

Title: PSI Lecture - Condensed Matter - Lecture 1

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Collection: PSI Lecture - Condensed Matter

Date: January 10, 2022 - 9:00 AM

URL: <https://pirsa.org/22010012>

# Condensed Matter

Today

What is CM?  
free  $e^-$  gas

What is Condensed Matter?

→ The study of the collective behavior of many particles

Subsets: - "Soft" CM: classical, eg. biophysics, polymers, ...

→ "Hard" CM: quantum CM, eg. solid state physics

This class

## Overview of Hard CM

"Realistic"  
"Practical"

Compute  
thermal  
conductivity  
for a particular  
metal

models that  
roughly capture  
qualitative behavior  
of real materials

"Abstract"

Predict new phase of  
matter using field theory

Part I:  
non-interacting  
systems

This class

quantum CM, eg. solid state physics

This course

models that  
roughly capture  
qualitative behavior  
of real materials

"Abstract"

Predict new phase of  
matter using field theory

compute  
normal  
activity  
a particular  
state

Perimeter-A

CAUTION  
DO NOT TOUCH THE SURFACE  
OR THE CONTENTS OF THE BOARD  
IT IS DANGEROUS TO YOUR  
HEALTH AND PROPERTY DAMAGE  
PLEASE REPORT ANY DAMAGE

Part I: (Weeks 1-3)  
non-interacting  
systems

This class

Part II: (4-5)  
Strong interactions

quantum CM, eg. solid state physics

"Realistic"  
"Practical"

Compute  
thermal  
conductivity  
for a particular  
metal

This course

models that  
roughly capture  
qualitative behavior  
of real materials

"Abstract"

Predict new phase of  
matter using field theory

# Condensed Matter

Free electron gas, simplest model of a metal

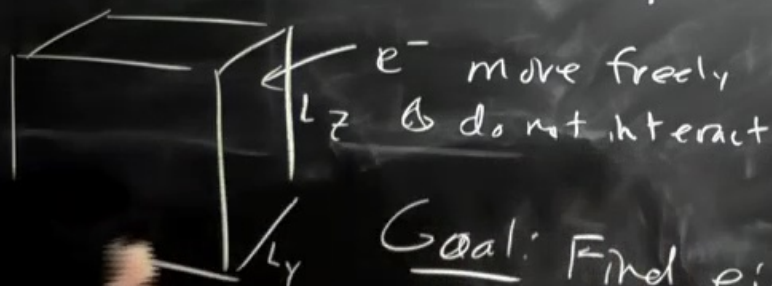


$$H = \sum_i \frac{p_i^2}{2m}$$

Goal: Find eigenstates & energies of  $H$ .  
← labels all the  $N$   $e^-$  in the box



Free electron gas, simplest model of a metal



$$H = \sum \frac{p_i^2}{2m}$$

$i$  labels all the  $N$   $e^-$  in the box

Goal: Find eigenstates & energies of  $H$ .

1: understand what many-particle  $H$  means:

$\frac{p_i^2}{2m}$  really means

$$\frac{p_i^2}{2m} \otimes I_2 \otimes I_3 \otimes \dots \otimes I_N$$

Annotations:   
 -  $\otimes I_2$  has an arrow pointing to it with the label "on  $e^- 2$ ".   
 -  $\otimes I_3$  has an arrow pointing to it with the label "on 3".   
 -  $\otimes I_N$  has an arrow pointing to it with the label "on  $N$ ".   
 - The first  $\otimes$  has an arrow pointing to it with the label "acts on  $e^- 1$ ".

Step 1: understand what  $\frac{p_i^2}{2m}$  really means: "non-interacting"

$$\frac{p_1^2}{2m} \otimes I_2 \otimes I_3 \otimes \dots \otimes I_N$$

acts on  $e^-_1$       on  $e^-_2$       on  $e^-_3$       on  $e^-_N$

Step 2: All terms commute

Hence, can simultaneously diagonalize

Def: non-interacting H.

$$H = \sum_{i=1}^N H_i$$

Thus, solve one term at a time

eg.  $\frac{p_1^2}{2m} \otimes I_2 \otimes \dots \otimes I_N$ , eigenstate will look like

$$|\phi_1\rangle \otimes |\text{anything}\rangle \otimes \dots \otimes |\text{anything}\rangle$$

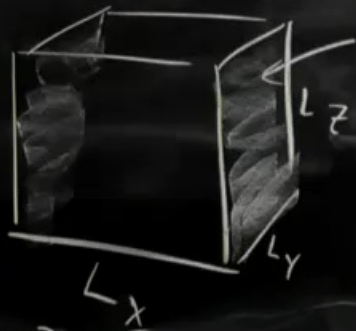
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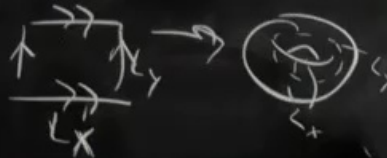
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# Condensed Matter

## Free electron gas



2D



Step 3: Find  $|\phi_{\vec{k}}\rangle$ , eig state of  $\frac{p^2}{2m}$

Solution: plane waves

$$|\phi_{\vec{k}}\rangle = A \cdot e^{i\vec{k} \cdot \vec{r}}$$

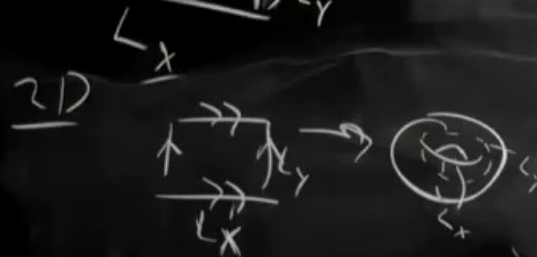
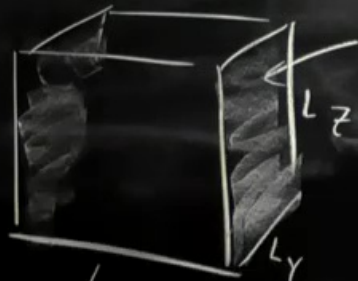
$$\vec{r} = (x, y, z)$$

$$\vec{k} = (k_x, k_y, k_z)$$

Subtlety: quantization

1st big assumption: Periodic boundary conditions

# Free electron gas



Solution: plane waves

$$|\phi_{\vec{k}}\rangle = A \cdot e^{i\vec{k} \cdot \vec{r}}$$

$$\vec{r} = (x, y, z)$$

$$\vec{k} = (k_x, k_y, k_z)$$

Subtlety: quantization

1st big assumption: Periodic boundary conditions

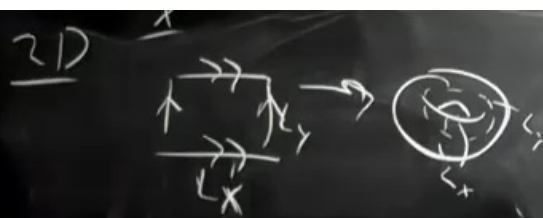
$|\phi_{\vec{k}}\rangle$  must be periodic

$$e^{i\vec{k} \cdot (\vec{r} + (L_x, 0, 0))} = e^{i\vec{k} \cdot \vec{r}}$$

Hence,  $\vec{k} = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right), n_\alpha \in \mathbb{Z}$

$$\Rightarrow e^{ik_x L_x} = 1$$

same for  $y, z$



$$e^{i\vec{n} \cdot (\vec{r}(L_y, 0, 0))} = e^{i\vec{k} \cdot \vec{r}}$$

Hence,  $\vec{k} = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right)$ ,  $n_\alpha \in \mathbb{Z}$

$A = \frac{1}{\sqrt{V}}$ ,  $V = L_x L_y L_z$

$e^{ik_x L_x}$  same for  $y, z$

Step 2: All  
Hence

Def: non-interacting

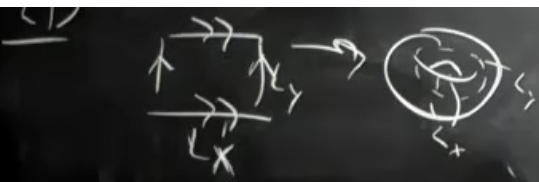
$$H = \sum_{\vec{r}} H_i$$

simultaneously diagonalize  
us, solve one term at a time

$$\frac{p_i^2}{2m} \otimes \text{Id} \otimes \dots \otimes \text{Id}, \text{ eigenstate will look like}$$

$$|\phi_i\rangle \otimes |\text{anything}\rangle \otimes \dots \otimes |\text{anything}_z\rangle$$

find this



Hence,  $\vec{k} = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right)$ ,  $n_\alpha \in \mathbb{Z}$  same for  $y, z$

$A = \frac{1}{\sqrt{V}}$ ,  $V = L_x L_y L_z$

Step 4 many-particle eigenstates

eigenstates of  $\frac{p_i^2}{2m} \otimes \mathbb{I} \dots \otimes \mathbb{I}$ ,  $|\phi_{\vec{k}_1}\rangle \otimes$

$\mathbb{I} \otimes \frac{p_i^2}{2m} \otimes \dots$

many-body eigenstates

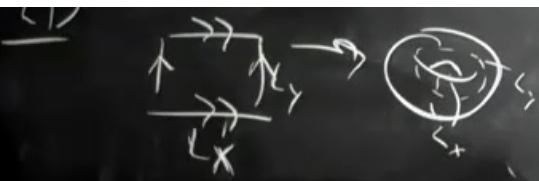
$|\phi_{\vec{k}_1}\rangle_1 \otimes |\phi_{\vec{k}_2}\rangle_2 \otimes \dots$

$E = \sum_i \frac{\hbar^2 k_i^2}{2m}$

$|\phi_{\vec{k}_n}\rangle_n$  each  $\vec{k}_i$  satisfies  $\vec{k}_i = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right)$

Step 5 continued  
Corresponding eigenenergies,  $\frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m} \vec{k} \cdot \vec{k}$   
 $= (2\pi)^2 \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$





Hence,  $\vec{k} = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right)$ ,  $n_\alpha \in \mathbb{Z}$  same for  $y, z$

$A = \frac{1}{\sqrt{V}}$ ,  $V = L_x L_y L_z$

$e^{ik \cdot r} = e^{ik_x L_x}$

Step 4 many-particle eigenstates

eigenstates of  $\frac{p_i^2}{2m} \otimes \mathbb{I} \otimes \dots \otimes \mathbb{I}$ ,  $|\phi_{\vec{k}_1}\rangle \otimes$

$\mathbb{I} \otimes \frac{p_i^2}{2m} \otimes \dots \otimes \mathbb{I}$

$\otimes |\phi_{\vec{k}_2}\rangle \otimes \dots \otimes \mathbb{I}$

many-body eigenstates

$|\phi_{\vec{k}_1}\rangle_1 \otimes |\phi_{\vec{k}_2}\rangle_2 \otimes \dots \otimes |\phi_{\vec{k}_N}\rangle_N$

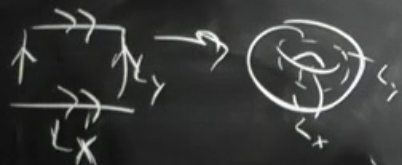
$E = \sum_i \frac{\hbar^2 k_i^2}{2m}$

$\vec{k}_1 = \vec{k}_2 = \vec{k}_3$

each  $\vec{k}_i$  satisfies  $\vec{k}_i = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right)$

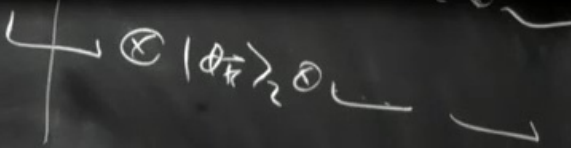
Step 5 continued  
Corresponding eigenenergies,  $\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \vec{k} \cdot \vec{k}$   
 $= \frac{\hbar^2}{2m} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$





Hence,  $\vec{H} = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right)$ ,  $n_\alpha \in \mathbb{Z}$  same for  $y, z$   
 $A = \frac{1}{\sqrt{V}}$ ,  $V = L_x L_y L_z$

$$\mathbb{Z} \otimes \frac{L^2}{2m} \otimes \dots$$



many-body eigenstates

$$|\phi_{\vec{H}_1}\rangle_1 \otimes |\phi_{\vec{H}_2}\rangle_2 \otimes \dots \otimes |\phi_{\vec{H}_N}\rangle_N$$

These are all eigenstates,  $E = \sum_i \frac{\hbar^2 \vec{H}_i^2}{2m}$   
But may not be physical

$\vec{H}_1 = \vec{H}_2 = \vec{H}_3 \rightarrow$  not anti-symmetric

$$\vec{H}_i = 2\pi \left( \frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right)$$

But eigenstates may not be physical

$$i \frac{2m}{\hbar^2}$$

$$\vec{k}_1 = \vec{k}_2 = \vec{k}_3 \rightarrow \text{not anti-symmetric}$$

$$\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right)$$

Physical subset of eigenstates:

Slater determinants:

$$|\Phi\rangle = \frac{1}{\sqrt{N}} \begin{vmatrix} |\phi_{\vec{k}_1}\rangle_1 & |\phi_{\vec{k}_1}\rangle_2 & \dots & |\phi_{\vec{k}_1}\rangle_N \\ \vdots & \vdots & \ddots & \vdots \\ |\phi_{\vec{k}_N}\rangle_1 & \dots & \dots & |\phi_{\vec{k}_N}\rangle_N \end{vmatrix}$$

← row all same 1-particle eigenstate

↑ col: acts on same particle

$$|\Phi\rangle = \frac{1}{\sqrt{N}} \sum_{\sigma \in S_N} (-1)^{\text{sign}(\sigma)} |\phi_{\vec{k}_{\sigma_1}}\rangle_1 \dots |\phi_{\vec{k}_{\sigma_N}}\rangle_N$$

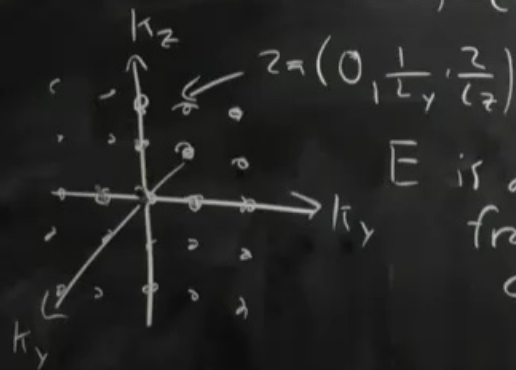
Physical many-body states

Note: Still many-body eigenstates w/ same energy

Reason: every component of sum has the same energy

col: acts on  
same particle

Now  $N$  electrons, eigenenergies  $E = \sum_i \frac{\hbar^2 k_i^2}{2m}$ ,  $\vec{k}$  form a grid in 3D



$E$  is distance  
from the  
origin,  $k^2$

With  $N$  particles, doubly fill (spin)  
the  $\frac{N}{2}$  orbitals closest to  $k=0$ .  
Doing so, there will be a maximal  
 $|\vec{k}|$  of filled states,  $k_F$ , Fermi momentum

Next time