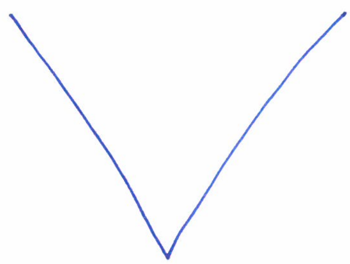
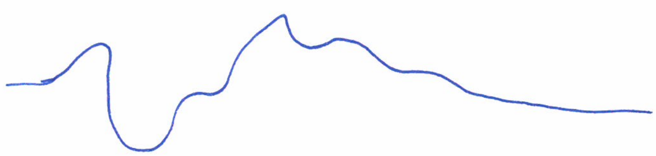
Sturm-Liouville Implications

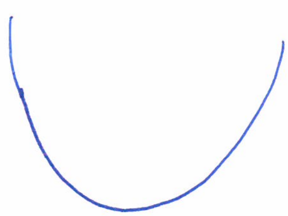
Pick any non-infinite potential, e.g.



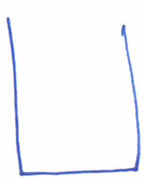
Eigenfunctions of that Hamiltonian can represent any $f(x)$ which $\to 0$ at $\pm\infty$.

e.g. $f(x) =$ 

Also, eigenfunctions of some other potential

e.g.  + vice versa.

But eigenfunctions of infinite potentials like

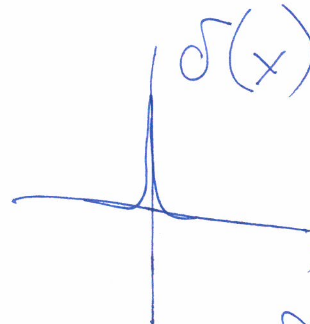


satisfy a more restrictive + different set of B.C.s, so they won't work as generic basis for larger space of functions.

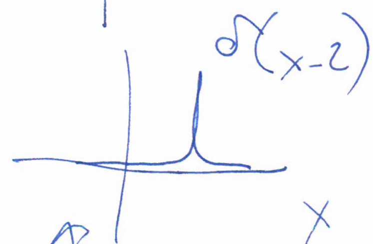
Periodic Boundaries, Plane Wave Decomposition

Dirac δ-function

Consider function $\delta(x)$ s.t.

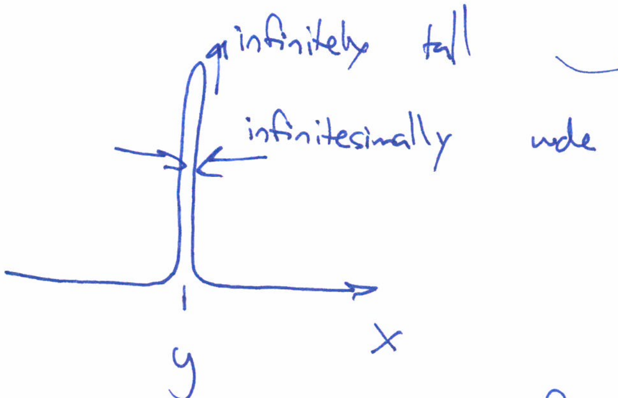


$$f(y) = \int dx\, \delta(x-y) f(x)$$



When integrated, Returns value of $f(x)$ @ $x=y$.

Must have strange form



But with area underneath $=1$

$$\int dx\, \delta(x-y) = 1$$

There are several represetations of $\delta(x-y)$, but one especially very useful for QM:

Recall that for non-infinite potentials,

operator $H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ satisfies Sturm-Liouville

theorem for $f(x)$ meeting B.C.'s of $f(x) \to 0$

at $x = \pm\infty$.

$\Rightarrow$ Eigenfunctions of H form complete set for

representing any $f(x)$.

If φ_n orthogonal:
(so non-degenerate suffices)

(0) $$f(x) = \sum_{n=1}^{\infty} c_n \varphi_n(x), \quad \text{where} \quad (3)\ c_m = \frac{1}{N_m}\int dx\, \varphi_m^*(x) f(x),$$

(2) $$\int dx\, \varphi_m^*(x) f(x) = \int \sum c_n \varphi_m^*(x)\varphi_n(x) = c_n N_n \delta_{n,m}$$ (if non-degenerate)

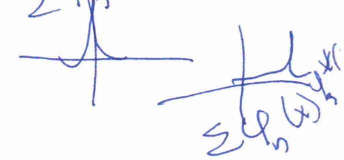
(Plug $f(x) = \Sigma\ldots$ in here & use:

(1) $$\int dx\, \varphi_n^*(x)\varphi_m(x) = \begin{cases} N_n, & n=m \\ 0, & n\neq m \end{cases}$$

integral over $y \cdot f(x)$ & stuff is acting like $\delta(x-y)$. Stuff must be δ.

(4) $$f(x) = \sum_{n=1}^{\infty} \int dy\, \varphi_n(x)\frac{1}{N_n}\varphi_n^*(y) f(y) = \int dy\, f(y)\,\delta(x-y)$$

$\sum \varphi_n(x)\varphi_n^*(0)$



That equation can only be true if

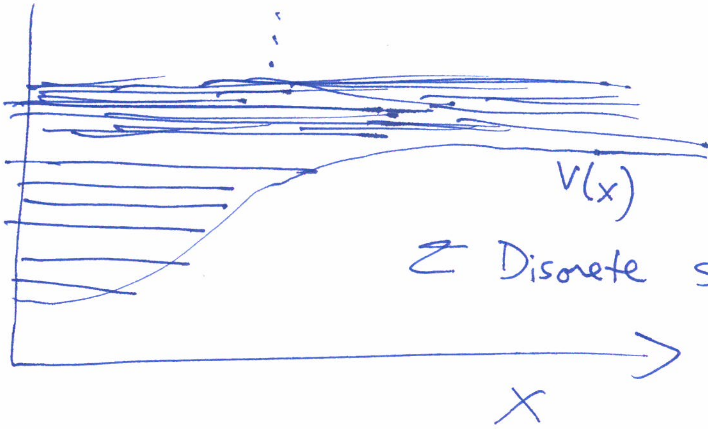
$$\boxed{\sum_{n=1}^{\infty} \varphi_n(x)\frac{1}{N_n}\varphi_n^*(y) = \delta(x-y)}$$

This is also just an alternative statement of $\boxed{\text{orthogonality/completeness}}$ of eigenfunctions

will need this in a few moments...

*eigenfunctions of any non-inf. potential!

Continuous Eigenvalues



- Lets consider first $V(x)=0$.

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\varphi = E\varphi$$

$\Rightarrow \varphi(x) = \sin kx,\ \cos kx,\ e^{\pm ikx}$ solves

with $E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$ using deBroglie

correspondence $p = \hbar k$

- We need some way to count these levels ~~&~~

sum over them.

- To do this, impose BCs at very large distance $L/2$ & take limit $L \to \infty$.

- We could ~~use a box~~ say $\varphi(x) = 0$ @ $x = \pm L/2$

Eigen functions satisfying these B.C.s are

$$\sin kx \quad , \quad k = \frac{2\pi n}{L} \quad n = 1, 2, \ldots$$

$$\cos kx \quad , \quad k = \frac{2\pi (n - \frac{1}{2})}{L} \quad n = 1, 2, \ldots$$

Pairs have Different wavelengths

- Alternatively, we could impose periodicity

$\cancel{\varphi(x+L) = \varphi(x)}$

(If you want to know φ further to right, you can just look back on left to find answer)

~~Equivalently~~

$$\varphi(-L/2) = \varphi(L/2) \qquad \varphi'(-L/2) = \varphi'(L/2)$$

Second-order dif eq. - these two BCs specify $\varphi(x)$

- Eigenfunctions satisfying this BC are

$$e^{ikx}, \quad k = \frac{2\pi n}{L}, \quad n \in \mathbb{Z}$$

(Pairs have same wavelength but dif sign of propagation), i.e. $n = \ldots -2, -1, 0, 1, 2, \ldots$

(Real part either @ max or min at ends. Imag. part @ 0)

- These two systems (both types of BC's) have 2 e.f. per increment of $|k|$:

$$\Delta |k| = \frac{2\pi}{L}$$

at $x = \pm L/2$ → $e^{ikx} = \pm 1$, cos & sin $= 0$

- Although different for finite L, they are ~~practically~~ identical as $L \to \infty$ & we are interested in local behavior

- It is most convenient to work with periodic BC, since e.f.s are also e.f.s of momentum operator $p = -i\hbar \frac{d}{dx}$, with eigenvalue $p = \hbar k$.

- From here, we will use "p" & "$\hbar k$" interchangeably

Note that $-i\hbar \frac{d}{dx} e^{ikx} = \hbar k e^{ikx}$ (e.f.)

But $-i\hbar \frac{d}{dx} \sin kx = -i\hbar k \cos kx$ (not e.f.)

- Sturm - Liouville, or just Fourier theorem, tells us that any fn periodic on interval $(-L/2, L/2)$, (or any fn in limit $L \to \infty$,) can be written as a linear combination of

expansion coefficients, could call them c_n, but will like this choice...

$$f(x) = \sum_{n=-\infty}^{\infty} e^{ik_n x} \tilde{f}_n \qquad \text{where } k_n = \frac{2\pi n}{L}$$

- As $L \to \infty$, k_n become closely spaced & replace $\Sigma \to \int$ as follows

$$\sum_{n=-\infty}^{\infty} = \sum_{k_n=-\infty}^{\infty} \underbrace{\Delta k \cdot \frac{L}{2\pi}}_{1}$$

, where Δk is spacing between levels $= \frac{2\pi}{L}$

$$\xrightarrow[\Delta k \to 0]{} \frac{L}{2\pi} \int_{-\infty}^{\infty} dk$$

- If we absorb factor ~~of~~ of L into $\tilde{f}_n$:

$\tilde{f}_k$ ~~$\tilde{f}(k)$~~ $= L\tilde{f}_n$ ($\longrightarrow \tilde{f}(k)$ as we go continuous)

$$\Rightarrow \boxed{f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx}\tilde{f}(k)}$$

We have just taken sum over discrete basis $\rightarrow$ integral over continuous. This is same statement we state with for $L \to \infty$

- Taking $L \to \infty$ ~~$\Rightarrow$ we can stop thinking about BCs~~
~~we~~ <u>Any</u> $f(x)$ (which $\to 0$ @ $\pm\infty$) can be represented this way.

- To find $\tilde{f}(k)$ we can use ~~δ-fn form of~~ orthogonality/completeness relation

$$\delta(x-y) = \sum_i \varphi_i^*(x)\frac{1}{N_i}\varphi_i(y), \quad N_i = \int dx\,|\varphi_i(x)|^2$$

(Back to periodic BCs) - For ~~...~~ $\varphi_n(x) = e^{ik_nx}$, $N_n = L$

$$\Rightarrow \boxed{\delta(x-y) = \sum_n \frac{e^{-ik_nx}e^{ik_ny}}{L} \longrightarrow \frac{1}{2\pi}\int dk\, e^{-ik(x-y)}}$$

Or, interchanging x & y ~~...~~ in integral (δ is even)

$$\boxed{\int_{-\infty}^{\infty}\frac{dk}{2\pi} e^{ik(x-y)} = \delta(x-y)}$$

Useful rep of δ function

This is one example of previous orth/comp. expression (for $V(x) \to 0$ as $L \to \infty$) for periodic B.C.s

Now, interchanging labels x, k, we have inverse identity

$$\boxed{\int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ix(k-l)} = \delta(k-l)}$$

Then we will see

$$\boxed{\tilde{f}(k) = \int_{-\infty}^{\infty} dx\, e^{-ikx} f(x)}$$

Proof: ~~Use~~ writing $f(x)$ as expansion of plane waves:

~~Evaluate RHS using~~ $\cancel{\int_{-\infty}^{\infty} dx}$

~~RHS~~

$$= \int_{-\infty}^{\infty} dx\, e^{-ikx} \int_{-\infty}^{\infty} \frac{dl}{2\pi} e^{ilx} \tilde{f}(l)$$

$$= \int \frac{dl}{\cancel{2\pi}} \cancel{2\pi}\, \delta(k-l)\, \tilde{f}(l) = \tilde{f}(k) \quad \checkmark$$

$\cancel{\tilde{f}(k}$

So we can represent any function ~~of x~~ either as a function of x or as a function of wavenumber k.

$$\cancel{f(x) = \int \frac{dk}{2\pi} e^{ikx} \tilde{f}(k) \qquad \tilde{f}(k) = \int_{-\infty}^{\infty} dx\, e^{-ikx} f(x)}$$

- And those boxed expressions tell us how to go back & forth between two representations

- $\tilde{f}(k)$ is called the Fourier transform of $f(x)$

- In QM $k \leftrightarrow p/\hbar$

$$\tilde{\psi}(p) = \int_{-\infty}^{\infty} e^{-ikx} \psi(x)$$

Describes x distribution

Describes p distribution