Chapter 9

The Schrödinger Equ. in 3-dim.

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x,y,z) \qquad (1)$$

or $$H = \frac{\bar{p}^2}{2m} + V(\bar{r}) \qquad (2)$$

where $$p = \frac{\hbar}{i}\bar{\nabla} \qquad (3)$$

For 2-particles: $$H = \frac{\bar{p}_1^2}{2m_1} + \frac{\bar{p}_2^2}{2m_2} + V(\bar{r}_1, \bar{r}_2) \qquad (4)$$

If $$V(\bar{r}_1, \bar{r}_2) = V(|\bar{r}_1 - \bar{r}_2|) \qquad (5)$$

$\rightarrow$ H is invariant under $\bar{r}_1 \rightarrow \bar{r}_1 + \bar{a}$, $\bar{r}_2 \rightarrow \bar{r}_2 + \bar{a}$ (6)

$\xrightarrow[\text{that}]{\text{this implies}}$ $\begin{cases} \bar{P}_{total} = \text{const} \\ \text{and a separation of variables} \end{cases}$ (7)

In what follows, we will achieve the separation by finding funcs that are <u>simultaneous</u> eigenfuncs. of H and $\bar{P} = \bar{P}_1 + \bar{P}_2$ which $[H, \bar{P}] = 0$ (8)

We have

$$P_{op} f(\bar{r}_1, \bar{r}_2) = P f(\bar{r}_1, \bar{r}_2) \quad (9) \quad \text{eigenvalue equ.}$$

$$\rightarrow \frac{\hbar}{i} (\bar{\nabla}_1 + \bar{\nabla}_2) f(\bar{r}_1, \bar{r}_2) = P f(\bar{r}_1, \bar{r}_2) \quad (10)$$

If we write $\quad f(\bar{r}_1, \bar{r}_2) = \Psi(\bar{r}_1 - \bar{r}_2, \alpha \bar{r}_1 + \beta \bar{r}_2) \quad (11)$

$$\text{with} \begin{cases} \bar{R} = \alpha \bar{r}_1 + \beta \bar{r}_2 \\ \bar{r} = \bar{r}_1 - \bar{r}_2 \end{cases} \quad (12)$$

$$(10) \rightarrow \frac{\hbar}{i} (\alpha + \beta) \bar{\nabla}_R \Psi(\bar{r}, \bar{R}) = P \Psi(\bar{r}, \bar{R}) \quad (13)$$

Where:

$$(12) \longrightarrow \begin{cases} \bar{X} = \alpha x_1 + \beta x_2 \\ \bar{Y} = \alpha y_1 + \beta y_2 \\ \bar{Z} = \alpha z_1 + \beta z_2 \end{cases} \qquad \begin{cases} x = x_1 - x_2 \\ y = y_1 - y_2 \\ z = z_1 - z_2 \end{cases} \quad (14)$$

$$\bar{\nabla}_1 = \hat{i} \frac{\partial}{\partial x_1} + \hat{j} \frac{\partial}{\partial y_1} + \hat{k} \frac{\partial}{\partial z_1} \quad \ldots\ldots \quad (15)$$

$$\frac{\partial \Psi}{\partial x_1} = \frac{\partial \Psi}{\partial x} \frac{\partial x}{\partial x_1} + \frac{\partial \Psi}{\partial y} \frac{\partial y}{\partial x_1} + \frac{\partial \Psi}{\partial z} \frac{\partial z}{\partial x_1} + \frac{\partial \Psi}{\partial X} \frac{\partial X}{\partial x_1} + \frac{\partial \Psi}{\partial Y} \frac{\partial Y}{\partial x_1} + \frac{\partial \Psi}{\partial Z} \frac{\partial Z}{\partial x_1}$$

$$= \left(\frac{\partial \Psi}{\partial x} + 0 + 0 \right) + \alpha \left(\frac{\partial \Psi}{\partial X} + 0 + 0 \right)$$

$$= \frac{\partial \Psi}{\partial x} + \alpha \frac{\partial \Psi}{\partial X} \quad (16)$$

Similarly;

$$\frac{\partial\psi}{\partial Y_1}=\frac{\partial\psi}{\partial y}+\alpha\frac{\partial\psi}{\partial Y}\quad,\quad\frac{\partial\psi}{\partial Z_1}=\frac{\partial\psi}{\partial z}+\alpha\frac{\partial\psi}{\partial Z}\qquad(17)$$

$$\rightarrow\begin{cases}\bar{\nabla}_1=\bar{\nabla}_r+\alpha\bar{\nabla}_R & ,\quad(18)\\ \bar{\nabla}_2=-\bar{\nabla}_r+\beta\bar{\nabla}_R\end{cases}$$

Similarly

$$\rightarrow\nabla_1+\nabla_2=(\alpha+\beta)\bar{\nabla}_R\qquad(19)$$

Note that $\bar{r}$ may be considered as a const. parameter in equ. (13).

The sol.,

$$\psi(\bar{r},\bar{R})=u(\bar{r})\,e^{iP.R/\hbar(\alpha+\beta)}\qquad(20)$$

The energy eigenvalue equ;

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2-\frac{\hbar^2}{2m_2}\nabla_2^2+V(|\bar{r}|)-E_{tot}\right]u(\bar{r})\,e^{iP.R/\hbar(\alpha+\beta)}=0\qquad(21)$$

$$(18)\rightarrow\begin{cases}\bar{\nabla}_1^2=\bar{\nabla}_r^2+\alpha^2\bar{\nabla}_R^2+2\alpha\bar{\nabla}_R\cdot\bar{\nabla}_r\\ \bar{\nabla}_2^2=\bar{\nabla}_r^2+\beta^2\bar{\nabla}_R^2-2\beta\bar{\nabla}_R\cdot\bar{\nabla}_r\end{cases}\qquad(22)$$

$$-\frac{\hbar^2}{2m_1}\left[\bar{\nabla}_r^2u(\bar{r})-\frac{\alpha^2P^2}{(\alpha+\beta)^2\hbar^2}u(\bar{r})+\frac{2i\alpha}{(\alpha+\beta)\hbar}P.\bar{\nabla}_r u(\bar{r})\right]$$

$$-\frac{\hbar^2}{2m_2}\left[\bar{\nabla}_r^2u(\bar{r})-\frac{\beta^2P^2}{(\alpha+\beta)^2\hbar^2}u(\bar{r})-\frac{2i\beta}{(\alpha+\beta)\hbar}P.\bar{\nabla}_r u(\bar{r})\right]$$

$$+V(|\bar{r}|)u(\bar{r})=E_{tot}u(\bar{r})\qquad(23)$$

If we choose $\begin{cases} \alpha = \gamma m_1 \\ \beta = \gamma m_2 \end{cases}$ (24)

the cross terms are eliminated;

$$-\frac{\hbar^2}{2\mu}\bar{\nabla}_r^2 u(\bar{r}) + V(|\bar{r}|)u(\bar{r}) = \left(E_{tot} - \frac{\bar{P}^2}{2(m_1+m_2)}\right)u(\bar{r}) \quad (25)$$

where $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$ (26)

This is really a one-particle Schrödinger equ. with energy;

$$E = E_{tot} - \frac{\bar{P}^2}{2(m_1+m_2)} \quad (27)$$

The quantity γ is not specified by the above equ. If however, we require that the variable $\bar{R}$ be canonically conjugate to the total momentum $\bar{P}$, that is, if we require that;

$$[P_x, R_x] = \frac{\hbar}{i} \quad (28)$$

and so on; we see that;

$$[P_{1x}+P_{2x}, \alpha X_1 + \beta X_2] = \frac{\hbar}{i}(\alpha+\beta) = \frac{\hbar}{i} \quad (29)$$

$$\rightarrow (\alpha+\beta) = 1 \quad (30)$$

$$\rightarrow \gamma = \frac{1}{m_1+m_2} \quad (31)$$

The method mentioned for separation of variables is possible whenever $V = V(|\bar{r}|) = V(r)$

$$\longrightarrow H = \frac{p^2}{2\mu} + V(r) \qquad (32) \quad \text{(rotationally invariant)}$$

Note that $V = V(r)$ and it doesnt depend on θ or φ.

$p^2 = P \cdot P$ is also scalar.

Equivalently; $p^2 = -\hbar^2 \vec{\nabla}^2$ is invariant under rot.

A check:

A rot. through an angle θ about z-axis;

$$\begin{cases} x' = x\, C\theta - y\, S\theta \\ y' = x\, S\theta + y\, C\theta \end{cases} \qquad (33)$$

$$r' = (x'^2 + y'^2 + z^2)^{1/2} = (x^2 + y^2 + z^2)^{1/2} = r \qquad (34)$$

$$\frac{\partial f}{\partial x'} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial x'} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial x'} = \left(C\theta \frac{\partial}{\partial x} - S\theta \frac{\partial}{\partial y} \right) f$$

$$\frac{\partial f}{\partial y'} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial y'} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial y'} = \left(S\theta \frac{\partial}{\partial x} + C\theta \frac{\partial}{\partial y} \right) f \qquad (35)$$

$$\left(\frac{\partial}{\partial x'}\right)^2+\left(\frac{\partial}{\partial y'}\right)^2=\left(C\theta\frac{\partial}{\partial x}-S\theta\frac{\partial}{\partial y}\right)^2+\left(S\theta\frac{\partial}{\partial x}+C\theta\frac{\partial}{\partial y}\right)^2$$

$$=\left(\frac{\partial}{\partial x}\right)^2+\left(\frac{\partial}{\partial y}\right)^2 \qquad (36)$$

Since H has an invariance property, we expect a <u>conservation</u> law.

To identify the ops. that commute with H, let us consider an infinitesimal rot. about z-axis;

For $\theta \to$ small

$$\begin{cases} x' = x-\theta y \\ y' = y+\theta x \end{cases} \qquad (37)$$

We require that;

$$H\,U_E(x-\theta y,\, y+\theta x,\, z) = E\,U_E(x-\theta y,\, y+\theta x,\, z) \qquad (38)$$

$$U_E(x-\theta y,\, y+\theta x, z) = U_E(x,y,z)-\theta y\frac{\partial U}{\partial x}+\theta x\frac{\partial U}{\partial y} \qquad (39)$$

Also $\qquad H\,U_E(x,y,z) = E\,U_E(x,y,z) \qquad$ 40)

$(39) \xrightarrow{\text{in}} (38)$:

$$H\left[u_E(x,y,z) - \theta y\frac{\partial u}{\partial x} + \theta x\frac{\partial u}{\partial y}\right] = E\left[u_E(x,y,z) - \theta y\frac{\partial u}{\partial x} + \theta x\frac{\partial u}{\partial y}\right] \quad (41)$$

Subtracting (40) from (41)

$$\rightarrow \quad H\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)u_E(x,y,z) = E\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)u_E(x,y,z) \quad (42)$$

Since $E\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)u_E(x,y,z) = \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)H\,u_E(x,y,z)$ (43)

and sine $\{u_E(\bar{r})\}$ form a complete set,

we conclude that;

$$[H, L_z] = 0 \quad (44)$$

where $L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = xP_y - yP_x$ (45)

L_z is the z-component of;

$$\bar{L} = \bar{r} \times \bar{p} \quad (46)$$

with taking rot. about x- and y-axex, we find;

$$\begin{aligned} [H, L_x] &= 0 \\ [H, L_y] &= 0 \end{aligned} \quad (47)$$

$\rightarrow [H, \bar{L}] = 0 \quad \rightarrow \bar{L}$: const of motion (48)

This parallels the classical result that central forces imply conservation of the ang. mom.

Now; $[L_x, L_y] = [yP_z - zP_y, zP_x - xP_z]$

$= [yP_z, zP_x] - [zP_y, zP_x] - [yP_z, xP_z] + [zP_y, xP_z]$

$= y[P_z, z]P_x + x[z, P_z]P_y = \frac{\hbar}{i}(yP_x - xP_y) = i\hbar L_z$

(49)

Similarly $\quad [L_y, L_z] = i\hbar L_x$

$[L_z, L_x] = i\hbar L_y \qquad (50)$

$\rightarrow H, L_x, L_y, L_z$ do not form a complete set of commuting variables.

$\rightarrow$ It is impossible to find simultaneous eigenfuncs for all of them.

Thus only one component $\bar{L}$ may be chosen with H to form the commuting set of observables.

Also,

$$[L_z, L^2] = [L_z, L_x^2 + L_y^2 + L_z^2] = [L_z, L_x^2] + [L_z, L_y^2]$$

$$= L_x [L_z, L_x] + [L_z, L_x] L_x + L_y [L_z, L_y] + [L_z, L_y] L_y$$

$$= i\hbar L_x L_y + i\hbar L_y L_x - i\hbar L_y L_x - i\hbar L_x L_y = 0 \qquad (51)$$

Similarly:

$$[L_x, L^2] = 0$$
$$[L_y, L^2] = 0 \qquad (52)$$

Also $[H, L^2] = [H, L_x^2] + [H, L_y^2] + [H, L_z^2]$

$$= [H, L_x] L_x + L_x [H, L_x] + [H, L_y] L_y + L_y [H, L_y] + [H, L_z] L_z + L_z [H, L_z]$$

$$= 0 \qquad (53)$$

$\rightarrow \{H, L_z, L^2\}$ complete set of commuting ops.

We could add the parity op. Π to this set (since $[H, \Pi] = 0$) but we shall see later, specification of L^2 determines the parity.

Now,

$$L^2 = (\bar{r} \times \bar{p})^2 = [(r \times p)_x]^2 + [(r \times p)_y]^2 + [(r \times p)_z]^2$$

$$L^2 = -\hbar^2 \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right)^2 - \hbar^2 \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right)^2 - \hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right)^2$$

$$= -\hbar^2 \Big[x^2 \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + y^2 \left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial x^2} \right) + z^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)$$

$$- 2xy \frac{\partial^2}{\partial x \partial y} - 2yz \frac{\partial^2}{\partial y \partial z} - 2zx \frac{\partial^2}{\partial z \partial x} - 2x\frac{\partial}{\partial x} - 2y\frac{\partial}{\partial y} - 2z\frac{\partial}{\partial z} \Big] \quad (54)$$

Similarly;

$$(r \cdot p)^2 = -\hbar^2 \left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z} \right)^2 =$$

$$= -\hbar^2 \Big(x^2 \frac{\partial^2}{\partial x^2} + y^2 \frac{\partial^2}{\partial y^2} + z^2 \frac{\partial^2}{\partial z^2} + 2xy \frac{\partial^2}{\partial x \partial y} + 2yz \frac{\partial^2}{\partial y \partial z} + 2zx \frac{\partial^2}{\partial z \partial x}$$

$$+ x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z} \Big) \quad (55)$$

$$L^2 + (r \cdot p)^2 = -\hbar^2 (x^2 + y^2 + z^2) \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \hbar^2 \left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z} \right) \quad (56)$$

$$\rightarrow L^2 + (r \cdot p)^2 = r^2 p^2 + i\hbar\, r \cdot p \quad (57)$$

$$(57) \rightarrow p^2 = \frac{1}{r^2} \left[L^2 + (r \cdot p)^2 - i\hbar\, r \cdot p \right]$$

$$= \frac{1}{r^2} L^2 - \hbar^2 \frac{1}{r^2} \left(r \frac{\partial}{\partial r} \right)^2 - \hbar^2 \frac{1}{r} \frac{\partial}{\partial r} \quad (58)$$

$$(58) \text{ in } (32) \rightarrow -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \left(r\frac{\partial}{\partial r} \right) \left(r\frac{\partial}{\partial r} \right) + \frac{1}{r}\frac{\partial}{\partial r} - \frac{1}{\hbar^2 r^2} L^2 \right] u_E(\bar{r})$$

$$+ V(r)\, u_E(\bar{r}) = E\, u_E(\bar{r}) \quad (59)$$

L^2: involves θ, φ (and not r) (we will see later)

If we pick eigenfuncs of the form;

$$u_E(\bar{r}) = Y_\lambda(\theta,\varphi)\, R_{E\lambda}(\bar{r}) \qquad (60)$$

where $$L^2 Y_\lambda(\theta,\varphi) = \lambda Y_\lambda(\theta,\varphi) \qquad (61)$$

Our procedure is really no different than the conventional separation of variables. It does however, stress the role of the symmetry in determining the complete commuting set of operators, and with this help the separation can be effected.

Now consider the pot. of the form;

$$V(x,y,z) = V_1(x) + V_2(y) + V_3(z) \qquad (62)$$

The schrödinger equ.;

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) u_E(x,y,z) + \left[V_1(x) + V_2(y + V_3(z)\right] u_E(x,y,z) =$$
$$= E\, u_E(x,y,z) \qquad (63)$$

$$u_E(x,y,z) = u_{E1}(x)\, v_{E2}(y)\, w_{E3}(z) \qquad (64)$$

Where,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_1(x)\right]u_{\epsilon_1}(x)=\epsilon_1 u_{\epsilon_1}(x)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}+V_2(y)\right]v_{\epsilon_2}(y)=\epsilon_2 v_{\epsilon_2}(y) \qquad (65)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V_3(z)\right]w_{\epsilon_3}(z)=\epsilon_3 w_{\epsilon_3}(z)$$

and $\quad E=\epsilon_1+\epsilon_2+\epsilon_3 \qquad (66)$

Ex. – 3-dim potential hole. If the 3-dim. box is cubical in shape, with side L, then;

$$V_1(x)=\begin{cases}\infty & x<0\\ 0 & 0<x<L\\ \infty & x>L\end{cases} \qquad V_2(y)=\Big\{ \;\cdots \quad \text{and so on,} \qquad (67)$$

Then aside from a normalization factor;

$$u_E(x,y,z)=\sin\frac{n_1\pi x}{L}\,\sin\frac{n_2\pi y}{L}\,\sin\frac{n_3\pi z}{L} \qquad (68)$$

and $\quad K_i^2=\dfrac{\pi^2 n_i^2}{L^2} \qquad i=1,2,3$

$$E=\frac{\hbar^2\pi^2}{2mL^2}\left(n_1^2+n_2^2+n_3^2\right) \qquad (69)$$

Note that there is quite a lot of degeneracy in the problem.

The degeneracy is usually associated with the existance of mutually commuting ops. Here these ops. are, H_x, H_y, and H_z,

$$H_x = \frac{p_x^2}{2m} + V_1(x) \quad , \quad H_y = \frac{p_y^2}{2m} + V_2(y) \; , \quad H_z = \frac{p_z^2}{2m} + V_3(z) \tag{70}$$

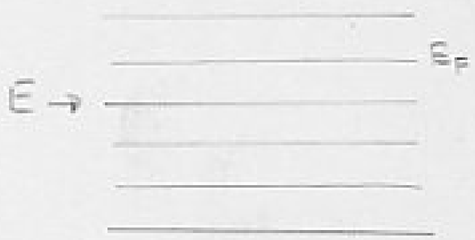
so that $\quad H = H_x + H_y + H_z \qquad (71)$

The ground state energy of N-noniteracting identical fermions, in the box of volume L^3:

For each triplet of integers $\{n_1, n_2, n_3\}$ two electrons can be accommodated.

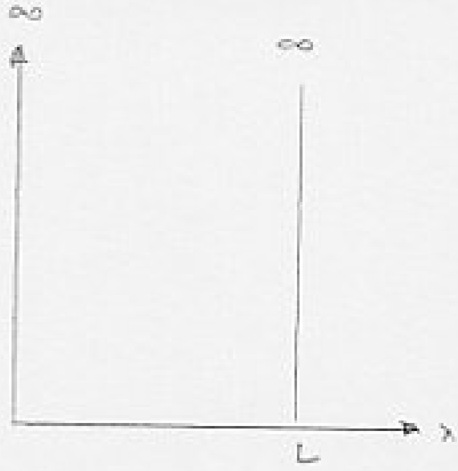
We can ask the ground state energy question in a different way: How many triplet of integers $\{n_1, n_2, n_3\}$ are there, such that E given by (69) is less than E_F ?

Each triplet forms a lattice in a 3-dim. space and if there are very many of them then it is a very good approx. to say that they must lie inside a sphere of radious R;



The Fermi Energy:

Consider non-interacting fermions in a one-dim box



$$u_E(x) = C \sin \frac{n\pi}{L} x$$

$$k^2 = \frac{\pi^2 n^2}{L^2} \qquad n = 1, 2, \ldots$$

$$E = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \qquad E_1 = \frac{\hbar^2\pi^2}{2mL^2} \qquad E_n = E_1 n^2$$

The N Fermions will fill up $N/2$ states (each state 2-Fermion)

At $T=0$ (no excitation) we have

$$E_F = E_{N/2} = \frac{\hbar^2\pi^2}{2mL^2}\left(\frac{N}{2}\right)^2 = \frac{\hbar^2\pi^2}{8m}\left(\frac{N}{L}\right)^2 = E_1\left(\frac{N}{2}\right)^2$$

$\frac{N}{L}$: number of Fermions / unit length (number density)

Ex. - The number of electrons in copper is $8.5 \times 10^{22} / cm^3$ assuming one free electron per atom. In one dimension, this is

$$\frac{N}{L} = (8.5 \times 10^{22})^{1/3} / cm = 4.4 \times 10^{7} / cm$$

$$E_F = \frac{\hbar^2\pi^2}{8m}\left(\frac{N}{L}\right)^2 = 1.8 eV$$

$$E_{ave} = \frac{1}{N} \sum_{n=1}^{N/2} \underset{\uparrow}{2} E_n = \frac{1}{N} \sum 2n^2 E_1$$

Spin up and down

For $N/2 \gg 1$; $\displaystyle\sum_{1}^{N/2} n^2 \approx \int_0^{N/2} n^2 dn = \frac{1}{3}\left(\frac{N}{2}\right)^3$

$$\rightarrow E_{ave} = \frac{2E_1}{N}\,\frac{1}{3}\left(\frac{N}{2}\right)^3 = \frac{1}{3}\left(\frac{N}{2}\right)^2 E_1 = \frac{E_F}{3}$$

Now let $n(E)\,dE$: the number of particles with energy between E and $E+dE$

we can write the distribution func. as:

$$n(E)\,dE = g(E)\,dE\,P(E)$$

$g(E)\,dE$: the number of states in dE

$P(E)$: the probability that a state will be occupied.

$$\text{At } T=0 \rightarrow \begin{cases} P(E)=1 & E<E_F \\ P(E)=0 & E>E_F \end{cases}$$

$$g(E) = \underset{\substack{\uparrow \\ \text{spin up and down}}}{2}\,\frac{dn}{dE} \qquad \text{the density of states}$$

$$E = E_0 n^2 \rightarrow dE = 2nE_0\,dn$$

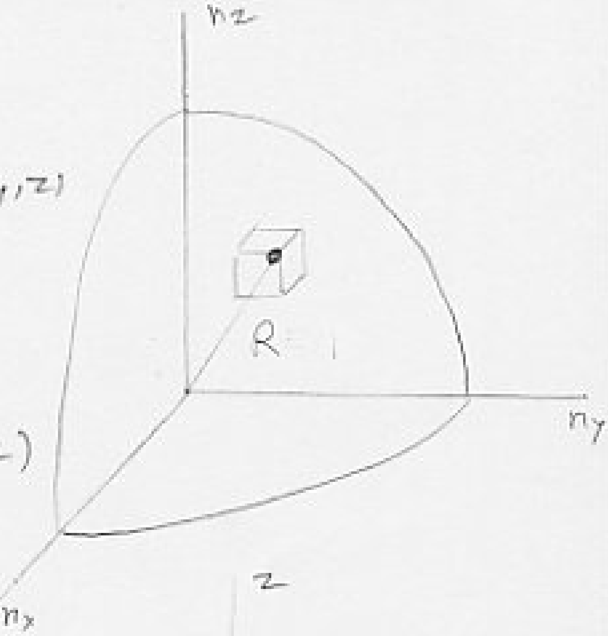
Since $n = \sqrt{\frac{E}{E_0}} \rightarrow dE = 2\sqrt{\frac{E}{E_0}}\,E_0\,dn = 2E^{1/2}E_0^{1/2}\,dn$

$$g(E) = 2\frac{dn}{dE} = 2\frac{1}{2nE_0} = \frac{1}{nE_0} = \frac{1}{\sqrt{\frac{E}{E_0}}\,E_0} = \frac{1}{\sqrt{EE_0}} = E_0^{-1/2}E^{-1/2}$$

$n(E)\,dE = g(E)\,dE\,F = E_0^{-1/2}E^{-1/2}\,dE\,F$ the energy distribution

In 3-dim.:

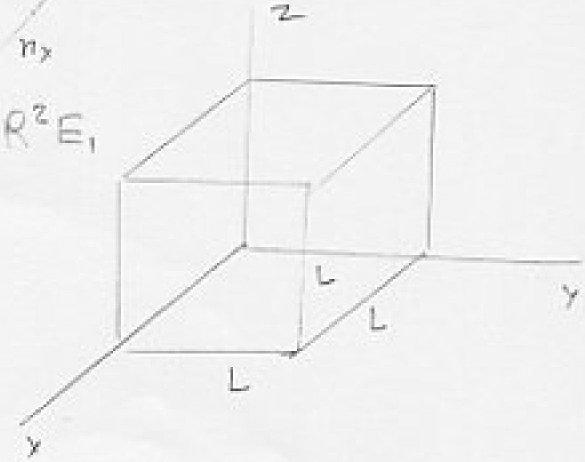
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)u_E(x,y,z) = E\,u_E(x,y,z)$$



$$u_E(x,y,z) \equiv u_{n_x,n_y,n_z}(x,y,z) =$$

$$= C\sin\left(\frac{n_x\pi}{L}x\right)\sin\left(\frac{n_y\pi}{L}y\right)\sin\left(\frac{n_z\pi}{L}z\right)$$

(standing waves)



$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2 = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2+n_y^2+n_z^2) = R^2E_1$$

$$K_i^2 = \frac{\pi^2 n_i^2}{L^2} \qquad i=1,2,3$$

$$n^2 = \frac{2mE}{\hbar^2\pi^2}L^2$$

$$\to R^2 = (n_1^2+n_2^2+n_3^2) = \frac{2mE_F}{\hbar^2\pi^2}L^2$$

Now, the number of states within the radius R is:

$$N = (2)\left(\frac{1}{8}\right)\left(\frac{4}{3}\pi R^3\right) = \frac{\pi}{3}L^3\left(\frac{2mE}{\hbar^2\pi^2}\right)^{3/2} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}V\,E^{3/2}$$

$$= \frac{\pi}{3}\left(\frac{E}{E_1}\right)^{3/2}$$

$$\to E_F = \left(\frac{3N}{\pi}\right)^{2/3}E_1 = \frac{\hbar^2\pi^2}{2mL^2}\left(\frac{3N}{\pi}\right)^{2/3} = \frac{\hbar^2\pi^2}{2m}\left(\frac{3}{\pi}\right)^{2/3}\left(\frac{N}{L^3}\right)^{2/3}$$

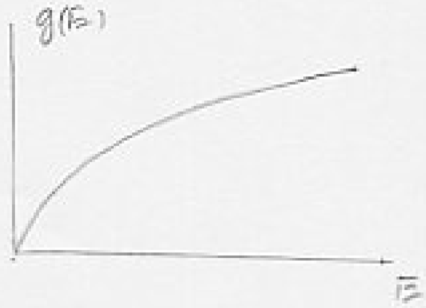
$\frac{N}{L^3}$: number density

Now

$$dN = \frac{\Omega}{2} E_1^{-3/2} E^{1/2} dE = \frac{\Omega}{2} \left(\frac{2mL^2}{\hbar^2 \pi^2} \right)^{3/2} E^{1/2} dE$$

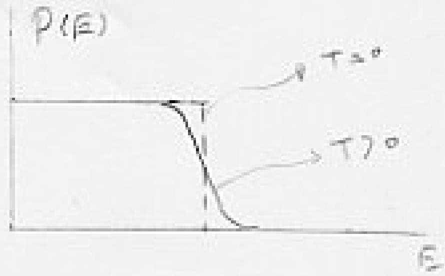
$$g(E) = \frac{dN}{dE} = \frac{\Omega}{2} \left(\frac{2mL^2}{\hbar^2 \pi^2} \right)^{3/2} E^{1/2}$$ density of states

Note that the factor of $\underline{2}$ (for spin up and down) has already been considered.



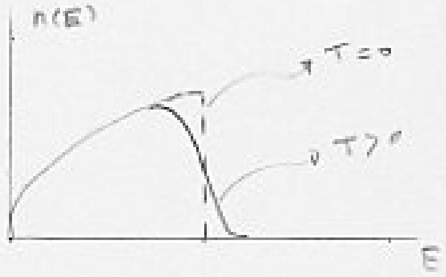
In terms of E_F,

$$g(E) = \frac{3}{2} N E_F^{-3/2} E^{1/2}$$



The number of Fermions in dE is thus

$$n(E)\,dE = g(E)\,dE\,P(E)$$



$$E_{ave} = \frac{1}{N} \int_0^{E_F} E\,(n(E)\,dE)$$

$$= \frac{1}{N} \int_0^{E_F} E\,(g(E)\,P(E)\,dE)$$

at $T=0$

$$E_{ave} = \frac{1}{N} \int_0^{E_F} E\,g(E)\,\theta(E-E_F)\,dE$$

$$= \frac{1}{N} \int_0^{E_F} \frac{3}{2} N E_F^{-3/2} E^{1/2} E\,dE = \frac{3}{5} E_F$$

$$E_{tot} = N E_{ave} = \frac{3N}{5} E_F = \frac{3N}{5} \frac{\hbar^2 \pi^2}{2mL^2} \left(\frac{3N}{\pi}\right)^{2/3} = \frac{\hbar^2 \pi^3}{10mL^2} \left(\frac{3N}{\pi}\right)^{5/3}$$

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

$\frac{N}{L^3}$: Fermion density

Note that we could equally calculate the E_{tot} using:

$$E_{tot} = \frac{1}{8} \underbrace{\int d n^3}_{\text{the number of lattice points}} (2E_n) = \frac{1}{8} \int_{|n| \leq R} n^2 dn d\Omega \left(2 \frac{\hbar^2 \pi^2}{2mL^2} n^2\right)$$

$$= \frac{\hbar^2 \pi^2}{mL^2} \frac{1}{8} (4\pi) \int_0^R n^4 dn = \frac{\pi^3 \hbar^2}{10mL^2} R^5$$

Note that;

$$\rho_{FB}(E) = \frac{1}{e^{(E-E_F)/kT} + 1} \qquad \text{Fermi-Dirac distribution}$$

$$\rho_{BE}(E) = \frac{1}{e^{(E-E_F)/kT} - 1} \qquad \text{Bose-Einstein} \quad ''$$

Remark: The Fermi temperature is defined by $k T_F = E_F$

Remark:

For travelling plane waves: $\psi = c\, e^{i[k_x x + k_y y + k_z z]}$

where $k_i = \frac{2\pi}{L} n_i$ $\qquad K_i = 0$, and positive and negative integers

$E_n = \frac{\hbar^2 k^2}{2m} = \frac{2\hbar^2 \pi^2}{mL^2} n^2 \qquad N_s = 2\,\frac{4}{3}\pi n^3 = \frac{8}{3}\pi \left(\frac{m}{2\hbar^2\pi^2}\right)^{3/2} V E^{3/2}$

$N_s = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E^{3/2}$ (the same result) $(V = L^3)$

Note also that

$$N = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E^{3/2} = \frac{1}{3\pi^2}\underbrace{\left(\frac{2mE}{\hbar^2}\right)}^{3/2} V = \frac{1}{3\pi^2} V K_F^2$$

Also $E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3} \quad \rightarrow \quad k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3}$

$$E_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m} p_F^2$$

Remark:

$(69) \rightarrow R^2 = n_1^2 + n_2^2 + n_3^2 = \frac{2mE_F}{\hbar^2 \pi^2} L^2$

and their number is given by the volume of the octant of the sphere for which all n_i are positive.

$$N_e = \frac{1}{8}\left(\frac{4}{3}\pi R^3\right) = \frac{1}{8}\frac{4\pi}{3}\left(\frac{2mE_F}{\hbar^2\pi^2}L^2\right)^{3/2} \quad (72)$$

the number of lattice points

$$N = 2N_e = \frac{\pi}{3} L^3 \left(\frac{2mE_F}{\hbar^2\pi^2}\right)^{3/2} \quad (73)$$

the number of electrons with $E < E_F$

i.e. $N \sim L^3$ (74)

In terms of density of electrons; $n = \frac{N}{L^3}$ (75)

$$(73)(75) \longrightarrow E_F = \frac{\hbar^2\pi^2}{2m}\left(\frac{3n}{\pi}\right)^{2/3} \quad (76)$$

Now $E_{tot} = ?$

$$(69) \rightarrow E = \frac{\hbar^2\pi^2}{mL^2}\,\bar{n}^2 \quad (77) \quad \text{(at each lattice point)}$$

$$E_{tot} = \frac{\hbar^2\pi^2}{mL^2}\left(\frac{1}{8}\int_{|n|\leq R} n^2\, d^3n\right) = \frac{\hbar^2\pi^2}{mL^2}\frac{1}{8}\int_0^R\int_0^{2\pi}\int_0^{\pi} n^2\,(n^2 \sin\theta\, d\theta\, d\varphi\, dn)$$

$$= \frac{\hbar^2\pi^2}{mL^2}\frac{1}{8}4\pi\int_0^R n^4\, dn = \frac{\pi^3\hbar^2}{10mL^2}R^5 \quad (78)$$

Since;

$$N = 2N_\ell = 2\,\frac{1}{8}\left(\frac{4}{3}\pi R^3\right) \quad (79)$$

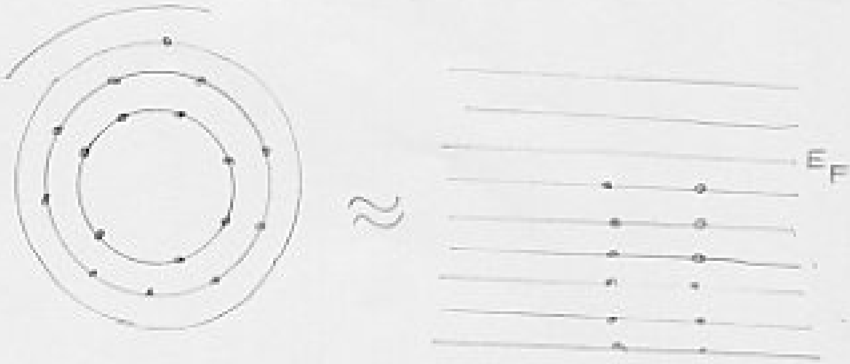
$$\rightarrow \quad E_{tot} = \frac{\pi^3\hbar^2}{10mL^2}\left(\frac{3N}{\pi}\right)^{5/3} \quad (80)$$

In terms of electron density $n = \frac{N}{L^3}$;

$$E_{tot} = \frac{\pi^3\hbar^2}{10m}\left(\frac{3n}{\pi}\right)^{5/3} L^3 \quad (81)$$

Ex. –

$E_F \sim 5\text{–}10$ eV Typical values of E_F



Thus at ordinary temperatures very few electrons can be thermally excited, most of them could only be excited to states that are already occupied.

If an electric field is applied to the metal, only the electrons near the top of Fermi sea can be accelerated, since those that lie deeper, cannot find available energy states. Those that are accelerated have long mean free path.

Collisions (of the electrons) with ions that would reduce their energies below E_F are inhibited because there are not available empty states.