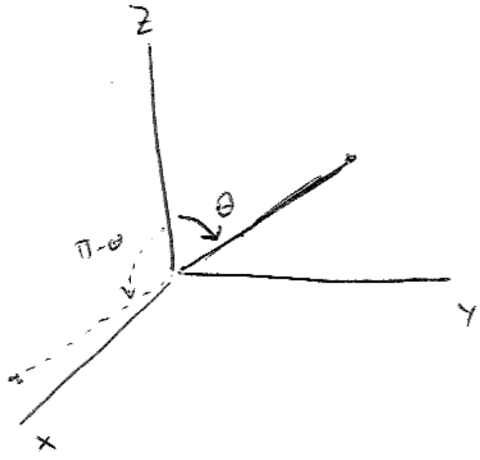
Parity

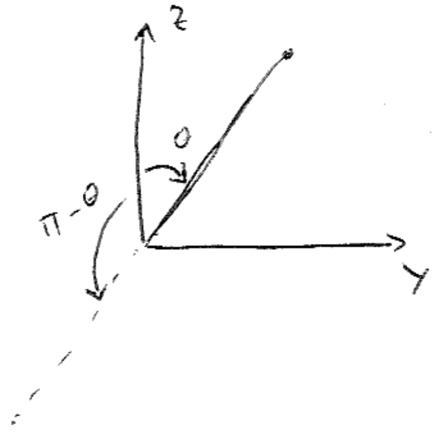
The parity operator $\hat{\Pi}$ is defined to change sign of all cartesian coordinates. For instance

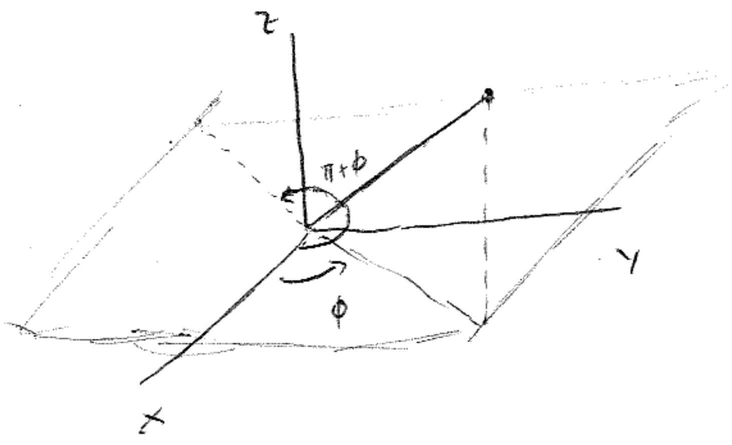
$$\hat{\Pi}\, f(x, y, z) = f(-x, -y, -z)$$

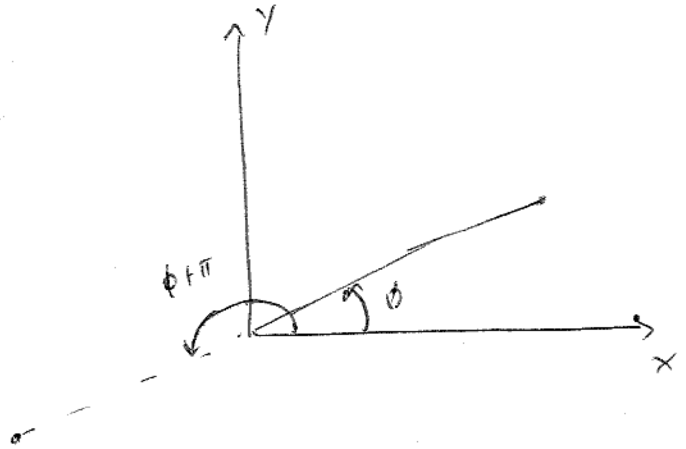
and in spherical coordinates

$$\hat{\Pi}\, f(r, \theta, \phi) = f(r, \pi - \theta, \pi + \phi)$$









By using

$$\begin{cases} \sin(\pi-\theta) = \sin\theta \\ \cos(\pi-\theta) = -\cos\theta \\ \sin(\pi+\phi) = -\sin\phi \\ \cos(\pi+\phi) = -\cos\phi \end{cases} \xrightarrow{\text{we get}} \left.\begin{matrix} \theta \to \pi-\theta \\ \phi \to \phi+\pi \end{matrix}\right\} \Rightarrow \left\{\begin{matrix} x \to -x \\ y \to -y \\ z \to -z \end{matrix}\right\}$$

Note that the parity operator is linear:

$$\hat{\Pi}\left(\alpha f(x,y,z) + g(x,y,z) \right) =$$

$$= \alpha f(x,-y,-z) + g(-x,-y,-z)$$

$$= \alpha \hat{\Pi} f(x,y,z) + \hat{\Pi} g(x,y,z)$$

Aiming to calculate the eigenvalues and eigenfunctions of the parity operator, consider the equation

$$\hat{\Pi} g_i = c_i g_i$$

and apply $\hat{\Pi}$ again

$$\hat{\Pi}\left(\hat{\Pi} g_i\right) = \hat{\Pi}\left(c_i g_i\right)$$

$$\hat{\Pi}^2 g_i = c_i \hat{\Pi} g_i$$

$$\hat{\Pi}^2 g_\alpha = c_\alpha^2 g_\alpha$$

But we know $\hat{\Pi}^2 = \mathbb{1}$ (the first $\hat{\Pi}$ changes sign and the second rechanges). Then we have

$$\mathbb{1} g_\alpha = g_\alpha = c_\alpha^2 g_\alpha$$

and we must have

$$\boxed{c_\alpha^2 = 1}$$

which implies

$$c_\alpha = \pm 1 .$$

By the way it is easy to check that $\hat{\Pi}$ is an Hermitian operator.

Thus the eigenvalues of the parity operator $\hat{\Pi}$ are ± 1. Concerning the eigenfunctions, we have

(i) for $c_1 = 1$

$$\hat{\Pi} g_1 = g_1 \longrightarrow g_1 \text{ is an even function}$$

(ii) for $c_2 = -1$

$$\hat{\Pi} g_2 = -g_2 \longrightarrow g_2 \text{ is an odd function}$$

Since we have only two eigenvalues and since it is possible to choose a basis of eigenvectors of $\hat{\Pi}$ ($\hat{\Pi}$ is Hermitian) we see depending on the specific problem usually these eigenvalues are highly degenerated.

<u>Theorem # 7</u> When the potential energy V is an even function we can choose the stationary-state wave functions with definite parity.

<u>proof</u>: Since both $\hat{\Pi}$ and $\hat{H}$ are Hermitian, it suffices to prove that $[\hat{\Pi}, \hat{H}] = 0$ because then we know there exists a common basis set of eigenfunctions of $\hat{H}$ (stationary-state wave functions) and $\hat{\Pi}$ (functions with definite parity).

From

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + V(x, y, z)$$

we get

$$[\hat{\pi}, \hat{H}] = -\frac{\hbar^2}{2m}[\hat{\pi}, \nabla^2] + [\hat{\pi}, V]$$

On account of

$$[\hat{\pi}, \nabla^2] f(x,y,z) = \hat{\pi}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) f(x,y,z) +$$

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \hat{\pi} f(x,y,z) =$$

$$= \left(\frac{\partial^2}{\partial (-x)^2} + \frac{\partial^2}{\partial (-y)^2} + \frac{\partial^2}{\partial (-z)^2}\right) f(-x,-y,-z)$$

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) f(-x,-y,-z) = 0$$

and of

$$[\hat{\pi}, V(x,y,z)] f(x,y,z) = \hat{\pi} V f - V \hat{\pi} f$$

$$= V(-x,-y,-z) f(-x,-y,-z) - V(x,y,z) f(-x,-y,-z)$$

$$= [V(-x,-y,-z) - V(x,y,z)] f(-x,-y,-z)$$

we see that, by using the theorem hypothesis of $V(-x,-y,-z) = V(x,y,z)$

we get

$$[\hat{\pi}, \hat{H}] = 0$$

and the desired result follows

<u>Theorem</u> # 8 Let $\hat{B}$ be an observable with eigenvalue equation

$$\hat{B}\, g_m = b_m\, g_m$$

and Ψ a general state which can be expanded as

$$\Psi = \sum_i c_i g_i$$

(i) If the eigenvalue b_m is nondegenerate, the probability of obtaining b_m in a measurement of B is $|c_m|^2$.

(ii) If the eigenvalue b_m is degenerate, the probability of obtaining b_m in a measurement of B is given by the sum of all $|c_i|^2$ corresponding to the eigenfunctions of eigenvalue b_m.

<u>proof</u>: Consider a normalized eigenstate

$$\Psi(q,t) = \sum_i c_i(t)\, g_i(q)$$

and write the expected value of B as

$$\langle B \rangle = \int \Psi^*(q,t)\, \hat{B}\, \Psi(q,t)\, d\tau$$

$$= \int \sum_j c_j^* g_j^* \, \hat{B} \sum_i c_i g_i \, d\tau$$

$$= \sum_{i,j} c_j^* c_i \int g_j^* b_i g_i \, d\tau$$

$$= \sum_{i,j} c_j^* c_i b_i \underbrace{\int g_j^* g_i \, d\tau}_{\delta_{ij}}$$

$$= \sum_i |c_i|^2 b_i$$

Now compare with

$$\langle B \rangle = \sum_{b_i} P_{b_i} b_i$$

We see that if b_i is non-degenerate then

$$P_{b_i} = |c_i|^2$$

and if b_i is degenerate then

$$P_{b_i} = \sum |c_i|^2$$

where the sum runs over the degenerated eigenvalues.

Position Eigenfunctions

Consider the position operator

$$\hat{x} = x .$$

Its eigenvalue equation reads

$$x\, g_a(x) = a\, g_a(x)$$

which means

$$(x - a)\, g_a(x) = 0$$

The eigenvalues are thus all real numbers $a \in \mathbb{R}$ and the eigenfunctions must satisfy

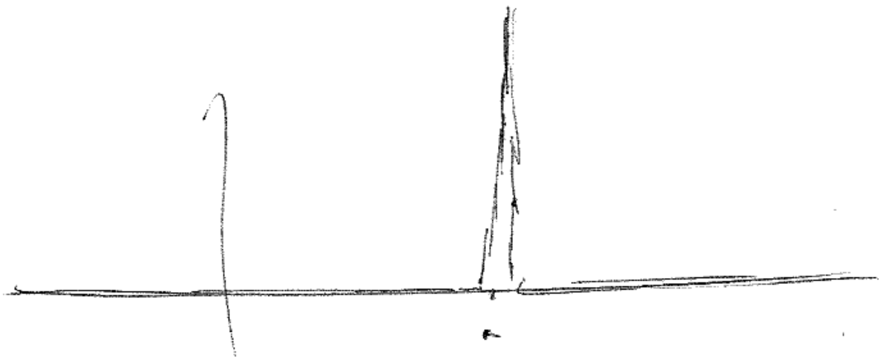
$$g_a(x) = 0 \quad \text{for } x \neq a$$

From the normalizing condition

$$\int_{-\infty}^{+\infty} g_a(x)\, dx = 0$$

We see we must have

$$g_a(x) = \delta(x-a)$$



Naturally the Dirac delta function satisfies

$$\int_{-\infty}^{+\infty} \delta(x-a)\,dx = 1$$

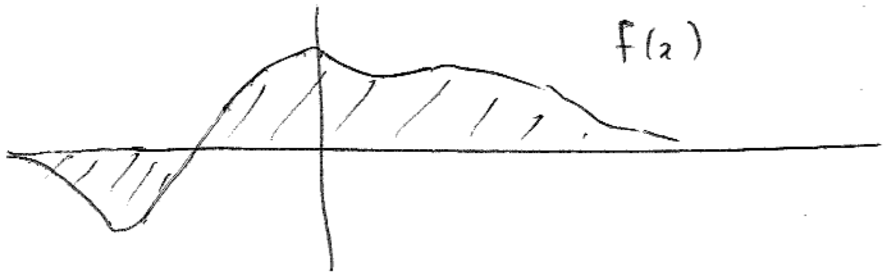
$$\int_{-\infty}^{+\infty} \delta(x-a)\, f(x)\, dx = f(a)$$

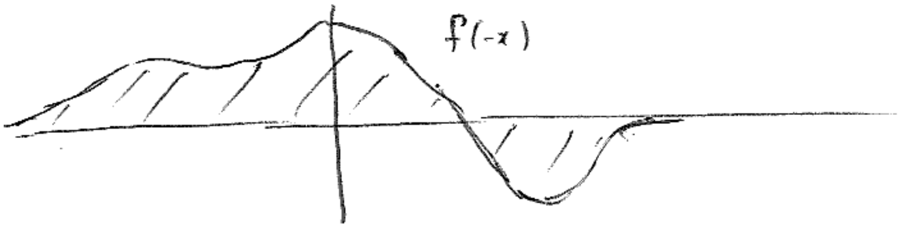
Remark: Checking the Hermicity of the parity operator $\hat{\Pi}$:

Note that $\int_{-\infty}^{+\infty} f(x)\, dx = \int_{-\infty}^{+\infty} f(-x)\, dx$. This holds

no matter what the parity of $f(x)$ happens to be.

Even if $f(x)$ has no definide parity.





Indeed we have

$$\int_{x=-\infty}^{x=+\infty} f(x)\, dx = \int_{-x=-\infty}^{-x=+\infty} f(-x)\, d(-x) = -\int_{x=+\infty}^{x=-\infty} f(-x)\, dx = \int_{x=-\infty}^{x=+\infty} f(x)\, dx$$

This property holds for higher number of dimensions as well. So, if q represents collectively the integration variables and $d\tau$ the integration element, we have

$$\int f(q)\, d\tau = \int f(-q)\, d\tau$$

where the implicity definite integration runs over the role range of the variables.

Then for arbitrary functions $f(q)$ and $g(q)$ we have

$$\int f^*(q) \left[\hat{\Pi}\, g(q) \right] d\tau =$$

$$= \int f^*(q)\, g(-q)\, d\tau$$

$$= \int f^*(-q)\, g(q)\, d\tau$$

$$= \int g(q) \left(\hat{\Pi}\, f(q) \right)^* d\tau$$

and we see that $\hat{\Pi}$ is Hermitian.

Incidentally note also that we have

$$\hat{\Pi}\left(f^*(q)\right) = \left(\hat{\Pi}\, f(q)\right)^*$$

because taking the complex conjugate first and then applying the parity operator is the same as the opposite. This can be seen from the following example

$$z : \mathbb{R} \longrightarrow \mathbb{C}$$

$$x \longmapsto a(x) + i\,b(x)$$

$$z(x) = a(x) + i\,b(x)$$

$$z(-x) = a(-x) + i\,b(-x)$$

$$(z(-x))^* = a(-x) - i\,b(-x)$$

$$z^*(x) = a(x) - i\,b(x)$$

$$z^*(-x) = a(-x) - i\,b(-x)$$

$$\therefore \quad (z(-x))^* = z^*(-x)$$

The Variational Method

The Variational Theorem

Consider a system described by a time independent Hamiltonian operator $\hat{H}$. If E_1 is the lowest eigenvalue for $\hat{H}$ and ϕ is any normalized wave function, we have

$$\int \phi^* \hat{H} \phi \, d\tau \geq E_1$$

proof:

Let ψ_k represent the eigenfunctions of $\hat{H}$

$$\hat{H} \psi_k = E_k \psi_k$$

and expand ϕ as

$$\phi = \sum_k a_k \psi_k$$

then we have

$$\int \phi^* \hat{H} \phi \, d\tau =$$

$$= \int \Big(\sum_k a_k \psi_k\Big)^* \hat{H} \Big(\sum_\ell a_\ell \psi_\ell\Big) \, d\tau$$

$$= \sum_{k,\ell} a_k^* a_\ell \int \psi_k^* \hat{H} \psi_\ell \, d\tau$$

$$= \sum_{k,\ell} a_k^* a_\ell E_\ell \int \psi_k^* \psi_\ell \, d\tau$$

$$= \sum_k |a_k|^2 E_k$$

Now, each E_k satisfies $E_k \geq E_1$ and thus

$$\int \phi^* \hat{H} \phi \, d\tau \geq \sum_k |a_k|^2 E_1$$

$$= \underbrace{\Big(\sum_k |a_k|^2\Big)}_{1} E_1 = E_1$$

and we obtain

$$\boxed{\int \phi^* \hat{H} \phi \, d\tau \geq E_1}$$

The variational theorem may be used to to look for approximated values for E_1. Namely, one tries different functions ϕ and calculates

$$E_\phi = \langle \phi | \hat{H} | \phi \rangle = \int \phi^* \hat{H} \phi \, d\tau$$

The ground state energy certainly satisfies

$$E_1 \leq E_\phi$$

In case ϕ is not normalized, we define $\phi' = N\phi$ with ϕ' normalized and we have

$$\int \phi'^* \hat{H} \phi' \, d\tau \geq E_1$$

$$\int N^* \phi^* \hat{H} N \phi \, d\tau \geq E_1$$

$$|N|^2 \int \phi^* \hat{H} \phi \, d\tau \geq E_1$$

From the normalization of ϕ' we have

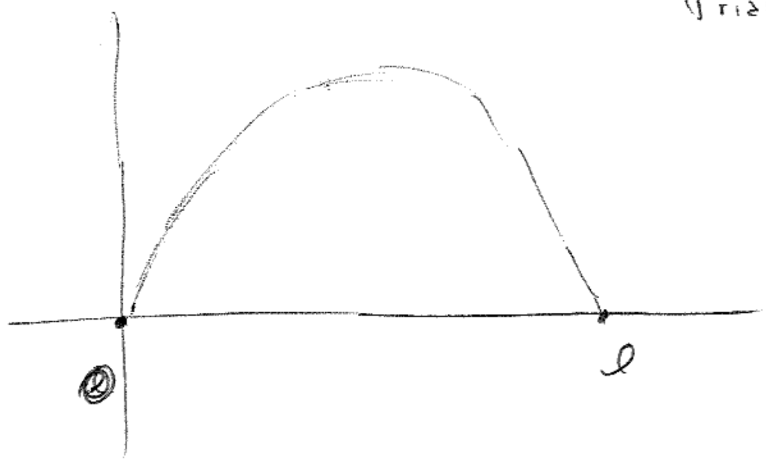
$$1 = \int (N\phi)^* N\phi \, d\tau = |N|^2 \int \phi^* \phi \, d\tau$$

which means $$|N|^2 = \frac{1}{\int \phi^* \phi \, d\tau}$$

Thus we may generalize the variational theorem to

$$\boxed{\frac{\int \phi^* \hat{H} \phi \, d\tau}{\int \phi^* \phi \, d\tau} \geq E_1}$$

<u>Example</u>: Let us estimate the ground state for the particle in a box



trial function:

$$\phi = x(l-x)$$

$$0 \leq x \leq l$$

$$\hat{H} = \frac{p_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \quad (\text{for } 0 \leq x \leq l)$$

Thus, considering the Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

and the trial function $\phi(x) = x(l-x)$,

for $0 \le x \le l$, we have

$$E_1 \le \frac{\int \phi^* \hat{H} \phi \, d\tau}{\int \phi^* \phi \, d\tau}$$

The ~~...~~ denominator integration reads

$$\int \phi^* \phi \, d\tau = \int_0^l [x(l-x)]^* [x(l-x)] \, dx$$

$$= \int_0^l x^2 (l-x)^2 \, dx$$

$$= \int_0^l (l^2 x^2 + x^4 - 2lx^3) \, dx$$

$$= l^5 \left[\frac{1}{3} + \frac{1}{5} - \frac{1}{2} \right]$$

$$= l^5/30$$

For the othe integration we need

$$\hat{H}\phi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\,x(x-\ell) = -\frac{\hbar^2}{m}$$

leading to

$$\int \phi^* \hat{H} \phi \, d\tau =$$

$$= \int_0^{\ell} x(x-\ell)\left(-\frac{\hbar^2}{m}\right) dx$$

$$= -\frac{\hbar^2}{m}\left(\frac{\ell^3}{3} - \frac{\ell^3}{2}\right) = \frac{\hbar^2 \ell^3}{6m}$$

Therefore we have

$$E_1 \leqslant \frac{\hbar^2 \ell^3/6m}{\ell^5/30} = \frac{5\hbar^2}{m\ell^2} = \frac{5h^2}{4\pi^2 m\ell^2}$$

$$\cong 0.12665 \frac{h^2}{m\ell^2}$$

Recall the exact value

$$E_1 = \frac{h^2}{8m\ell^2} = 0.125 \frac{h^2}{m\ell^2}$$