1_23_08

Note Title 1/23/2008

Review of special matrices

$A \in R^{N \times M}$

$(A^T)_{ij} = A_{ji}$ transpose

$(A^*)_{ij} = A^*_{ij}$ C. Conj.

$(A^+)_{ij} = A^*_{ji}$ Hermitian adjoint

$x, y \in R^N$

$(x, y) = \sum_{i=1}^{N} x_i y_i$

$$\boxed{\begin{array}{l} x, y \in C^N \\ (x, y) = \sum_{i=1}^{N} x_i^* y_i \end{array}}$$

Henceforth assume complex

Consequences $\alpha \in C$

$(\alpha x, y) = \alpha^* (x, y)$

$(x, \alpha y) = \alpha (x, y)$

$(x, y) = (y, x)^*$

For general matrix A

$$(x, Ay) \equiv (A^+x, y)$$

This is the definition of A^+

if $A^+ = A$, then $(x, Ay) = (Ax, y)$

For matrices $A^+ = A \Rightarrow A$ is Hermitian

For operators $A^+ = A \Rightarrow A$ self-adjoint

A matrix is the representation of a matrix in a particular coordinate system

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$$(AB)^T = B^T A^T$$

$$(AB)^+ = B^+ A^+$$

suppose $\quad Ax = \lambda x \quad$ ①

Take $+$ $\quad (Ax)^+ = \lambda^* x^+$

$$= x^+ A^+ = \lambda^* x^+ \quad ②$$

So $$x^+ A x = \lambda x^+ x \qquad (1)$$
$$x^+ A^+ x = \lambda^* x^+ x \qquad (2)$$

if $A^+ = A$ then

$$\lambda x^+ x = \lambda^* x^+ x$$

$$\Leftrightarrow \quad \lambda = \lambda^*$$

Eigenvalues of Hermitian (self-adjoint) matrices (operators) are real.

suppose
$$A = A^+$$

$$A x_1 = \lambda_1 x_1$$
$$A x_2 = \lambda_2 x_2$$

$$\Rightarrow \quad x_1^+ A = \lambda_1 x_1^+$$
$$x_2^+ A = \lambda_2 x_2^+$$

$$x_1^+ A x_2 = \lambda_1 x_1^+ x_2$$

$$\Rightarrow \quad \lambda_2 x_1^+ x_2 = \lambda_1 x_1^+ x_2$$

$$\Rightarrow \quad (\lambda_2 - \lambda_1) x_1^+ x_2 = 0$$

So either $\lambda_1 = \lambda_2$ or

$$X_1^{+} X_2 = 0$$

i.e. if the ε-values are different then the ε-vectors must be orthogonal.

Same stuff different notation

suppose $Ax = \lambda x$ $A^{+} = A$

$$(Ax, x) = (x, Ax)$$

$$\downarrow$$

$$(\lambda x, x) = (x, \lambda x)$$

$$\Downarrow$$

$$\lambda^{*}(x, x) = \lambda (x, x) \Rightarrow \lambda^{*} = \lambda.$$

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is the operator p self adjoint?

Need to show $(p\psi, \psi) = (\psi, p\psi)$

i.e.

$$\int_{-\infty}^{\infty} (p\psi)^{+} \psi \, dx = \int_{-\infty}^{\infty} \psi^{+} p \psi \, dx$$

for wavefunctions we don't

distinguish ψ^* from $\psi^\dagger$

$$(\psi, \hat{p}\psi) \equiv \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx$$

Now $\displaystyle\int \psi^* \hat{p} \psi \, dx = -i\hbar \int \psi^* \frac{\partial}{\partial x} \psi \, dx$

$$= \underbrace{-i\hbar \, \psi^* \psi \Big|_{-\infty}^{\infty}}_{0} + i\hbar \int \frac{\partial \psi^*}{\partial x} \psi \, dx$$

$$= \int \left(i\hbar \frac{\partial \psi^*}{\partial x} \right) \psi \, dx$$

$$= \int \left(-i\hbar \frac{\partial}{\partial x} \psi \right)^* \psi \, dx$$

$$= (\hat{p}\psi, \psi)$$

So $\quad (\psi, \hat{p}\psi) = (\hat{p}\psi, \psi)$

Looking ahead slightly: p 97-99

observables are represented by Hermitian operators

Determinate states are eigenfunctions of the corresponding operator

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E.g. $\hat{p}\,\psi = p_0\,\psi$

$$-i\hbar \frac{\partial \psi}{\partial x} = p_0\,\psi$$

$$\Rightarrow \quad \frac{\partial \psi}{\partial x} = \frac{-i p_0}{\hbar}\,\psi$$

$$\Rightarrow \quad \psi = \psi_0\, e^{-i p_0 x/\hbar}$$

As we would have expected, a definite momentum is associated with an (infinite) plane wave spatially

Recall from 1/21 a stationary state is an E-state of the Hamiltonian:

$$H\psi = E\psi \Rightarrow$$

$$\langle H \rangle = \int \psi^* H \psi \, dx$$
$$= \int \psi^* E \psi \, dx = E \underbrace{\int \psi^* \psi \, dx}_{=E}$$

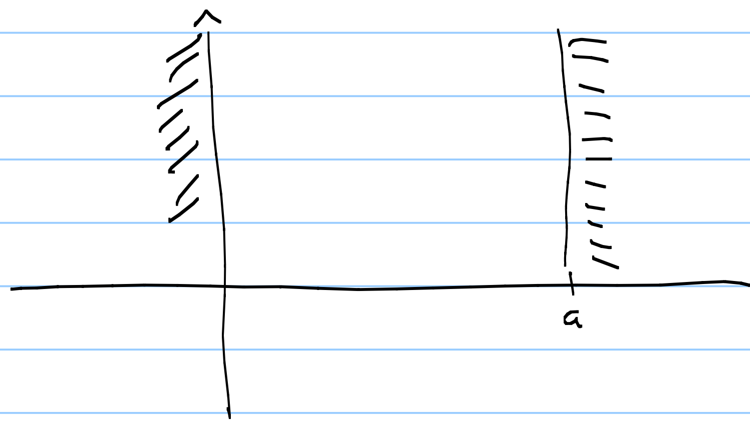
$$\langle H^2 \rangle = \int \psi^* H H \psi \, dx = E \int \psi^* H \psi \, dx$$
$$= E^2 \int \psi^* \psi \, dx$$
$$= E^2$$

So variance(H) $= \langle H^2 \rangle - \langle H \rangle^2$
$= E^2 - E^2 = 0$

if the state of a system is an eigenstate of H, then there is no uncertainty in the energy.

Try this for $\langle \hat{p} \rangle$ assuming ψ is an eigenstate of $\hat{p}$

$$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le a \\ \infty & \text{otherwise} \end{cases}$$



The fact that $V = \infty$ means there can be no prob. of finding the particle there. Obviously this is an idealization

$\psi(x,t) = 0$ if x not in $[0, a]$.

inside the box $V = 0$ so the TISE is

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

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \text{Let } k^2 = \frac{2mE}{\hbar^2}$$

and this is just the S. H. O.

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \Rightarrow \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi(x) = A \sin kx + B \cos kx$$

we require that $\psi(x)$ be continuous

thus $\psi(0) = \psi(a) = 0$ so

1) $B = 0$

2) $ka = n\pi$

just like for clamped string

$$\psi(x) = A \sin k_n x \qquad k_n = \frac{n\pi}{a}$$

$$k_n = \frac{n\pi}{a} = \frac{\sqrt{2mE_n}}{\hbar}$$

$$\Rightarrow \boxed{\frac{n^2\pi^2\hbar^2}{2ma^2} = E_n}$$

Energy levels of particle in Box.

Since $\psi(x) = A \sin(kx)$

we must normalize to find A

$$\int_0^a A^2 \sin^2(kx)\,dx \qquad kx = y \qquad k\,dx = dy$$

$$\frac{1}{k}\underbrace{\int_0^{ka} A^2 \sin^2 y\, dy}$$

$$\frac{y}{2} - \cancel{\frac{1}{4}\sin(2y)}$$

$$\frac{1}{k}\,\frac{ka}{2}$$

$$A^2\,\frac{a}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

$$\boxed{\begin{aligned} \psi_n(x) &= \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi}{a}\right)x \\ E_n &= \frac{n^2\pi^2\hbar^2}{2ma^2} \end{aligned}}$$

Stationary states

$$\psi_n(x)\, e^{-iE_n t/\hbar}$$

Ball park estimate.

suppose the box is the "size" of an H atom (i.e. 1 Bohr radius)

$a = 52 \times 10^{-12}$ m

suppose $m = m_e = 9 \times 10^{-31}$ kg

$\hbar = 1 \times 10^{-34}$ Js

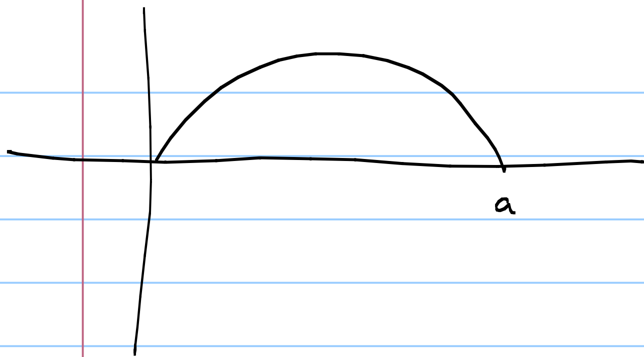
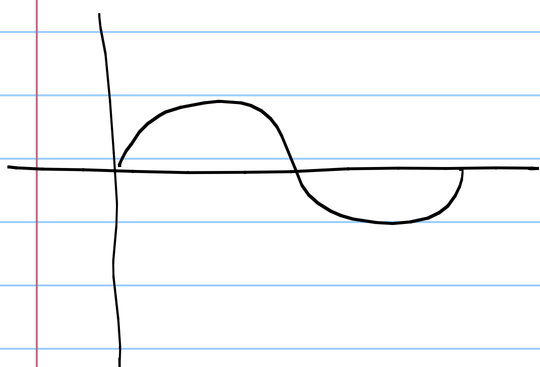
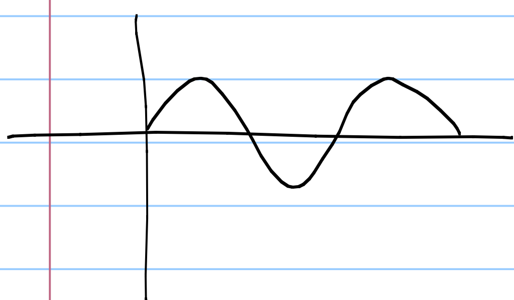
what do you get for E_1?

$$\frac{\pi^2 \hbar^2}{2ma^2} \approx 5 \times 10^{-18} \text{ Joules} \approx 30\,\text{eV}$$

As an ord. of mag. comparison
Binding energy of H ~ 13.6 eV.

Verify that the $\psi_n(x)$ satisfy

$$(\psi_n(x), \psi_m(x)) \equiv \int_{-\infty}^{\infty} \psi_n^* \psi_m \, dx = \delta_{nm}$$

ψ_N	E_N	# nodos
	$\frac{\pi^2 \hbar^2}{2ma^2} \cdot 1$	0
	$\frac{\pi^2 \hbar^2}{2ma^2} \cdot 4$	1
	$\frac{\pi^2 \hbar^2}{2ma^2} \; 9$	2

completeness of ψ_N. <u>any</u> $f(x)$

$$f(x) = \sum_{N=1}^{\infty} c_N \psi_N(x)$$

$$c_N = (\psi_N, f) = \int_{-\infty}^{\infty} \psi_N^* f(x)\, dx$$

The next step requires you to calculate of Fourier series. Review this.