Notes of 137A
Quantum Mechanics

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目录

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HW 30%, Mid 30%, Final 40%
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Mid – Th Oct 18 in class, Final – Tu Dec 12

Text
Griffths, Intro QM
Feynman
Morrison, Understanding Quantum Mechanics

1 The Wavefunction

1.6 The Uncertainty Principle

Uncertainty

$$\sigma_Q = \sqrt{\langle Q^2 \rangle - \langle Q \rangle^2} \tag{1.6.1}$$

Uncertainty Principle

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \tag{1.6.2}$$

2 Time-independent Schrödinger Eq.

2.1 Stationary State

$$\mathrm{i}\hbar \frac{\partial \Psi}{\partial t} = \hat{\mathbf{H}} \Psi \tag{2.1.1}$$

Assume

$$V = V(x) \tag{2.1.2}$$

$$\Psi(x,t) = \phi(t)\psi(x) \tag{2.1.3}$$

thus

$$\frac{\partial}{\partial t}\Psi(x,t) = \frac{\mathrm{d}\phi(t)}{\mathrm{d}t}\psi(x) \quad \frac{\partial^2}{\partial x^2}\Psi(x,t) = \phi(t)\frac{\partial^2 \psi(x)}{\partial x^2} \tag{2.1.4}$$

$$\mathrm{i}\hbar \frac{\mathrm{d}\phi(t)}{\mathrm{d}t}\psi(x) = -\frac{\hbar^2}{2m}\phi(t)\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\phi(t)\psi(x) \tag{2.1.5}$$

$$\frac{\mathrm{i}\hbar}{\phi(t)}\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = -\frac{\hbar^2}{2m\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) \tag{2.1.6}$$

thus

$$\frac{\mathrm{i}\hbar}{\phi(t)}\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = E = -\frac{\hbar^2}{2m\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) \tag{2.1.7}$$

right side – TISE
left side –

$$\mathrm{i}\hbar\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = E\phi(t) \tag{2.1.8}$$

$$\phi(t) = \mathrm{e}^{-\mathrm{i}Et/\hbar} \tag{2.1.9}$$

No time dependence of physically measurable quantities

$$p(x,t) = |\Psi(x,t)|^2 = \psi^*(x)\,\mathrm{e}^{\mathrm{i}Et/\hbar}\,\psi(x)\,\mathrm{e}^{-\mathrm{i}Et/\hbar} \tag{2.1.10}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle Q(x, -\mathrm{i}\hbar\frac{\partial}{\partial x})\rangle = 0 \tag{2.1.11}$$

$$\sigma_H = \sqrt{\langle\hat{\mathbf{H}}^2\rangle - \langle\hat{\mathbf{H}}\rangle^2} = 0 \tag{2.1.12}$$

Every solution of TDSE can be written as linear combination of solutions with definite energies (sol of TISE)
Assume "discrete spectrum" ...

most general sol of SE

$$\Psi(x,t) = \sum_n^\infty c_n\psi_n(x)\,\mathrm{e}^{-\mathrm{i}E_nt/\hbar} \tag{2.1.13}$$

where $c_n \in \mathbb{C}$.
How to find c_n?
Assume initial condition $\Psi(x,0)$
Assume discrete & non-degenerate spectrum: $E_n \neq E_m$ if $n \neq m$
thus

$$\Psi(x,0) = \sum_n^\infty c_n\psi_n(x) \tag{2.1.14}$$

$$c_n = \int \mathrm{d}x\Psi(x,0)\,\psi^*{}_n(x) \tag{2.1.15}$$

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1-D hamil has no-degenerate eigenvalues

if so

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_1}{\mathrm{d}x^2}+V(x)\psi_1=E\psi_1 \tag{2.1.16}$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_2}{\mathrm{d}x^2}+V(x)\psi_2=E\psi_2 \tag{2.1.17}$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_1}{\mathrm{d}x^2}\frac{1}{\psi_1}=-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_2}{\mathrm{d}x^2}\frac{1}{\psi_2} \tag{2.1.18}$$

$$\psi_1\psi_2''-\psi_2\psi_1''=0 \tag{2.1.19}$$

$$\mathrm{d}x\left(\psi_2\psi_1'-\psi_1\psi_2'\right)=0 \tag{2.1.20}$$

$$\psi_2\psi_1'-\psi_1\psi_2'=Cons. \tag{2.1.21}$$

since when $x\to\infty$, $\psi_2\psi_1'-\psi_1\psi_2'\to 0$

$$\psi_2\psi_1'-\psi_1\psi_2'=0 \tag{2.1.22}$$

$$\frac{\psi_1'}{\psi_1}=\frac{\psi_2'}{\psi_2} \tag{2.1.23}$$

$$\ln\psi_1=\ln\psi_2+Cons. \tag{2.1.24}$$

$$\psi_1=\psi_2\cdot Cons. \tag{2.1.25}$$

superposition state is not 定态

$$\Psi(x,t)=\frac{1}{\sqrt{2}}\left(\psi_1(x)\,\mathrm{e}^{-\mathrm{i}E_1t/\hbar}+\psi_2(x)\,\mathrm{e}^{-\mathrm{i}E_2t/\hbar}\right) \tag{2.1.26}$$

...

$$\langle x\rangle=\frac{1}{2}(\langle\psi_1|\,x\,|\psi_1\rangle+\langle\psi_2|\,x\,|\psi_2\rangle)+\langle\psi_1|\,x\,|\psi_2\rangle\cos\frac{(E_2-E_1)t}{\hbar} \tag{2.1.27}$$

2.2 The Infinite Square Well

2.3 SH Oscillator

$$V(x)=\frac{1}{2}m\omega^2x^2 \tag{2.3.1}$$

Expand near a minimum

$$V(x)=V(x_0)+\frac{1}{2}\frac{\mathrm{d}^2V(x)}{\mathrm{d}x^2}(x-x_0)^2+\cdots \tag{2.3.2}$$

def $k_{eff}=\frac{\mathrm{d}^2}{\mathrm{d}x^2}V(x)$

TISE for SHO

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi(x)+\frac{1}{2}m\omega^2x^2\Psi(x)=E\Psi(x) \tag{2.3.3}$$

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{p}}^2}{2m} + \frac{1}{2} m\omega^2 x^2 \tag{2.3.4}$$

def

$$\hat{\mathbf{H}} = \frac{1}{2}\hbar\omega(\hat{\mathbf{a}}_+ \hat{\mathbf{a}}_- + \hat{\mathbf{a}}_- \hat{\mathbf{a}}_+) \tag{2.3.5}$$

or

$$\hat{\mathbf{H}} = \hbar\omega(\hat{\mathbf{a}}_+ \hat{\mathbf{a}}_- + \frac{1}{2}) \tag{2.3.6}$$

where

$$\hat{\mathbf{a}}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp \mathrm{i}\, \hat{\mathbf{p}} + m\omega x) \tag{2.3.7}$$

$$[\hat{\mathbf{a}}_-, \hat{\mathbf{a}}_+] = 1 \tag{2.3.8}$$

Noticing

$$\begin{aligned} [\hat{\mathbf{H}}, \hat{\mathbf{a}}_+] &= \hbar\omega[\hat{\mathbf{a}}_+ \hat{\mathbf{a}}_- + \frac{1}{2}, \hat{\mathbf{a}}_+] \\ &= \hbar\omega\, \hat{\mathbf{a}}_+ \end{aligned} \tag{2.3.9}$$

we have

$$\hat{\mathbf{H}}(\hat{\mathbf{a}}_+ \psi(x)) = (E + \hbar\omega)(\hat{\mathbf{a}}_+ \psi(x)) \tag{2.3.10}$$

Similarly

$$\begin{aligned} [\hat{\mathbf{H}}, \hat{\mathbf{a}}_-] &= \hbar\omega[\hat{\mathbf{a}}_+ \hat{\mathbf{a}}_- + \frac{1}{2}, \hat{\mathbf{a}}_-] \\ &= \hbar\omega\, \hat{\mathbf{a}}_- \end{aligned} \tag{2.3.11}$$

$$\hat{\mathbf{H}}(\hat{\mathbf{a}}_\psi(x)) = (E - \hbar\omega)(\hat{\mathbf{a}}_- \psi(x)) \tag{2.3.12}$$

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Ex.

$$\Psi(x,0) = A\Big(3\,\mathrm{e}^{\mathrm{i}\theta_0}\sin\frac{\pi x}{a} + 2\cos\frac{\pi x}{2a}\Big) \tag{2.3.13}$$

Calc A, $\Psi(x,t)$.

Sol:

$$\langle\Psi|\Psi\rangle = |A|^2\int_{-a}^{a}\Big(3\,\mathrm{e}^{-\mathrm{i}\theta_0}\sin\frac{\pi x}{a} + 2\cos\frac{\pi x}{2a}\Big)\Big(3\,\mathrm{e}^{\mathrm{i}\theta_0}\sin\frac{\pi x}{a} + 2\cos\frac{\pi x}{2a}\Big)\mathrm{d}x = 1 \tag{2.3.14}$$

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suppose

$$\hat{\mathbf{a}}_+ \, \hat{\mathbf{a}}_- \, \psi(x) = u\psi(x) \tag{2.3.15}$$

$$\langle\psi| \, \hat{\mathbf{a}}_+ \, \hat{\mathbf{a}}_- \, |\psi\rangle = u \tag{2.3.16}$$

$$\langle\psi| \, \hat{\mathbf{a}}_+ \, \hat{\mathbf{a}}_- \, |\psi\rangle = \langle \hat{\mathbf{a}}_- \, \psi | \hat{\mathbf{a}}_- \, \psi\rangle \tag{2.3.17}$$

thus $\hat{\mathbf{a}}_- \, \psi(x) = 0$ iff $u = 0$.

??

2.4 Free particle

$\psi_k(x,t)$ is not a quantum state of a free particle

$$\psi(x,t) = \sum_k a_k \psi_k(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \phi(k) \, \mathrm{e}^{\mathrm{i}k(x - \hbar k t/2m)} \tag{2.4.1}$$

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$$\langle Q^2 \rangle = \langle Q \rangle^2 \tag{2.4.2}$$

$$\langle Q\psi | Q\psi \rangle \langle \psi | \psi \rangle = |\langle \psi | Q\psi \rangle|^2 \tag{2.4.3}$$

3 Formalism

3.1 Eigenfunctions of a Hermitian Operator

3.1.1 Discrete Spectra

Let $\{|f_{q,A}\rangle\}_A$ be a collection of orthogonal eigenvectors of eigenvalue q.

$$\langle f_{q,A} | f_{q',B} \rangle = \delta_{qq'} \delta_{AB} \tag{3.1.1}$$

3.2 Generalized Statistical Interpretation

If

$$|\Psi\rangle = \sum_{q,A} c_{q,A} |f_{q,A}\rangle \tag{3.2.1}$$

thus

$$c_{q,A} = \langle f_{q,A} | \Psi \rangle \tag{3.2.2}$$

Identity operator

$$\hat{I} = \sum_{q,A} |f_{q,A}\rangle \langle f_{q,A}| \tag{3.2.3}$$