 0} \int_{-\pi/a}^{\pi/a} \frac{\Gamma}{\epsilon + 2t \cos k - i\Gamma} dk$$

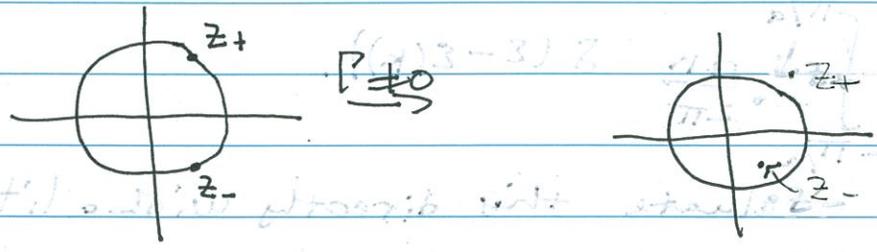
as before  $z = e^{ika}$ ;  $dz = ia z dk$

$\Rightarrow$  integration over unit circle  $\Rightarrow \boxed{dk = \frac{dz}{ia z}}$

$$\Rightarrow D(\epsilon) = \frac{1}{\pi^2} \lim_{\Gamma \rightarrow 0} \int \frac{dz}{z^2 + 1 + z \frac{\epsilon - i\Gamma}{t}} = \frac{1}{\pi^2} \lim_{\Gamma \rightarrow 0} \int \frac{dz}{(z - z_+)(z - z_-)}$$

Poles (singularities) at  $z_{\pm} = -\frac{\epsilon - i\Gamma}{2t} \pm \sqrt{\left(\frac{\epsilon - i\Gamma}{2t}\right)^2 - 4}$

clearly  $|z_{\pm}|^2 \Big|_{P=0} = 1$



only  $z_+$  lies within the unit circle. Recall Cauchy's theorem

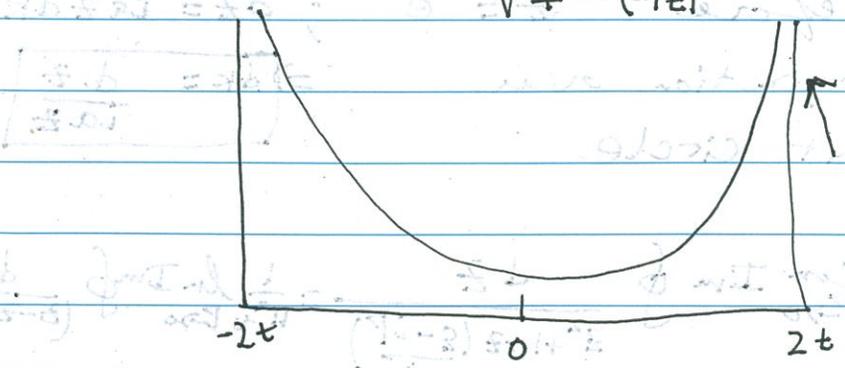
$$2\pi i f(z_0) = \oint \frac{f(z)}{z-z_0}$$

In our problem  $f(z) = \frac{1}{z-z_+}$

$$\Rightarrow D(\epsilon) = \frac{1}{\pi^2 \alpha t} \lim_{\Gamma \rightarrow 0} \frac{\text{Im}}{2\pi i} \frac{1}{z_- - z_+}$$

$$= -\frac{1}{\pi^2 \alpha t} \frac{\text{Im} 1}{\sqrt{(\frac{\epsilon}{t})^2 - 4}} \leftarrow \text{Imaginary part only if } (\epsilon/t) \leq 2$$

$$= \frac{1}{\pi^2 \alpha t} \frac{1}{\sqrt{4 - (\epsilon/t)^2}} \quad |\epsilon/t| \leq 2$$



V.H.S.  
density of states diverges at band edges.

### 3.) Geometric Phases

When we wrote down the Wannier functions, we did not include the most general form:

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

↑ phase

$\phi(\vec{k})$  is an arbitrary real function.

There are a number of geometric phases.

$$\begin{aligned} \text{S.E.} \quad i\hbar |\dot{\psi}\rangle &= H|\psi\rangle \\ &= E|\psi\rangle \\ \Rightarrow |\psi\rangle &= \underbrace{e^{-iE/\hbar t}}_{\text{Phase.}} |\psi\rangle \end{aligned}$$

What if  $H$  depends on a series of parameters  $\lambda \in (\lambda_1(t), \lambda_2(t), \dots, \lambda_n(t))$ . Let's assume they vary slowly with time. Guess a solution of the form

$$\begin{aligned} i\hbar |\dot{\psi}\rangle &= H_{\lambda(t)} |\psi(t)\rangle \\ |\psi(t)\rangle &= e^{-\frac{i}{\hbar} \int_0^t \epsilon_{\lambda(t')} dt'} e^{i\phi(t)} |\psi_{\lambda}(t)\rangle \end{aligned}$$

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

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

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

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

$R_\lambda$  is the Berry connection (Phase). If  $\psi_\lambda$  is a periodic fn. of  $\vec{\lambda}$ , then

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

4.) Interactions:

$$V_{ee} = \frac{e^2}{|r_1 - r_2|}$$

$$H = \frac{p^2}{2m} + V_{ee} + V_{ext}$$

Various levels of approximation.

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

b.) Hartree-Fock:

We evaluate the energy with a single Slater determinant. Consider 2-e's

$$\psi(r_1, r_2) = \frac{1}{\sqrt{2}} [\phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1)]$$

$$= \text{Det} \begin{vmatrix} \phi_1(r_1) & \phi_2(r_1) \\ \phi_1(r_2) & \phi_2(r_2) \end{vmatrix}$$

$$\Psi = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \phi_1(r_1) \dots \phi_N(r_N)$$

P  
permutations

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & & & \phi_N(r_1) \\ & \ddots & & \vdots \\ & & \ddots & \vdots \\ \phi_1(r_N) & & & \phi_N(r_N) \end{vmatrix}$$

$\phi_x = \chi_x \chi_x \rightarrow$  spin state.

Consider a 2-body interaction  $g(r_1, r_2)$

Let's just use a 2-particle w.f. for simplicity,  $\Psi(r_1, r_2)$

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

There are 2 types of terms.

$$\langle g \rangle = \int dr_1 dr_2 n_{\phi_1}(r_1) g(r_1, r_2) n_{\phi_2}(r_2) = U_{\phi_1 \phi_2}$$

$$n_{\phi_i} = |\phi_i(r_i)|^2$$

This is the direct term.

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### Exchange interaction:

$$J = - \int \phi_1^*(r_2) \phi_2^*(r_1) g(r_1, r_2) \phi_1(r_1) \phi_2(r_2) dr_1 dr_2$$

$$\langle \chi_{1, \sigma_2} | \chi_{1, \sigma_1} \rangle = \delta_{\sigma_1, \sigma_2}$$

⇒ the exchange term is non-zero only if the spins are the same.

$$\Rightarrow \langle g \rangle = U_{\phi_1 \phi_2} - J_{\phi_1 \phi_2}$$

For a general N-particle problem.

$$U_{\lambda \nu} = \int dr_1 dr_2 |\phi_\lambda(r_1)|^2 \frac{e^2}{|r_1 - r_2|} |\phi_\nu(r_2)|^2$$

Classical term.

Exchange interaction.

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