

§ Degenerate Fermi systems.

Zn 8.05:

wave function describing identical fermions must be anti-symmetric under the exchange of any two particles.

⇒ Pauli ^{exclusion} ~~principle~~ principle: no two fermions can occupy the same state.

an important application: atomic structure

(~~as~~ briefly discussed in 8.05)

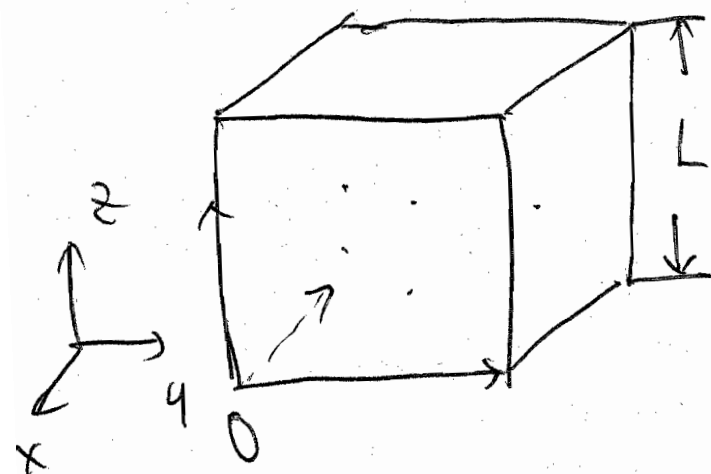
Here: we consider

= ~~the~~ some further ^{applications} examples in condensed matter and astrophysics.

We start by solving an idealized simple problem,
and then consider its physical applications.

8.1 Free electron gas:

Consider N non-interacting electrons confined inside
a 3-d box, with length L on each side.



would like to know:

- 1) Ground state wave function and energy
- 2) physical properties of the ground state.

8.1.1



8.1.1 A Digression: (8.05 review)

General Strategy for Solving problems involving ~~multiple~~ ^{multiple} ~~non-interacting~~ fermions: (say electrons, spin $\frac{1}{2}$)

1) ^{Solve} ~~write down~~ single particle schrodinger equation.

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \psi_n = E_n \psi_n$$

— E_{n+1}
↓ E_n

2) ~~Full~~ multi-particle states are

constructed by occupying electrons

↑ ↓ E_0
↑ E_1
↓ E_2

in different single-particle states (Pauli principle).

($\oplus$) including spin

3) Ground State: occupy ^{lowest} ~~minimum possible~~ available state.

Note: Strategy does not work for interacting fermions,
in which case one must solve full problem

$$\left(-\frac{\hbar^2}{2m} \nabla_1^2 - \dots - \frac{\hbar^2}{2m} \nabla_N^2 + V(x_1 \dots x_N) \right) \psi(x_1 \dots x_N) = E \psi(x_1 \dots x_N)$$

In reality: electrons always interact with each other.

Non-interacting electron is an approximation.

when mutual interaction is not important.



8.1.2

60 Single-particle wave functions

Single-particle wave functions inside the box: (3d infinite square well)

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi$$

$$\psi|_{\text{boundary}} = 0$$

$$\Rightarrow \psi(x, y, z) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin k_x x \sin k_y y \sin k_z z$$

$$k_i = \frac{n_i \pi}{L} \quad i=1, 2, 3$$

$$n_1, n_2, n_3 = \underline{1}, 2, \dots \quad (\text{positive integers})$$

$$E = \frac{\hbar^2}{2m} (k_1^2 + k_2^2 + k_3^2)$$

2/2

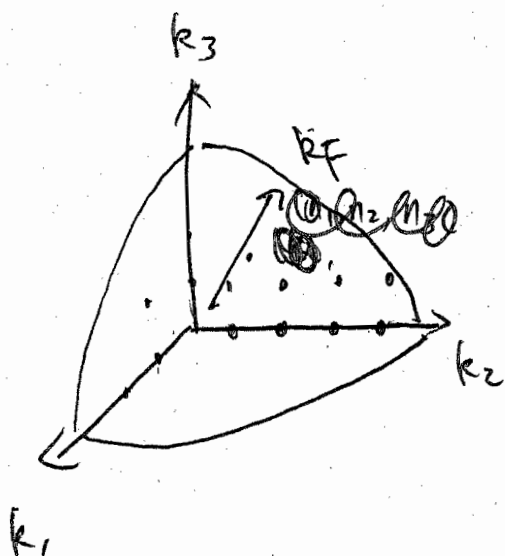
Visualization:

Single particle

State $\longleftrightarrow$

(k_1, k_2, k_3) : lattice points

in the positive octant
of $\vec{k}$ -space.



Lattice spacing: $\frac{\pi}{L}$ in all

directions

Note: 1) each state occupies a volume $(\frac{\pi}{L})^3$

2) Energy of a state is proportional

to the distance of the point from

the origin in $\vec{k}$ -space

3) Each lattice points allow 2 electrons,

($\uparrow\downarrow$) 3



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8.1.3
Q

Ground State energy:

Ground State: Choose $\frac{N}{2}$ points closest to
the origin. (spin $\frac{1}{2}$)

When N is very large (say, $10^{20})$

$\frac{N}{2}$ points can be considered as filling a

$\frac{1}{8}$ ball ~~of radius $\frac{1}{2}$~~ in k -space, (draw)

- points on the surface of the ball may or may not be filled. ~~But~~ Their number is small compare to N , if ~~the~~ ball is big enough.



• Denote the radius of the ball by k_F .

• Then

~~Recall~~

$$\frac{1}{8} \cdot \frac{4}{3} \pi k_F^3 = \frac{N}{2} \cdot \left(\frac{\pi}{L}\right)^3$$

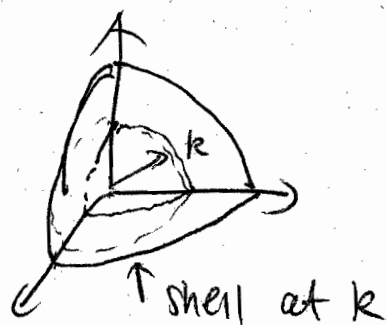
$\uparrow$ positive octant $\uparrow$ Spin- $\frac{1}{2}$ $\uparrow$ volume occupied by a single state

$$\Rightarrow k_F = \left(\frac{3\pi^2 N}{L^3} \right)^{\frac{1}{3}} = \left(3\pi^2 \frac{N}{V} \right)^{\frac{1}{3}}$$

The sphere with $|\vec{k}| = k_F$ is called Fermi surface.

$p_F = \hbar k_F$ is Fermi - momentum

$\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$: Fermi energy



Total ~~energy~~ ground state energy:

$$E_{\text{tot}} = \int_0^{k_F} \frac{4\pi k^2 dk \cdot \frac{1}{8}}{\left(\frac{\pi}{L}\right)^3} \cdot 2 \cdot \frac{\hbar^2 k^2}{2m}$$

$$= \frac{\hbar^2 V}{2\pi^2 m} \frac{k_F^5}{5}$$

$$= \frac{\hbar^2 V}{10\pi^2 m} \left(3\pi^2 \frac{N}{V} \right)^{\frac{5}{3}}$$



$\frac{4}{3}\pi$

Remarks:

$$(1) \quad \bar{e} = \frac{E_{\text{tot}}}{N} = \frac{\frac{\hbar^2 k_F^2}{2m} \frac{V k_F^3}{5\pi^2 N}}{N} = \frac{3}{5} \epsilon_F$$

$\uparrow$
 average
 energy
 per particle

$$(2) \quad E_{\text{tot}} \propto N^{\frac{2}{3}} V^{-\frac{2}{3}}$$

$V \downarrow \quad E \uparrow$, it costs energy to

compress the electron gas

$\Rightarrow$ pressure.

(3) Degenerate pressure:

$$p = - \frac{dE_{\text{tot}}}{dV} \bigg|_N$$

$$= \frac{\frac{\hbar^2 (3\pi^2)^{\frac{2}{3}}}{5m} \left(\frac{N}{V} \right)^{\frac{5}{3}}}{} \propto n^{\frac{5}{3}}$$

$\uparrow$
 density

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(4) $p \propto \frac{1}{m}$

More massive particle needs a larger # density

(that's even larger
 @ the mass density) to ~~achieve~~ achieve the same pressure

will see electron v.s. neutron.

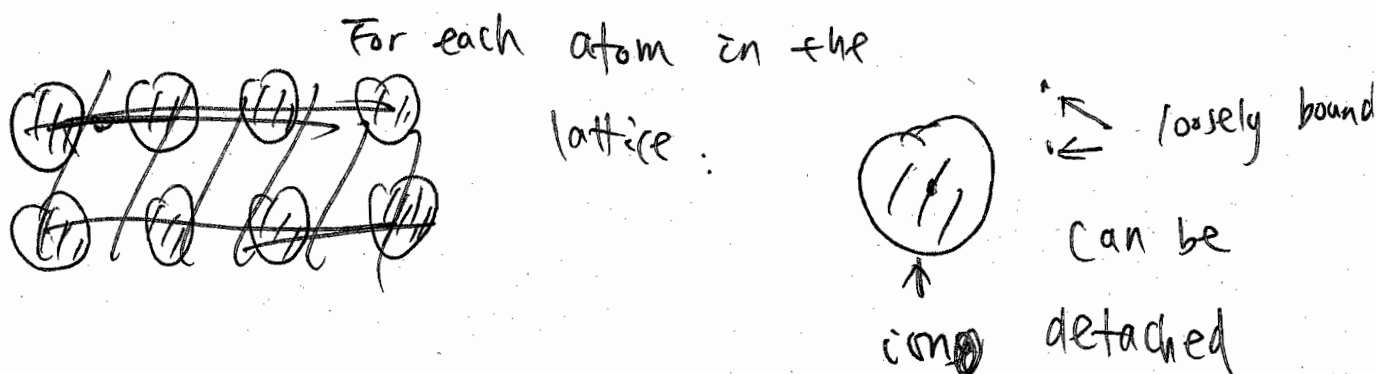
(5) when N is very large, the
 expressions for k_F , E_{tot} , P
 should ~~do~~ not depend ~~on~~ ^{sensitively} on the
shape of the box.

(Bulk properties of ^a system does not
 depend sensitively on boundary conditions
shape)

End of lecture 1

8-1-4 An application: ~~metal~~ metallic properties of Solids
(alkali metals)

Solids: atoms or molecules closed packed together
and (typically) arranged in a periodic structure
conductors, semi-conductors, insulators.



E.g. Copper: ~~1 electron~~ one such electron per atom

of atoms / cm³ ~ 8.5×10^{22}

$\Rightarrow \frac{N}{V} \sim 8.5 \times 10^{22} / \text{cm}^3$ (pret 1 #4)

lowest order approximation: ~~the~~ ~~great~~

1) ignore the potential due to ions

2) ignore Coulomb interaction between electron.

⇒ Free electron gas in a box (size of metal)

⇒ Sommerfeld electron gas theory

which ^{can be used to} explain ~~electric~~, ~~thermal conductivities~~, ~~spec~~

~~law~~ ^{of various metals} metallic properties ~~reasonably well~~, such

as electric and thermal conductivity, specific heat

Very important in early days of solid state physics.

We will ^{not} go into details here.

(In part 1, you will also check that:

1) treating electrons as non-relativistic
is justified for metals (using example of
Copper)

2) at room temperature, the material ~~can~~

be "cold", i.e. the state of the

electron gas is very close to g.s.

Ask yourself: how to check the other two assumptions.

In metals, electron degenerate pressure does not play a

major role. We will now examine an application that

the pressure plays an essential role.



8.2 White dwarf stars

8.2-1 Introduction

~~physics underlying the~~
life of ^{an} Ordinary star: (like sun)

- fusion $\longrightarrow$ heat $\longrightarrow$ thermal pressure
($4H \rightarrow {}^4\text{He} + 2e^+ + 2\nu_e$)

- pressure balances gravity $\longrightarrow$ star stable

- when H is gone, burns ${}^4\text{He} \rightarrow$ ~~C, O~~ C, O

Very heavy stars burn C, O, if not

- e.g. for sun, C, O cannot burn

What will happen?



⇒  No more heat, No more pressure

⇒ Collapse

⇒ Atoms crashed together, electrons squeezed out

Collapse stopped by degenerate pressure
of the electron gas

⇒ White dwarf: ~~Star~~ force due to gravity

is balanced by degenerate pressure of

electrons confined inside the star.

Q: Given the mass M_x of a white dwarf,
what is its radius R_x , at which the
star is stabilized?

A proper treatment is rather involved.

but somewhat crude

Use a simple, rather qualitative treatment.



8.2.2 Radius of a white dwarf

Idea: 1) Assume the star has radius R ,

find the total energy of the system:

$$E(R) = E_{\text{grav}}(R) + E_{\text{electron}}(R)$$

2) R_* : minimize $E(R)$ w.r.t. R

i.e. $\frac{dE}{dR} \Big|_{R_*} = 0$ (force balance)

$$\frac{d^2E}{dR^2} \Big|_{R_*} > 0 \quad (\text{stable balance})$$

Note: $\bar{F}_{\text{grav}} = - \frac{dE_{\text{grav}}}{dR}$ $\bar{F}_{\text{elec}} = - \frac{dE_{\text{elec}}}{dR}$ (force balance)



parameters:

N : total number of ~~the~~ nucleons (proton + neutron)

$N = \frac{M_*}{m_p}$ (m_p : proton mass, $m_p \approx m_n$)

f : # of electrons per nucleon

$N_e = f N$: total # of electrons

$= f \frac{M_*}{m_p}$

^{initial}
Assumptions: (will check later)

1) Star has uniform density ρ

$$\frac{4}{3}\pi\rho R^3 = M_*$$

2) electron gas ~~are~~ non-interacting -

3) electrons non-relativistic

check it later



Finding ~~E_{el}~~ $E_{\text{electron}}(R)$

$$E_{\text{electron}}(R) = \frac{V \hbar^2}{10 \pi^2 m_e} \left(3 \pi^2 \frac{N_e}{V} \right)^{\frac{5}{3}}$$

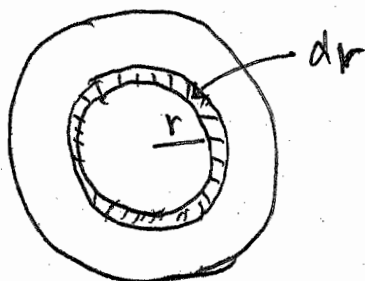
apply ~~using~~ [↑] previous ~~paper~~
formula for a
cubic box

$$= \frac{V \hbar^2}{10 \pi^2 m_e} \left(3 \pi^2 \frac{f N}{V} \right)^{\frac{5}{3}}$$

$$= \frac{k_1 N^{\frac{5}{3}}}{R^2} \quad \left(k_1 = \frac{\hbar^2 f^{\frac{5}{3}}}{m_e} \frac{3}{10} \left(\frac{9\pi}{4} \right)^{\frac{2}{3}} \right) \quad (1)$$

$$p = - \frac{\partial E}{\partial R} > 0 \quad (\text{want to increase } R)$$

Finding $E_{\text{grav}}(R)$



$$E_{\text{grav}}(R) = - \int_0^R \frac{G m(r)}{r} dm(r)$$

$$m(r) = \frac{4}{3}\pi r^3 \rho : \text{ mass enclosed by the shell}$$

$$\Delta m(r) = 4\pi r^2 dr \rho : \text{ mass of the shell}$$

$$\rho = \frac{M_x}{\frac{4}{3}\pi R^3}$$

$$\Rightarrow E_{\text{grav}} = - \int_0^R r^4 dr \cdot \frac{3GM_x^2}{R^6}$$

$$= - \frac{3GM_x^2}{5R} = - \frac{k_2 N^2}{R}$$

(2)

$$k_2 = \frac{3G m_p^2}{5}$$

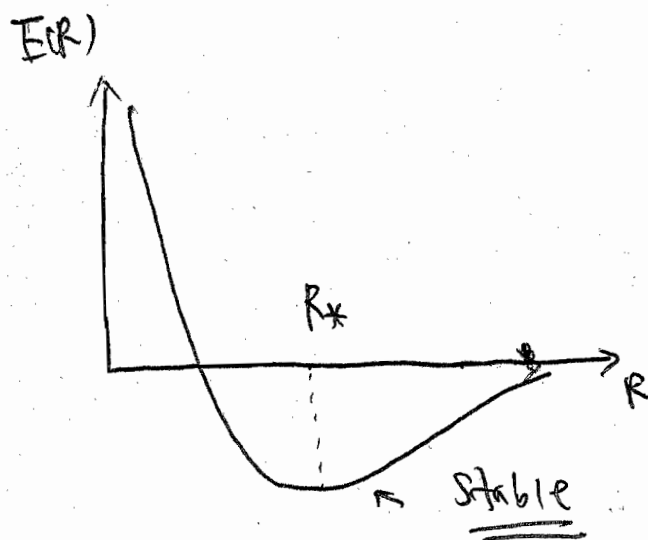
$$F_{\text{grav}} = - \frac{\partial E_{\text{grav}}}{\partial R} < 0 \quad (\text{want to decrease } R)$$



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combining ① and ②

$$E(R) = -\frac{K_2 N^2}{R} + \frac{K_1 N^{\frac{5}{3}}}{R^2}$$



$$\frac{dE(R)}{dR} = 0 \Rightarrow$$

$$R_* = \frac{2K_1}{K_2} N^{-\frac{1}{3}}$$

$$\frac{2K_1}{K_2} = \left(\frac{9\pi}{4}\right)^{\frac{2}{3}} \frac{\hbar^2 f^{\frac{5}{3}}}{G m_e m_p^2}$$

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Break

High density

4) a teaspoon of white dwarf would weigh 5 tons.

a white dwarf with ~~a~~ solar mass ~~would~~ would be
about the size of ~~the~~ the earth.

(from your pset 1)

~~5) pset 1 check interaction~~



• Remarks:

$$1) \quad N \uparrow, M_* \uparrow \Rightarrow R_* \downarrow$$

The more massive the star, the smaller radius

Ordinary star: $M_* \uparrow \Rightarrow R_* \uparrow$

GOTO (2)

$$3) \quad \text{Notice: if } M_* \rightarrow \infty, \quad R_* \rightarrow 0$$

the density of star will become infinite ?

In order to see whether we need to trust this

conclusion, check our assumptions: (non-interacty, ~~non-relativistic~~
non-relativistic

both of which will likely to break down.



4) Check non-relativistic assumption (~~check of~~ ~~non-interacting~~ ~~see pset 1~~)

Criterion: OK if $\frac{P_F}{m_e c} < 1$ or $\frac{E_F}{m_e c^2} < 1$

$$P_F = \hbar k_F \quad E_F = \frac{\hbar^2 k_F^2}{2m_e}$$

$$\frac{\hbar k_F}{m_e c} = \frac{\hbar \left(\frac{3\pi^2 N_e}{V} \right)^{\frac{1}{3}}}{m_e c} = \frac{\hbar \left(\frac{3\pi^2 f N}{\frac{4}{3}\pi R_*^3} \right)^{\frac{1}{3}}}{m_e c}$$

(after plug in = $\left(\frac{4}{9\pi} \right)^{\frac{1}{3}} \frac{N^{\frac{2}{3}} G m_p^2}{\hbar c f^{\frac{4}{3}}} < 1$

the expression
for R_*
 $\Rightarrow$

$$N < N_0 \quad \left(\frac{9\pi}{4} \right)^{\frac{1}{2}} f^2 \frac{\left(\frac{\hbar c}{G} \right)^{\frac{3}{2}}}{m_p^3} \equiv N_0$$

$$= \left(\frac{9\pi}{4} \right)^{\frac{1}{2}} f^2 \left(\frac{M_{pe}}{m_p} \right)^3 \equiv N_0$$

$\uparrow$ involve only M_{pe}
and m_p



$$M_{pe} = \sqrt{\frac{\hbar c}{G}} \quad : \quad \underline{\text{Planck mass}} \quad (\text{see Pref 1})$$

$$\Rightarrow M_* = N m_p < \underline{M_0} = N_0 m_p$$

For a typical heavy element heavier than H

$$f = \frac{1}{2} \quad (\text{e.g. He, C, O} \dots)$$

$$M_{pe} = \frac{1.2 \times 10^{19}}{\cancel{1.2 \times 10^{19}}} \frac{\text{GeV}}{c^2}$$

$$M_p = \frac{1 \text{ GeV}}{c^2} = 1.78 \times 10^{-24} \text{ g}$$

$$\Rightarrow M_0 \approx 2 \times 10^{33} \text{ g}$$

$$\approx M_\odot !$$

Thus for $M_* > M_\odot$
should use relativistic
electrons.



8.3 Relativistic electron gas and the Chandrasekhar mass

Relativistic electrons:

$$E_{\text{kin}} = \sqrt{m_e^2 c^4 + \hbar^2 k^2 c^2} \quad \text{(only difference)}$$

Ultra-relativistic: $\hbar k c \gg m_e c^2$

$$E_{\text{kin}} \approx \hbar k c + \dots$$

Let us see what happens if we assume most electrons are ultra-relativistic:

$$E_{\text{electron}} \approx 2 \int_0^{k_F} \frac{4\pi k^2 dk}{8 \left(\frac{\pi}{2}\right)^3} \cdot \hbar k c$$

$3\frac{1}{4}$



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$\Rightarrow$

$$E_{\text{elec}} = \frac{V \hbar c}{4\pi^2} k_F^4 = \frac{V \hbar c}{4\pi^2} \left(3\pi^2 \frac{N e}{V} \right)^{\frac{4}{3}} \uparrow$$

power change

$$= \frac{k_3}{R} N^{\frac{4}{3}} \quad \left(k_3 = \frac{3}{4} \left(\frac{q\pi}{4} \right)^{\frac{1}{3}} f^{\frac{4}{3}} \hbar c \right)$$

Now $E_{\text{tot}} = -\frac{k_2 N^2}{R} + \frac{k_3}{R} N^{\frac{4}{3}}$

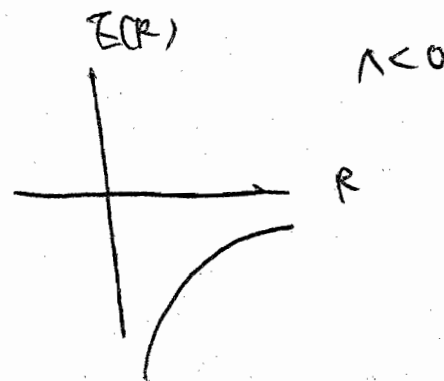
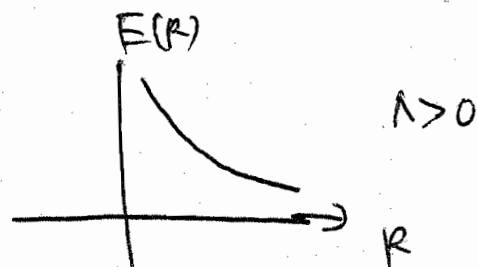
$$= \frac{\Lambda}{R}$$

Ask yourself what happens for $\Lambda > 0$

If $\Lambda < 0$, ~~$k_2 N^2$~~

i.e. $k_2 N^2 > k_3 N^{\frac{4}{3}}$

or $N > \left(\frac{k_3}{k_2} \right)^{\frac{3}{2}} \equiv N_c$



$$N_c = \left(\frac{K_3}{K_2} \right)^{\frac{3}{2}} = \left(\frac{5}{4} \right)^{\frac{3}{2}} \left(\left(\frac{9\pi}{4} \right)^{\frac{1}{3}} f^{\frac{4}{3}} \frac{\hbar c}{G m_p^2} \right)^{\frac{3}{2}}$$

$$= 3.1 f^2 \left(\frac{M_{pe}}{m_p} \right)^3$$

$$\approx 1.4 M_\odot$$

$$\Rightarrow M_c = 1.4 M_\odot \quad \text{Chandrasekhar mass.}$$

When $M_x > M_c \Rightarrow$ Collapse

Two possibilities:

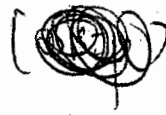
$$1) e + p \rightarrow n$$

neutron star, supported by the degenerate
neutron pressure.

$$2) M > M_c^{(n)} \quad (\text{for neutron } \odot, \text{ @ about } 3 M_\odot)$$

Collapse to form a black hole.

A little bit history



1862

A. Clark discover

Sirius B

$$T = 25,000 \text{ K}$$

much fainter 10,000 than

Sirius A

 $\Rightarrow$ small radius

① mass of the same as Sun

 $\Rightarrow$ extremely dense

start here

 $\rightarrow$ 1920Eddington suggested high densities of were

due to complete ionization of the atoms in the interior.

1926

R.H. Fowler :

electron degenerate gas, a few

months after Fermi-Dirac statistics

1930: Chandrasekhar, at age 19 on a ship
to England, applied relativistic theory to

Fowler's results $\Rightarrow$ Mc

It took long time for people to be convinced
of his results, in particular Eddington.

(Chandrasekhar himself did not know what to expect when ~~the~~ Mc
is exceeded.

Chandrasekhar got 1983 Nobel Prize.

8.4 Electrons in a periodic potential.

Last Lecture, metal: ^{lattice} ions surrounded by

free electron gas.

~~ions~~ ~~ions~~ ~~ions~~ ignore: ion potential
mutual coulomb interact.

Now Let us examine whether ignoring ion potential is reasonable or not.

be inclined to
✓ include
~~ions~~

If you think a bit about it, one would ~~have~~

~~great difficulty~~ the opposite: electrons should have ~~could have~~

great difficulty going around.

radius of ion: a few angstrom

lattice spacings: a few angstrom

It turns out neither
both intuitions

is correct
quite right.

(ignore potential)
electrons have difficulty moving around

(We will see that, when including the in

potentials: (electrons still ~~not~~ non-interacting)

due to $\leftarrow$ 1) electrons can still move around smoothly and easily, almost as free.

(Block theorem) (b) is wrong.

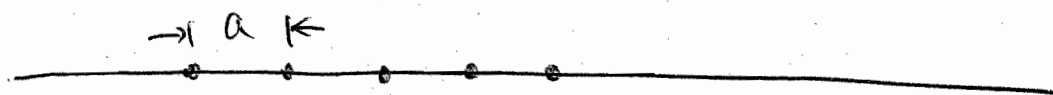
2) Single-particle wave functions have qualitative

different from free electron gas. (Band structure)

$\Rightarrow$ ~~met~~ conductor, semi conductor, insulator

8.4.1 Bloch theorem.

Consider a single electron moving in a lattice of ions. Let us consider a ~~1-d~~ ^{1-d} version for simplicity.



potential is periodic; $V(x) = V(x+a)$

Single-particle Schrodinger equation:

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi(x) = E \psi(x) \quad (*)$$

Bloch theorem:

$$\psi(x) = e^{ik \cdot x} u_k(x)$$

k real:

$$u_k(x) = u_k(x+a)$$

Proof: (i) Define ~~an~~ operator $\hat{T}_a$ such that

$$\hat{T}_a \psi(x) = \psi(x+a) \quad (1)$$

e.g. $T_a = e^{a \frac{d}{dx}} \quad T_a^\dagger = T_{-a} = (T_a)^{-1} \quad (2)$

unitary operator.

Since $V(x+a) = V(x)$

$$[\hat{T}_a, H] = 0$$

$\Rightarrow$ We can choose eigenstates of H that are also eigenstates of $\hat{T}_a$, i.e.

$$\hat{T}_a \psi(x) = c(a) \psi(x) \quad (3)$$

~~(2)~~

(ii) determine $c(a)$

Acting $\hat{T}_a$ n times.

On the one hand, (from (3))

$$\hat{T}_a^n \psi(x) = C^n(a) \psi(x)$$

On the other hand (from (2))

$$\hat{T}_a^n = T_{na}$$

$$(3) \Rightarrow \hat{T}_a^n \psi(x) = C^n(a) \psi(x)$$

$$\Rightarrow \underline{C^n(a) = C(na)}$$

$$\Rightarrow \boxed{C(a) = e^{ika}} \quad (4) \text{ for some constant } k$$

Since $T_a^\dagger = T_a^{-1} \Rightarrow e^{-ik^*a} = e^{-ika}$
 k real.

(iii)
 Equation (3) (1):

$$\hat{T}_a \psi = \underline{\psi(x+a) = e^{ika} \psi(x)} \quad (5)$$

Now let

$$\psi(x) = e^{ikx} u_k(x)$$

from eq (5) $\Rightarrow$

$$\Rightarrow u_k(x+a) = u_k(x)$$

Q.E.D.

Remarks:

1. physical implication

Recall free particle

$$\psi(x) = ce^{ikx}$$

$$|\psi(x)|^2 = \text{const}$$

Periodic potential : $\psi(x)$ is a plane wave modulated by a periodic function profile $u(x)$.

$$|\psi|^2 = |u(x)|^2 \text{ is periodic}$$

$\Rightarrow$ wave functions are delocalized.
electrons can move around

despite the presence of ~~close~~ ^{of} closely packed ions.

2. Range of Values of k :

$$\hat{T}_a \psi_k(x) = e^{ika} \psi_k(x)$$

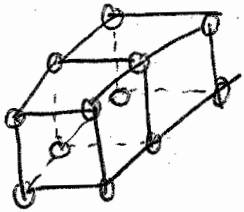
~~thus~~ Since ~~thus~~ e^{ika} is periodic in ka ,

we can restrict k to range

$$\underline{\underline{-\frac{\pi}{a} < k \leq \frac{\pi}{a}}}$$

3. 3-dimensional ~~generalization~~ generalization is immediate.

$$\psi(\vec{x}) = e^{i\vec{k} \cdot \vec{x}} u(\vec{x})$$

E.g. for a  cubic lattice

$$\vec{k} \in \left(-\frac{\pi}{a}, \frac{\pi}{a} \right]$$

Different lattice structure $\Rightarrow$ different allowed values to $\vec{k}$ (Brillouin Zone)

§4.2 ^{Band} ~~Block~~ structure (tight ~~to~~ binding model)

while Bloch theorem tells us that electrons can move around in a solid, it does not ~~to~~ give us direct physical intuition ~~to~~ how

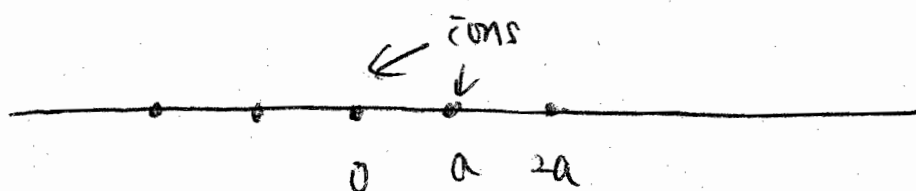
this happens. To get more physical ~~the purpose~~

intuition, let us ^{now} look at a simple model.

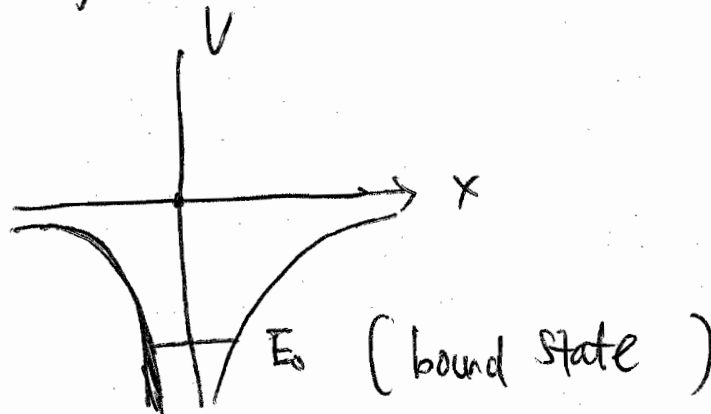
From this model, ~~we~~ ^{another} we also learn an important effect

of a periodic potential, (write section title)

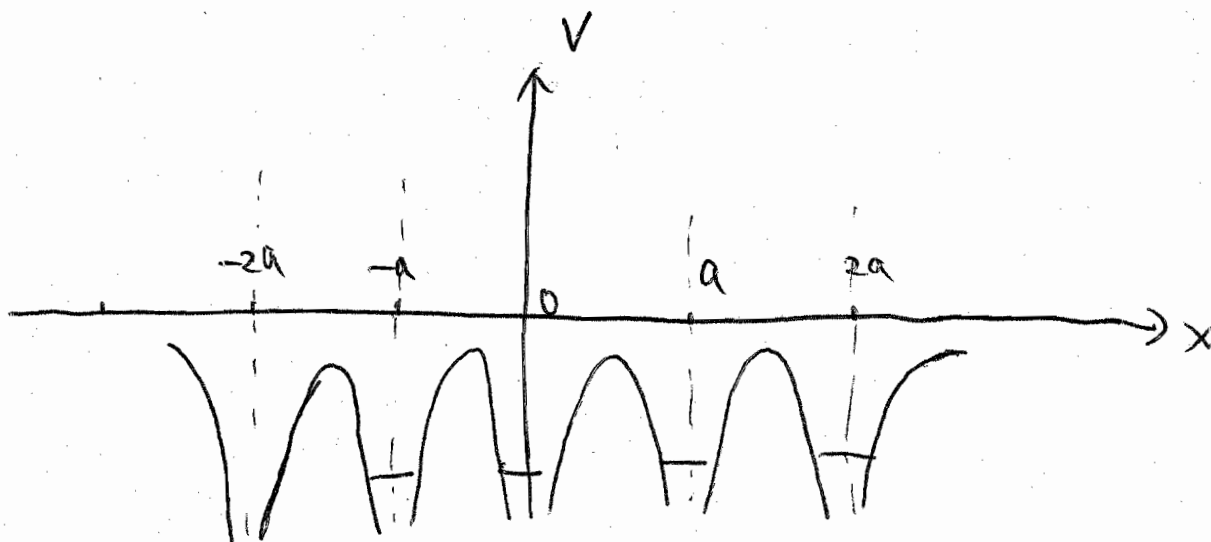
Consider a one-dimensional lattice (at the moment infinite,



~~atom~~ potential of a single atom:



~~Full~~ Full lattice potential:



What are the energy eigenstates?

Directly solving Schrodinger equation with such a potential is ~~course~~ very difficult, and not necessary.

~~We~~ want to know: How does the presence of other ions affect the state E_0 ?

Key effect: an electron can tunnel from one atom to a neighboring one,

e.g. $x=0 \longrightarrow x=\pm a$

Let ~~Define~~ $|n\rangle$ to be the state that the

electron is ~~at~~ trapped by the atom at $x=na$.

Assuming $\langle m|n\rangle = \delta_{nm}$, $\sum_n |n\rangle\langle n| = 1$

Ignore effects of other atoms:

$$H_0 = \sum_{n=-\infty}^{+\infty} E_0 |n\rangle \langle n|$$

in the basis of $|n\rangle$. (a complete set)

Now taking into account of tunneling:

$$H = \sum_{n=-\infty}^{+\infty} \left[E_0 |n\rangle \langle n| - \Delta |n+1\rangle \langle n| - \Delta |n-1\rangle \langle n| \right]$$

tunneling to neighboring atoms

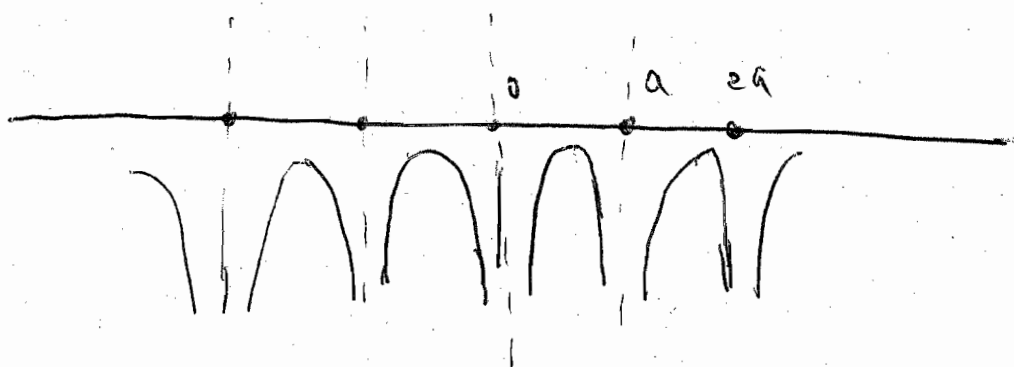
Now solve

$$\underline{H \psi = E \psi}$$

End of lect. 3.

Lec. 4.

§ 4.2 Band structure (continued)



Mathematical idealization:

1) $|n\rangle$, states localized at $x=na$.

$$\langle n|m\rangle = \delta_{nm}$$

2) An electron at $x=na$ can hop to

$$x = (n \pm 1)a \quad (\text{tunnelling})$$

Convenient to write the Hamiltonian in $|n\rangle$ basis

The translation operator is

$$T|n\rangle = |n+1\rangle \quad \text{or} \quad T = \sum_{n=-\infty}^{+\infty} |n+1\rangle \langle n|$$

$$T^{-1} = \sum_{n=-\infty}^{+\infty} |n\rangle \langle n+1|$$

• ~~Since~~ Since H does not depend on the labelling

$$[H, T] = 0$$

In fact:

$$H = E_0 \mathbb{1} - \Delta (T + T^{-1})$$

Since $|n\rangle$ is a complete set.

Bloch theorem: choose eigenstates of T

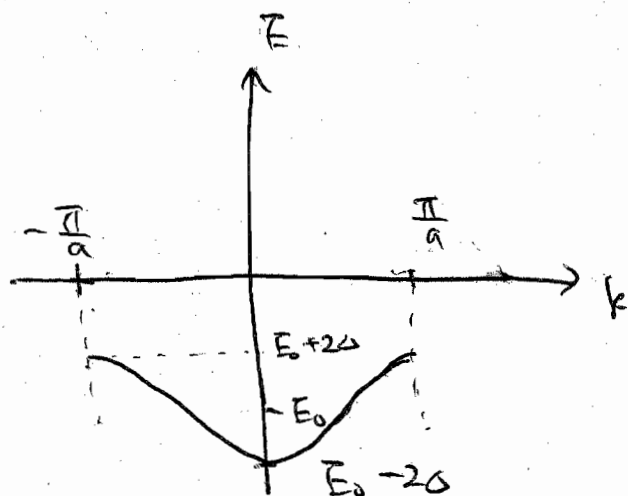
$$T|\psi_k\rangle = e^{ika} |\psi_k\rangle$$

$$\Rightarrow H|\psi_k\rangle = E_k |\psi_k\rangle$$

With

$$E_k = E_0 - \Delta (e^{ika} + e^{-ika})$$

$$= E_0 - 2\Delta \cos ka$$



$$-\frac{\pi}{a} < k \leq \frac{\pi}{a}$$

Remarks

1) In pset 2 you will find $|\psi_k\rangle$.

2) And see explicitly $|\psi_k\rangle$ is delocalized.

Skip:

Intuitively: even though tunneling rate is typically very small, constructive interference due to periodic structure.

total # of states in a ~~solid~~ solid:

2. Zn ^{reality} ~~reality~~ solid is not infinite.

We consider

~~there are~~ N sites with periodic

boundary conditions on the wave function.

i.e., $L = Na$, $\psi(0) = \psi(L)$

$$\Rightarrow T^N |\psi\rangle = |\psi\rangle$$

energy eigenstates: $T^N |\psi_k\rangle = e^{iNka} |\psi_k\rangle = |\psi_k\rangle$

$$\Rightarrow Nka = 2\pi n$$

$$\Rightarrow k = \frac{2\pi n}{Na}, \quad -\frac{N}{2} < n \leq \frac{N}{2}$$

total N states.

Effect of tunneling:

3. 0 a 2a

E_0 — — — — —

→ tunneling

a band
of
 N
states

— $E_0 + 2\alpha$

— $E_0 - 2\alpha$

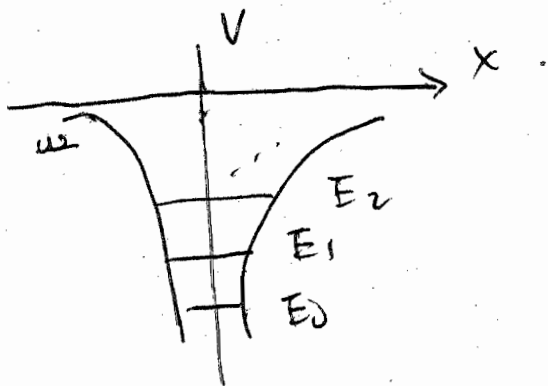
↑

each state is delocalized

with equal probability at any
site.

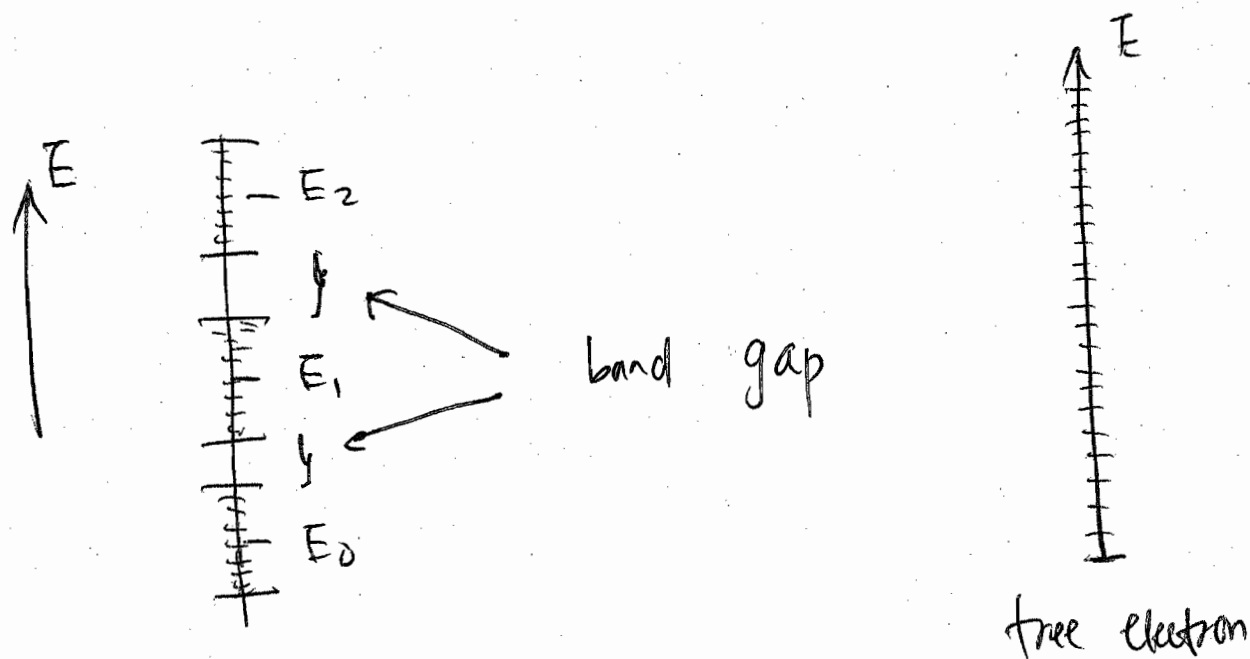
4. Band structure

A single atom has more than one energy levels



Δ is ~~typically~~ much smaller than the energy differences
(simplest situation)

Then in a lattice:



~~So Band structure Zn~~

Zn more generally, different bands can cross ...
complicated situations,

5. Conductors, ~~the~~ semi-conductors and insulators.

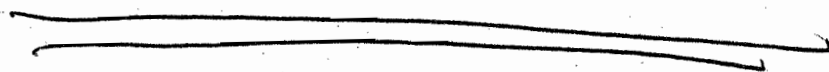
Now consider N electrons: fill single-particle states.

Each band can hold $2N$ electrons.

~~conductor~~



Ground state: no net current.



Conductors: partial filled

semi-conductor: ← → Shallen band gap
insulator } filled