Notes on Quantum Mechanics

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Contents

1 The Wave Function

1.1 The Schrodinger Equation

Goal of Quantum Mechanics: Determine the wave function $\Psi(x,t)$ of the particle.

Schrodinger Equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

Given the initial conditions: $\Psi(x,0)$; the Schrodinger equation determines $\Psi(x,t)$ for all future time.

1.2 Probability

$|\Psi(x,t)|^2\,dx$ represents the probability of finding the particle between x and $x+dx$.

$N(j)$ - number of people with j:

$$N = \sum_{j=0}^{\infty} N(j)$$

$P(j)$ - probability of getting j:

$$P(j) = \frac{N(j)}{N}$$

$$\sum_{j=0}^{\infty} P(j) = 1$$

Expectation value (average):

$$\langle j \rangle = \frac{\sum jN(j)}{N} = \sum_{j=0}^{\infty} jP(j)$$

$$\langle f(j) \rangle = \frac{\sum jN(j)}{N} = \sum_{j=0}^{\infty} f(j)P(j)$$

Variance:

$$\Delta j = j - \langle j \rangle$$

$$\sigma^2 = \left\langle (\Delta j)^2 \right\rangle$$

Standard deviation - σ

$$\sigma^2 = \left\langle j^2 \right\rangle - \langle j \rangle^2$$

$\rho(x)\,dx$ - probability that individual is between x and $x+dx$
$\rho(x)$ - probability density

$$P_{ab} = \int_a^b \rho(x)\,dx$$

Continuous distributions:

$$\int_{-\infty}^{\infty} \rho(x)\,dx = 1$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x\rho(x)\,dx$$

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\rho(x)\,dx$$

$$\sigma^2 = \left\langle x^2 \right\rangle - \langle x \rangle^2$$

1.3 Normalization

Particle must be somewhere:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = 1$$

Non-normalizable solutions cannot represent particles.
Wave function remains normalized as time goes on.

1.4 Momentum

Average of measurements performed on particles all in the state Ψ:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x,t)|^2 \, dx$$

Through integration by parts and discarding boundary terms:

$$\frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{m} \int \Psi^* \frac{\partial \Psi}{\partial x} \, dx$$

Expectation value of velocity:

$$\langle v \rangle = \frac{d\langle x \rangle}{dt}$$

Expectation value of momentum:

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = -i\hbar \int \left(\Psi^* \frac{\partial \Psi}{\partial x} \right) dx$$

Notation with operators:

$$\langle x \rangle = \int \Psi^* (x) \Psi \, dx$$

$$\langle p \rangle = \int \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx$$

Expectation value of dynamical variables:

$$\langle Q(x,p) \rangle = \int \Psi^* Q \left(x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx$$

1.5 The Uncertainty Principle

de Broglie formula:

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$$

Heisenberg uncertainty principle:

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

2 The Time-Independent Schrodinger Equation

2.1 Stationary States

Separation of Variables:

$$\Psi(x,t) = \psi(x)f(t)$$

Using the Schrodinger equation:

$$i\hbar\frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + V$$

Crucial argument: Left side is a function of only t, right side is a function of only x, therefore both sides are **constant** denoted by E.

$$\frac{df}{dt} = -\frac{iE}{\hbar}f$$

$$f(t) = e^{-iEt/\hbar}$$

Time-independent Schrodinger equation:

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

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

Separable Solutions

1. They are **stationary states** - the probability density does not depend on time.

2. They are states of definite total energy.

   Hamiltonian:

$$H(x,p) = \frac{p^2}{2m} + V(x)$$
$$\langle H \rangle = E$$
$$\sigma_H^2 = 0$$

3. The general solution is a **linear combination** of separable solutions. There is a different wave function for each **allowed energy**.

$$\Psi_1(x,t) = \psi_1(x)e^{-iE_1t/\hbar}$$
$$\Psi_2(x,t) = \psi_2(x)e^{-iE_2t/\hbar}$$

Time-dependent Schrodinger equation has the property that **any linear combination of solutions** is itself a **solution**.
General solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar}$$

2.2 The Infinite Square Well

$V = 0$ if $0 \le x \le a$, and $V = \infty$ otherwise.

Outside the well: $\psi(x) = 0$
Inside the well: $V = 0$

Simple harmonic oscillator:

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

General solution:

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

Boundary Conditions:

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

Hence:

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

$$ka = 0, \pm\pi, , \pm 2\pi, \pm 3\pi, ...$$

Distinct solutions:

$$k_n = \frac{n\pi}{a}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Normalize ψ:

$$A = \sqrt{\frac{2}{a}}$$

Solutions:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

ψ_1 - **ground state**, other waves are **excited states**

Important properties of $\psi_n(x)$

1. They are alternately **even** and **odd** (true when potential is an even function).
2. Each successive state has one more **node** (universal).
3. They are mutually orthogonal (quite general).

$$\int \psi_m(x)^* \psi_n(x)\, dx = 0, m \neq n$$

$$\int \psi_m(x)^* \psi_n(x)\, dx = \delta_{mn}$$

δ_{mn} - Kronecker delta

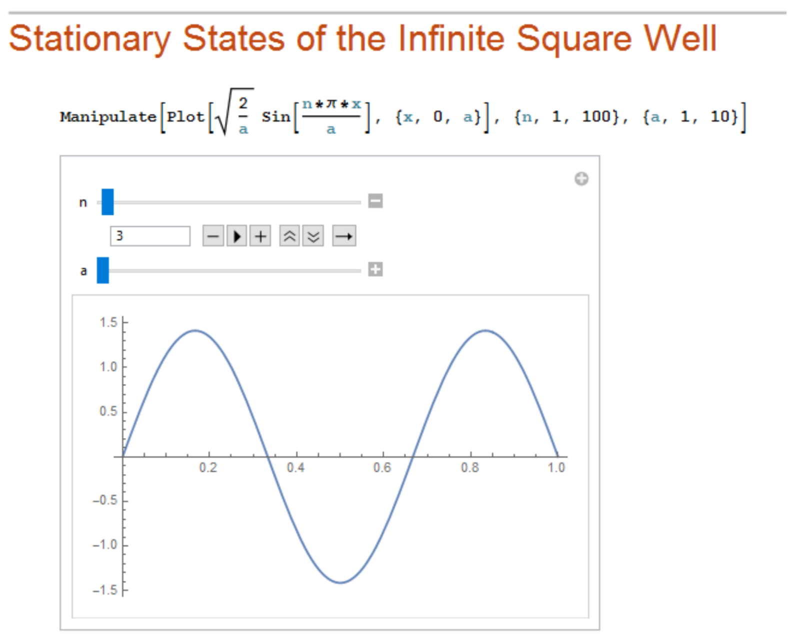
4. They are **complete**, in the sense that any other function, $f(x)$, can be expressed as a linear combination of them

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a} x\right)$$

Expansion coefficients can be evaluated by **Fourier's trick**:

$$\int \psi_m(x)^* f(x) d = \sum_{n=1}^{\infty} c_n \int \psi_m(x)^* \psi_n(x)\, dx = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$

$$c_m = \int \psi_m(x)^* f(x)\, dx$$



Stationary States for Infinite Square Well:

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

General Solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a} x\right) \Psi(x,0)\, dx$$

2.3 The Harmonic Oscillator

Practically any potential is approximately parabolic. Virtually any oscillatory motion is approximately simple harmonic.

$$V(x) \cong \frac{1}{2}V''(x_0)(x-x_0)^2$$

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

Solve:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$$

2.3.1 Algebraic Method

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right]\psi = E\psi$$

Ladder Operators:

$$a_\pm = \frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx} \pm im\omega x\right)$$

$$a_-a_+ = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right] + \frac{1}{2}\hbar\omega$$

$$a_+a_- = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right] - \frac{1}{2}\hbar\omega$$

$$a_-a_+ - a_+a_- = \hbar\omega$$

Schrodinger equation:

$$(a_-a_+ - \frac{1}{2}\hbar\omega)\psi = E\psi$$

$$(a_+a_- + \frac{1}{2}\hbar\omega)\psi = E\psi$$

Important: If ψ satisfies the Schrodinger equation with energy E, then $a_+\psi$ satisfies the Schrodinger equation with energy $(E+\hbar\omega)$. $a_-\psi$ is a solution with energy $(E-\hbar\omega)$.

There must exist a "lowest rung":

$$a_-\psi_0 = 0$$

$$\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d\psi_0}{dx} - im\omega x\psi_0\right) = 0$$

$$\psi_0 = A_0 e^{-\frac{m\omega}{2\hbar}x^2}$$

$$E_0 = \frac{1}{2}\hbar\omega$$

Excited states:

$$\psi_n(x) = A_n(a_+)^n e^{-\frac{m\omega}{2\hbar}x^2}$$

$$E_n = (n + \frac{1}{2})\hbar\omega$$

2.3.2 Analytic Method

Substitution:

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x$$

Schrodinger equation:

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi$$

$$K = \frac{2E}{\hbar\omega}$$

Large ξ:

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi$$

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{+\xi^2/2}$$

Asymptotic form:

$$\psi(\xi) \rightarrow ()e^{-\xi^2/2}$$

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}$$

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K = 1)h = 0$$

Look for a solution in the form of a power series:

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + ... = \sum_{j=0}^{\infty} a_j\xi^j$$

Recursion formula:

$$a_{j+2} = \frac{(2j + 1 - K)}{(j + 1)(j + 2)}a_j$$

The power series must terminate for the solution to be normalizable. One series must truncate, the other must be zero from the start.

$$K = 2n + 1$$

$$E_n = (n + \frac{1}{2})\hbar\omega$$

$$a_{j+2} = \frac{-2(n - j)}{(j + 1)(j + 2)}a_j$$

Stationary states:

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

Stationary States for the Harmonic Oscillator

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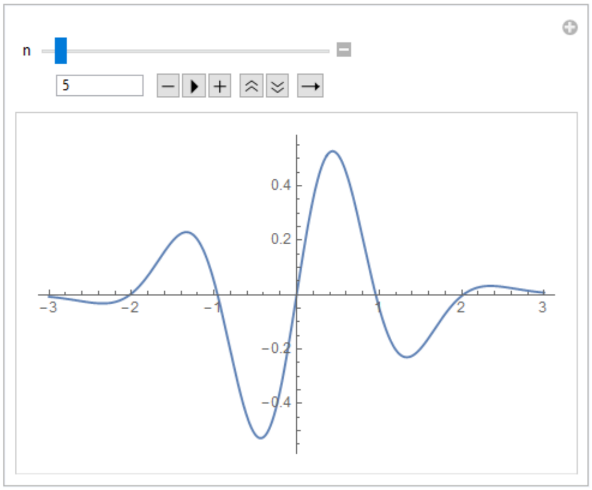

2.4 The Free Particle

$V(x) = 0$ everywhere.

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\Psi(x,t) = Ae^{ik(x - \frac{\hbar k}{2m}t)} + Be^{-ik(x + \frac{\hbar k}{2m}t)}$$

Special combination: $(x \pm vt)$ represents a wave of fixed profile, traveling in the $\mp x$ direction, at speed v.

$$\Psi_k(x,t) = Ae^{i(kx - \frac{\hbar k^2}{2m}t)}$$

$k > 0$: Wave traveling to the right
$k < 0$: Wave traveling to the left

$$v_{quantum} = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$$

A free particle cannot exist in a stationary state; there is no such thing as a free particle with a definite energy.

Wave packet:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx-\omega t)} \, dk$$

$$\omega = \frac{\hbar k^2}{2m}$$

Plancherel's theorem:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} \, dx$$

$$v_{group} = \frac{d\omega}{dk}$$

$$v_{phase} = \frac{\omega}{k}$$

2.5 The Delta-Function Potential

Bound State: If V(x) rises higher than the particle's total energy E on either side, then the particle is stuck in the potential well.

Scattering State: If E exceeds V(x) on one side or both, the the particle comes in from infinity and returns to infinity.

Tunneling allows the particle to leak through any finite potential barrier.

$E < V(-\infty)$ and $V(+\infty)$ - **Bound State**
$E > V(-\infty)$ or $V(+\infty)$ - **Scattering State**

Real life: Most potentials go to zero at infinity.

$E < 0$: Bound State $E > 0$: Scattering State

Infinite square well and harmonic oscillator admit **bound states** only. Free particle only allows **scattering states**.

Dirac delta function

$$\delta(x) = 0, x \neq 0$$

$$\delta(x) = \infty, x = 0$$

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

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

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

Potential:

$$V(x) = -\alpha\delta(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi$$

2.5.1 Bound States: $E < 0$

$$x < 0, V(x) = 0$$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$

General Solution:

$$\psi(x) = Be^{\kappa x}, x < 0$$

$$\psi(x) = Fe^{-\kappa x}, x > 0$$

Boundary Conditions:

1. ψ is always continuous.
2. $\frac{d\psi}{dx}$ is continuous except at points where the potential is infinite.

$$F = B$$

Integrate the Schrodinger equation from $-\epsilon$ to ϵ and take the limit as $\epsilon \to \infty$:

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} V(x)\psi(x)\,dx = -\frac{2m\alpha}{\hbar^2}\psi(0) = -2B\kappa$$

$$\kappa = \frac{m\alpha}{\hbar^2}$$

$$B = \frac{\sqrt{m\alpha}}{\hbar}$$

One bound state:

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|\hbar^2}$$

$$E = -\frac{m\alpha^2}{2\hbar^2}$$

2.5.2 Scattering States: $E > 0$

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, x < 0$$

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}, x > 0$$

In a typical scattering experiment particles are fired in from one direction. In that case the amplitude of the wave coming in from the right will be zero.

$$G = 0$$

A - amplitude of the **incident wave**
B - amplitude of the **transmitted wave**

$$\beta = \frac{m\alpha}{\hbar^2 k}$$

$$B = \frac{i\beta}{1 - i\beta}A$$

$$F = \frac{1}{1 - i\beta}A$$

Reflection Coefficient

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2} = \frac{1}{1 + (2\hbar^2 E/m\alpha^2)}$$

Transmission Coefficient

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2} = \frac{1}{1 + (m\alpha^2/\hbar^2 E)}$$

$$R + T = 1$$

2.6 Finite Square Well

$V(x) = -V_0$ for $-a < x < a$
$V(x) = 0$ for $|x| > a$

2.6.1 Bound States: $E < 0$

$x < -a$, $V(x) = 0$:

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$

$$\psi(x) = Be^{\kappa x}$$

$-a < x < a$, $V(x) = V_0$:

$$\frac{d^2\psi}{dx^2} = l^2\psi$$

$$l = \frac{\sqrt{2m(E + V_0}}{\hbar}$$

$$\psi(x) = C\sin(lx) + D\cos(lx)$$

$x > a$, $V(x) = 0$:

$$\psi(x) = Fe^{-\kappa x}$$

1. **Wide, deep well**

$$E_n + V_0 \cong \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

2. **Shallow, narrow well**: There is always one bound state, no matter how weak the well becomes.

2.6.2 Scattering States: $E > 0$

$x < -a$:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$-a < x < a$:

$$\psi(x) = C\sin(lx) + D\cos(lx)$$

$$l = \frac{\sqrt{2m(E + V_0}}{\hbar}$$

$x > a$ (assuming there is no incoming wave in this region):

$$\psi(x) = Fe^{ikx}$$

$$B = i\frac{\sin(2la)}{2kl}(l^2 - k^2)F$$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{\sin(2la)}{2kl}(k^2 + l^2)}$$

$$T^{-1} = 1 + \frac{v_0^2}{4E(E+V_0} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0}\right)$$

Energies for perfect transmission:

$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

2.7 The Scattering Matrix

Arbitrary Localized Potentials

Region 1:

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}$$

Region 2:

$$\psi(x) = Cf(x) + Dg(x)$$

Region 3:

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}$$

$$B = S_{11}A + S_{12}G$$

$$F = S_{21}A + S_{22}G$$

Scattering Matrix

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

$$\begin{pmatrix} \mathrm{B} \\ \mathrm{F} \end{pmatrix} = S \begin{pmatrix} \mathrm{A} \\ \mathrm{G} \end{pmatrix}$$

Scattering from the left:

$$R_l = |S_{11}|^2$$

$$T_l = |S_{21}|^2$$

Scattering from the right:

$$R_r = |S_{22}|^2$$

$$T_r = |S_{12}|^2$$

If you want to locate the bound states, put in $k \to i\kappa$.