8.04 Quantum Physics I — Course Summary

Zwiebach, *Mastering Quantum Mechanics* Part I (Ch 1–11, 29) + MIT 8.04 notes (2016)

The course in 8 ideas

1. **State** = complex wavefunction Ψ; $|\Psi|^2$ = probability density. Superpositions are allowed; overall phase is not physical.
2. **Dynamics:** $i\hbar\partial_t\Psi = \hat{H}\Psi$. Energy eigenstates only pick up a phase $e^{-iEt/\hbar}$; every motion is a superposition of them.
3. **Observables** = Hermitian operators. A measurement gives an eigenvalue with probability $|c_i|^2$ and leaves the eigenstate.
4. **Uncertainty** comes from non-commuting operators ($[\hat{x},\hat{p}] = i\hbar$) and is Fourier analysis: narrow in x ⇔ wide in k.
5. **Bound states quantize energy:** normalizability + matching conditions pick discrete E_n; state n has $n-1$ nodes; $E_{gs} > V_{min}$.
6. **Scattering:** unbound states; current conservation gives $R+T=1$; phase shifts give time delays; δ jumping by π marks a resonance.
7. **Oscillator:** $\hat{a},\hat{a}^\dagger$ give $E_n = \hbar\omega(n+\frac{1}{2})$ by algebra alone, the template for later courses.
8. **3D central potentials:** $\psi = \frac{u}{r}Y_{\ell m}$ turns 3D into a 1D problem with a centrifugal barrier. Hydrogen: $E_n = -13.6\,\text{eV}/n^2$, n^2-fold degenerate.

1 · Key features of QM L1 · Ch 1

- **Linearity.** If Ψ_1, Ψ_2 are solutions, so is $\alpha\Psi_1 + \beta\Psi_2$ — the Schrödinger eq. is linear, unlike Maxwell+matter or Newton in general.
- **Complex numbers are essential:** $i\hbar\partial_t\Psi = \hat{H}\Psi$ has an explicit i; Ψ cannot be real for all t.
- **Loss of determinism.** Identical states can give different outcomes; QM predicts probabilities.
- **Superposition** $|\psi\rangle = \alpha|A\rangle + \beta|B\rangle$: a measurement gives A w.p. $|\alpha|^2$, B w.p. $|\beta|^2$ — never "half of each". Adding a state to itself gives the *same* state ($|A\rangle + |A\rangle \sim |A\rangle$); overall phase is unphysical.
- **Entanglement.** $|\psi\rangle = |u\rangle_1|u\rangle_2 + |d\rangle_1|d\rangle_2$ can't be written as $|\cdot\rangle_1 \otimes |\cdot\rangle_2$. Measuring 1 fixes 2 instantly; no signalling.
- Photon polarization: a photon at angle α passes an x-polarizer w.p. $\cos^2\alpha$, then is x-polarized.
- **Making atoms possible.** A classical orbiting electron radiates and spirals into the proton in $\sim 10^{-11}$ s. In QM, squeezing the electron raises its kinetic energy ($p \sim \hbar/r$), so a stable ground state of size a_0 exists.

2 · Photon interferometry L2 · Ch 2

Photon state in two arms: $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$, $|\alpha|^2+|\beta|^2=1$. A beam splitter is a **unitary 2×2** matrix (columns orthonormal), e.g.

$$\text{BS1} = \tfrac{1}{\sqrt2}\begin{pmatrix}-1 & 1\\ 1 & 1\end{pmatrix},\quad \text{BS2} = \tfrac{1}{\sqrt2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix},\quad \text{BS2}\cdot\text{BS1} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$$

Mach–Zehnder: photon in lower arm → output D_0 with prob 1 (interference). Blocking one arm destroys interference: each detector fires w.p. ¼, absorbed w.p. ½.

Elitzur–Vaidman bomb (live bomb = detector in one arm): explode ½, D_0 ¼ (inconclusive), D_1 ¼ → **live bomb found without photon touching it**. Dud: always D_0. Interaction-free measurement.

Phase shifter $e^{i\delta}$ in one arm: $P(D_0)$, $P(D_1)$ oscillate as $\cos^2(\delta/2)$, $\sin^2(\delta/2)$.

Toward perfect bomb detection (quantum Zeno). Put the photon in a cavity with a high-reflectivity splitter: each pass rotates its state by $\pi/2N$, so after N passes it has moved fully to the other side (dud). A live bomb on that side "measures" the photon every pass and resets it. Survival:

$$P_{\text{no boom}} = \left(\cos^2\frac{\pi}{2N}\right)^N \simeq 1 - \frac{\pi^2}{4N} \to 1$$

Photon still on the original side after N passes ⇒ bomb is live, and it almost never explodes.

3 · Particle nature of light, wave nature of matter L3 · Ch 2

$$E = h\nu = \hbar\omega,\qquad p = \frac{h}{\lambda} = \hbar k,\qquad E^2 = p^2c^2 + m^2c^4$$

$$\textbf{de Broglie: } \lambda = \frac{h}{p},\qquad \textbf{Photoelectric: } \hbar\omega = W + K_{\max}$$

$$\textbf{Compton: } \lambda_f - \lambda_i = \lambda_C(1-\cos\theta),\quad \lambda_C = \frac{h}{m_e c} \approx 2.43\,\text{pm}$$

- Photoelectric: $K_{\max}$ depends on ω not intensity; threshold $\omega_0 = W/\hbar$; no time lag. Intensity ∝ number of photons.
- Compton: photon–electron elastic collision; derive with 4-momentum conservation. Shift is independent of λ; visible only for X/γ-rays.
- Davisson–Germer: electron diffraction off nickel crystal confirms $\lambda = h/p$.
- Nonrel. $\lambda = h/\sqrt{2mK}$; electron: $\lambda[\text{nm}] \approx 1.226/\sqrt{K[\text{eV}]}$.

4 · Free-particle waves; Galilean transformations L4 · Ch 2–3

$$\Psi(x,t) = e^{i(kx-\omega t)},\quad p = \hbar k,\quad E = \hbar\omega = \frac{\hbar^2k^2}{2m}$$

$$v_{\text{phase}} = \frac{\omega}{k} = \frac{v}{2},\qquad v_{\text{group}} = \frac{d\omega}{dk}\Big|_{k_0} = \frac{\hbar k_0}{m} = v$$

- Choose $e^{i(kx-\omega t)}$ (not $\sin$/$\cos$, not $e^{-i(kx-\omega t)}$): a first-order-in-time equation must map a momentum state to itself; the convention $E>0 \Leftrightarrow e^{-iEt/\hbar}$.
- de Broglie waves are not Galilean-invariant (λ depends on frame) ⇒ Ψ is not directly measurable; under a boost Ψ picks up a (x,t)-dependent phase, $|\Psi|^2$ is invariant.
- **Stationary phase:** a packet $\int \Phi(k)e^{i(kx-\omega(k)t)}dk$ with Φ peaked at k_0 has its peak where $\frac{d}{dk}[kx-\omega t]_{k_0} = 0 \Rightarrow x = \omega'(k_0)t$.

5 · Schrödinger equation & wavefunction L5–6 · Ch 3

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\Psi$$

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x},\qquad [\hat{x},\hat{p}] = i\hbar,\qquad \hat{E} \leftrightarrow i\hbar\partial_t$$

Born rule: $\rho(x,t) = |\Psi(x,t)|^2$ is a probability density; $\int_{-\infty}^{\infty}|\Psi|^2dx = 1$. Requires $\Psi \to 0$ faster than $|x|^{-1/2}$.

Conservation of normalization holds iff $\hat{H}$ is Hermitian (V real).

$$\textbf{Current: } J = \frac{\hbar}{2mi}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right) = \frac{\hbar}{m}\,\text{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)$$

$$\frac{\partial\rho}{\partial t} + \frac{\partial J}{\partial x} = 0,\qquad \frac{dP_{ab}}{dt} = J(a,t) - J(b,t)$$

$$\textbf{3D: } \vec{J} = \frac{\hbar}{m}\text{Im}(\Psi^*\nabla\Psi),\quad \partial_t\rho + \nabla\cdot\vec{J} = 0$$

- Plane wave Ae^{ikx}: $J = |A|^2\hbar k/m$ = density × velocity. Real Ψ (up to const phase) ⇒ $J = 0$.
- Units: $[\Psi] = L^{-1/2}$ (1D), $L^{-3/2}$ (3D); $[J] = T^{-1}$ (1D).

6 · Fourier, wavepackets & momentum space L7–8 · Ch 4–5

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int\Phi(k)e^{ikx}dk,\qquad \Phi(k) = \frac{1}{\sqrt{2\pi}}\int\Psi(x,0)e^{-ikx}dx$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int\Phi(k)\,e^{i(kx-\omega(k)t)}dk,\quad \omega = \frac{\hbar k^2}{2m}$$

$$\textbf{Parseval: } \int|\Psi(x)|^2dx = \int|\Phi(k)|^2dk\quad \left(=\int|\tilde{\Phi}(p)|^2dp\right)$$

$$\tilde{\Phi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int\Psi(x)e^{-ipx/\hbar}dx,\qquad \Delta x\,\Delta k \gtrsim 1$$

Free evolution recipe: $\Psi(x,0) \xrightarrow{\text{FT}} \Phi(k) \xrightarrow{\times e^{-i\omega(k)t}} \xrightarrow{\text{FT}^{-1}} \Psi(x,t)$.

Shape change comes from the k^2 term in $\omega(k)$: expand $\omega(k) = \omega_0 + \omega'(k-k_0) + \frac{1}{2}\omega''(k-k_0)^2$. Packet distorts when $\frac{\hbar t}{2m}(\Delta k)^2 \sim 1$, i.e. $t \sim m(\Delta x)^2/\hbar$.

Gaussian packet $\Psi(x,0) = \frac{1}{(2\pi)^{1/4}\sqrt{a}}e^{-x^2/4a^2}$, $\Delta x(0) = a$, $\Delta p = \frac{\hbar}{2a}$ (minimum uncertainty):

$$\Delta x(t) = a\sqrt{1+\left(\frac{\hbar t}{2ma^2}\right)^2},\qquad \Delta p \text{ constant}$$

FT of a Gaussian of width a is a Gaussian of width $\propto 1/a$. Momentum distribution of a free particle never changes.

Expectation values $\langle\hat{Q}\rangle = \int\Psi^*\hat{Q}\Psi\,dx$. E.g. $\langle\hat{p}\rangle = \int\Psi^*\frac{\hbar}{i}\Psi'dx = \int p|\tilde{\Phi}(p)|^2dp$.

$$\frac{d\langle\hat{Q}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$$

Ehrenfest: $\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m},\qquad \frac{d\langle\hat{p}\rangle}{dt} = -\left\langle\frac{\partial V}{\partial x}\right\rangle$

Note $\langle V'(x)\rangle \neq V'(\langle x\rangle)$ in general (equal for V at most quadratic).

7 · Observables, Hermitian operators, uncertainty L9 · Ch 5

Inner product $(\phi,\psi)=\int \phi^*\psi\,dx$. Hermitian: $(\phi,\hat{Q}\psi)=(\hat{Q}\phi,\psi)\ \forall\ \phi,\psi$. $\hat{x}$, $\hat{p}$, $\hat{H}$ are Hermitian; $\hat{p}$'s hermiticity uses integration by parts + decay at ∞.

- Expectation values of Hermitian operators are **real**.
- Eigenvalues are real; eigenfunctions with distinct eigenvalues are **orthogonal**; eigenfunctions form a **complete** basis: $\Psi=\sum_i \alpha_i\psi_i$, $\alpha_i=(\psi_i,\Psi)$.

Measurement postulate. Measuring $\hat{Q}$ on $\Psi=\sum_i \alpha_i\psi_i$ yields eigenvalue q_i with probability $|\alpha_i|^2$, and the state collapses to ψ_i. $\sum_i|\alpha_i|^2=1$, $\langle\hat{Q}\rangle=\sum_i q_i|\alpha_i|^2$.

$$(\Delta Q)^2=\langle\hat{Q}^2\rangle-\langle\hat{Q}\rangle^2=\langle(\hat{Q}-\langle\hat{Q}\rangle)^2\rangle=\int|(\hat{Q}-\langle\hat{Q}\rangle)\Psi|^2\geq 0$$

$\Delta Q=0 \iff \Psi$ is an eigenstate of $\hat{Q}$.

$$\Delta A\,\Delta B\ \geq\ \left|\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right|\ \Rightarrow\ \Delta x\,\Delta p\geq\frac{\hbar}{2}$$

$$\textbf{Energy–time: } \Delta E\,\Delta t\geq\frac{\hbar}{2},\qquad \Delta t\equiv\frac{\Delta Q}{|d\langle\hat{Q}\rangle/dt|}$$

Estimating ground energies: set $p\sim\hbar/\Delta x$ in $E(\Delta x)=\frac{\hbar^2}{2m\Delta x^2}+V(\Delta x)$ and minimize. Works for SHO, hydrogen (a_0), etc.

8 · Stationary states & the TISE L10 · Ch 6

$$\Psi(x,t)=\psi(x)e^{-iEt/\hbar},\qquad -\frac{\hbar^2}{2m}\psi''+V(x)\psi=E\psi$$

$$\Psi(x,t)=\sum_n c_n\,\psi_n(x)\,e^{-iE_nt/\hbar},\qquad c_n=\int\psi_n^*(x)\Psi(x,0)\,dx$$

$$\sum_n|c_n|^2=1,\qquad \langle\hat{H}\rangle=\sum_n|c_n|^2E_n\ \textbf{(time-indep.)}$$

- Stationary states: $|\Psi|^2$ and all $\langle\hat{Q}\rangle$ (time-indep. $\hat{Q}$) are constant. $\Delta H=0$.
- E is real (normalizability). Normalizable solutions require $E>V_{\min}$.
- **Superposition of two energies:** $|\Psi|^2$ oscillates at $\omega=(E_1-E_2)/\hbar$.

$V(x)$ has…	ψ	ψ'
finite jumps	continuous	continuous
delta function	continuous	jumps
hard wall (∞)	continuous, $\psi=0$ at wall	jumps

Particle on a circle ($x\sim x+L$): $\psi_n=\frac{1}{\sqrt{L}}e^{2\pi inx/L}$, $E_n=\frac{2n^2\hbar^2n^2}{mL^2}$, $n\in\mathbb{Z}$; $\pm n$ degenerate (allowed: no 1D non-degeneracy theorem on a circle). $p_n=2\pi\hbar n/L$.

9 · Square wells L11 · Ch 6

Infinite well, $0<x<a$

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a},\qquad E_n=\frac{n^2\pi^2\hbar^2}{2ma^2},\quad n=1,2,\dots$$

(Symmetric well $-a/2<x<a/2$: even $\cos$ states for odd n, odd $\sin$ states for even n.) ψ_n has $n-1$ nodes; $\langle x\rangle=a/2$.

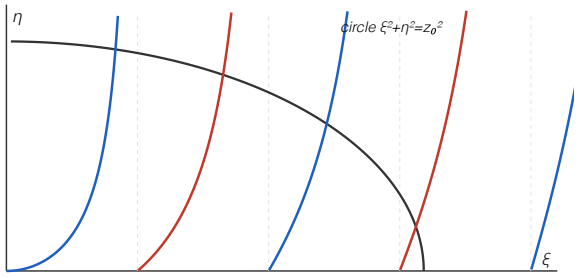
Finite well, $V=-V_0$ for $|x|<a$ $(-V_0<E<0)$

Inside $\psi\sim\cos kx$ or $\sin kx$, $k^2=\frac{2m(V_0+E)}{\hbar^2}$; outside $\psi\sim e^{-\kappa|x|}$, $\kappa^2=\frac{2m|E|}{\hbar^2}$. Let $\xi=ka$, $\eta=\kappa a$:

$$\xi^2+\eta^2=z_0^2\equiv\frac{2mV_0a^2}{\hbar^2}$$

$$\textbf{even: } \eta=\xi\tan\xi,\qquad \textbf{odd: } \eta=-\xi\cot\xi$$

Number of bound states $=\lceil 2z_0/\pi\rceil$; always ≥ 1 (even) bound state. $E=-V_0+\frac{\hbar^2\xi^2}{2ma^2}$.



Graphical solution: circle radius z_0 (here 5) vs. $\xi\tan\xi$ (blue, even) and $-\xi\cot\xi$ (red, odd). Each crossing = a bound state.

Deep well ($z_0\to\infty$): $\xi\to n\pi/2$, recovers infinite well of width $2a$. Shallow ($z_0\ll 1$): one state, $\eta\approx z_0^2$.

10 · General properties of 1D bound states L12 · Ch 7

1. **No degenerate bound states** in 1D (Wronskian argument).
2. Energy eigenstates can be chosen **real**; a 1D bound state is real up to a constant phase.
3. If $V(-x)=V(x)$: eigenstates can be chosen even/odd; **bound states are automatically even or odd**.
4. **Node theorem:** the n-th bound state ($n=1$ ground) has $n-1$ nodes; ground state has none.

$$\frac{\psi''}{\psi}=\frac{2m}{\hbar^2}\big(V(x)-E\big)$$

$E>V$ (allowed): ψ curves **toward** axis, oscillates. $E<V$ (forbidden): curves **away**, exponential.
Turning points $E=V(x)$: inflection points of ψ.

Slowly varying V: local momentum $p(x)=\sqrt{2m(E-V(x))}$, local wavelength $\lambda(x)=h/p(x)$. Where $E-V$ is larger: shorter wavelength and **smaller amplitude**, amplitude $\propto 1/\sqrt{p(x)}$ (classical particle spends less time there). Validity: $|d\lambda/dx|\ll 1$. Quantization estimate $\int_a^b k(x)\,dx\approx(n-\frac{1}{2})\pi$.
Shooting method: fix $\psi(0),\psi'(0)$ (by parity), integrate outward; ψ blows up $\pm\infty$ unless E = eigenvalue. Sign flip of the blow-up brackets an eigenvalue.

Four general tools (Ch 7.6–7.9)

- **Remove units:** $x=Lu$, $E=\frac{\hbar^2}{mL^2}\varepsilon$ with L built from the potential; only unit-free combinations (like z_0) matter.
- **Virial:** in a stationary state ($[\hat{H},\hat{x}\hat{p}]\rangle=0\Rightarrow 2\langle T\rangle=\langle xV'(x)\rangle$. For $V\propto|x|^k$: $2\langle T\rangle=k\langle V\rangle$ (SHO: $T=V=E/2$; Coulomb: $E=-\langle T\rangle=\frac{1}{2}\langle V\rangle$).
- **Variational:** $E_{gs}\leq\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$ for any trial ψ. Any 1D potential with $\int V\,dx<0$ (and $V\to 0$) has a bound state.
- **Hellmann–Feynman:** $\frac{\partial E_n}{\partial\lambda}=\langle\psi_n|\frac{\partial\hat{H}}{\partial\lambda}|\psi_n\rangle$. E.g. differentiate hydrogen E_n w.r.t. e^2 to get $\langle 1/r\rangle$.

11 · Delta-function & linear potentials L13 · Ch 6

$V=-\alpha\,\delta(x)$, $\alpha>0$:

$$\psi'(0^+)-\psi'(0^-)=-\frac{2m\alpha}{\hbar^2}\psi(0)$$

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

Exactly **one** bound state. General: integrate TISE over $(-\epsilon,\epsilon)$ to get the jump in ψ'. Units: $[\delta(x)]=1/L$, so $[\alpha]=E\cdot L$. Scattering off $-\alpha\delta$: $T=\frac{1}{1+m\alpha^2/(2\hbar^2E)}$.

Linear potential $V=gx$ $(x>0$, wall at $0)$

Easiest in **momentum space**, where the TISE is first order: $i\hbar g\varphi'(p)=\big(E-\frac{p^2}{2m}\big)\varphi\Rightarrow\varphi\propto\exp\big[-\frac{i}{\hbar g}\big(Ep-\frac{p^3}{6m}\big)\big]$. In position space this is an Airy function:

$$\psi(x)\propto\mathrm{Ai}\Big(\frac{x-E/g}{\ell}\Big),\quad \ell=\Big(\frac{\hbar^2}{2mg}\Big)^{1/3},\qquad E_n=a_n\Big(\frac{\hbar^2g^2}{2m}\Big)^{1/3}$$

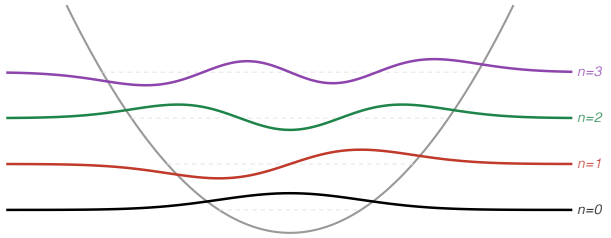
a_n = n-th zero of Ai at $-a_n$: $2.338,\ 4.088,\ 5.521,\dots$ Uses: neutrons bouncing in gravity ($V=mgx$), WKB near turning points.

12 · Harmonic oscillator L13–15 · Ch 9

$$V=\tfrac{1}{2}m\omega^2x^2,\qquad E_n=\hbar\omega\big(n+\tfrac{1}{2}\big),\quad n=0,1,2,\dots$$

$$\psi_n(x)=\Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4}\frac{1}{\sqrt{2^nn!}}H_n(u)\,e^{-u^2/2},\quad u=\frac{x}{L},\ L=\sqrt{\frac{\hbar}{m\omega}}$$

$H_0=1$, $H_1=2u$, $H_2=4u^2-2$, $H_3=8u^3-12u$. Parity $(-1)^n$. Series method: $\psi=h(u)e^{-u^2/2}$; series must terminate $\Rightarrow\mathcal{E}\equiv\frac{2E}{\hbar\omega}=2n+1$.



$\psi_0\dots\psi_3$ drawn at height E_n inside $V=\frac{1}{2}m\omega^2x^2$.

Algebraic method

$$\hat{a}=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}+\frac{i\hat{p}}{m\omega}\right),\quad \hat{a}^\dagger=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}-\frac{i\hat{p}}{m\omega}\right),\quad [\hat{a},\hat{a}^\dagger]=1$$

$$\hat{x}=\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger),\qquad \hat{p}=i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger-\hat{a})$$

$$\hat{H}=\hbar\omega\left(\hat{N}+\tfrac{1}{2}\right),\quad \hat{N}=\hat{a}^\dagger\hat{a},\quad [\hat{N},\hat{a}^\dagger]=\hat{a}^\dagger,\ [\hat{N},\hat{a}]=-\hat{a}$$

$$\hat{a}^\dagger\varphi_n=\sqrt{n+1}\,\varphi_{n+1},\quad \hat{a}\varphi_n=\sqrt{n}\,\varphi_{n-1},\quad \varphi_n=\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\varphi_0$$

- Ground state: $\hat{a}\varphi_0=0\Rightarrow\varphi_0\propto e^{-m\omega x^2/2\hbar}$. Spectrum bounded below because $\langle\hat{H}\rangle\geq\frac{1}{2}\hbar\omega$ (since $\langle\hat{a}^\dagger\hat{a}\rangle=\|\hat{a}\psi\|^2\geq 0$).
- $\hat{a}^\dagger$ raises E by $\hbar\omega$; $\hat{a}$ lowers. $[\hat{H},\hat{a}^\dagger]=\hbar\omega\,\hat{a}^\dagger$.
- $\langle x\rangle_n=\langle p\rangle_n=0$; $\langle x^2\rangle_n=\frac{\hbar}{m\omega}(n+\frac{1}{2})$; $\langle p^2\rangle_n=m\hbar\omega(n+\frac{1}{2})$; $\Delta x\Delta p=\hbar(n+\frac{1}{2})$. Virial: $\langle T\rangle=\langle V\rangle=E_n/2$.

Trick: to get $\langle x^k\rangle$, $\langle p^k\rangle$, write in $\hat{a},\hat{a}^\dagger$; only terms with equal numbers of $\hat{a}$ and $\hat{a}^\dagger$ survive in $\langle n|\cdot|n\rangle$.

13 · Step potential & 1D scattering L16–17 · Ch 8

$V=0$ for $x<0$, V_0 for $x>0$. Incident from left: $\psi=Ae^{ikx}+Be^{-ikx}$ ($x<0$), $Ce^{i\bar{k}x}$ ($x>0$).

$E>V_0$: $k=\frac{\sqrt{2mE}}{\hbar}$, $\bar{k}=\frac{\sqrt{2m(E-V_0)}}{\hbar}$

$$\frac{B}{A}=\frac{k-\bar{k}}{k+\bar{k}},\quad \frac{C}{A}=\frac{2k}{k+\bar{k}}$$

$$R=\left|\frac{B}{A}\right|^2=\left(\frac{k-\bar{k}}{k+\bar{k}}\right)^2,\qquad T=\frac{\bar{k}}{k}\left|\frac{C}{A}\right|^2=\frac{4k\bar{k}}{(k+\bar{k})^2}$$

$R+T=1$ (current conservation, $J_A=J_B+J_C$).

Pitfall: $T\neq|C/A|^2$ — transmission is a ratio of currents, include the velocity factor $\bar{k}/k$. Classically $R=0$ for $E>V_0$; QM reflects even off a step down.

$E<V_0$: $\psi=Ce^{-\kappa x}$, $\kappa=\frac{\sqrt{2m(V_0-E)}}{\hbar}$

$$\frac{B}{A}=-\frac{\kappa+ik}{\kappa-ik}=-e^{2i\delta(E)}\ \Rightarrow\ R=1,\ T=0$$

Penetration depth $\sim 1/\kappa$; reflected packet is **delayed** by $\Delta t=2\hbar\,\delta'(E)$.

Finite square well (scattering, $E>0$), $V=-V_0$ on width $2a$

$$\frac{1}{T}=1+\frac{V_0^2}{4E(E+V_0)}\sin^2(2k_2a),\quad k_2=\frac{\sqrt{2m(E+V_0)}}{\hbar}$$

Resonant transmission $T=1$ when $2k_2a=n\pi$: well width = integer # half-wavelengths (the would-be bound states of an infinite well of width $2a$).

Ramsauer–Townsend effect: slow electrons (~1 eV) pass almost freely through noble-gas atoms — resonant transmission; no classical explanation.

Barrier V_0 of width $2a$, $E<V_0$ (tunneling)

$$\frac{1}{T}=1+\frac{V_0^2}{4E(V_0-E)}\sinh^2(2\kappa a)\xrightarrow{\kappa a\gg 1}T\approx\frac{16E(V_0-E)}{V_0^2}e^{-4\kappa a}$$

(For $E>V_0$ replace $\sinh\to\sin$, $\kappa\to\bar{k}$, $V_0-E\to E-V_0$.)

Wavepackets: peak of $\int\Phi(k)e^{i(kx-\omega t)}e^{i\phi(k)}$ shifted by $\phi'(k_0)$ — phases of B/A, C/A give spatial shifts/time delays.

14 · Scattering on the half-line; phase shifts L18 · Ch 29

Wall at $x=0$, $V(x)=0$ for $x>R$. Free solution $\phi=\sin kx$. With potential, for $x>R$:

$$\psi(x)=e^{i\delta}\sin(kx+\delta)=\tfrac{1}{2i}\left(-e^{-ikx}+e^{ikx+2i\delta}\right)$$

$$\psi=\phi+\psi_s,\qquad \psi_s=A_se^{ikx},\quad A_s=e^{i\delta}\sin\delta,\quad |A_s|^2=\sin^2\delta$$

$$\textbf{Time delay: }\Delta t=2\hbar\frac{d\delta}{dE}=\frac{2m}{\hbar k}\frac{d\delta}{dk}$$

- $\delta(E)$ real (current conservation: outgoing $|\cdot|$ = incoming). δ and $\delta\pm\pi$ give the same ψ.
- $\delta>0$: wave pulled in by δ/k — **attractive**. $\delta<0$: pushed out — **repulsive**.
- Hard wall at $x=a$: $\delta=-ka$. $\Delta t<0$ possible (advance), bounded below.
- Square well ($V=-V_0$, $0<x<a$), $k'=\sqrt{2m(E+V_0)}/\hbar$: match $A\sin k'a=e^{i\delta}\sin(ka+\delta)\Rightarrow k\cot(ka+\delta)=k'\cot k'a$.
- Unit-free delay $\frac{1}{a}\frac{d\delta}{dk}$ = delay / free transit time.

15 · Levinson's theorem & resonances L19 · Ch 29

$$\textbf{Levinson: }N_b=\frac{1}{\pi}\left(\delta(0)-\delta(\infty)\right)$$

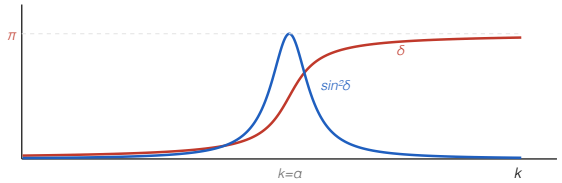
Number of bound states = phase-shift excursion / π. Proof: add a regulator wall at $x=L$, count states.

Resonance: δ increases rapidly by $\sim\pi$ near E_α; large time delay; $|A_s|^2=\sin^2\delta$ peaks at $\delta=\pi/2$. Physically: quasi-bound state trapped behind a barrier. Model:

$$\delta=\tan^{-1}\frac{\beta}{\alpha-k},\quad A_s=\frac{\beta}{\alpha-k-i\beta}\ \ (\text{pole at } k=\alpha-i\beta)$$

$$\textbf{Breit–Wigner: }|A_s|^2=\frac{\frac{1}{4}\Gamma^2}{(E-E_\alpha)^2+\frac{1}{4}\Gamma^2},\qquad \Gamma=\frac{2\alpha\beta\hbar^2}{m}$$

Γ = full width at half max. Lifetime $\tau=\hbar/\Gamma$; peak delay $\Delta t=4\hbar/\Gamma$.



Resonance near $k=\alpha$: phase δ jumps by π (red) while $\sin^2\delta$ (blue) peaks, width ∝ β.

16 · QM in 3D; angular momentum L20–21 · Ch 10

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V(\vec{r})\psi=E\psi,\quad \hat{\vec{p}}=\frac{\hbar}{i}\nabla,\quad [\hat{x}_i,\hat{p}_j]=i\hbar\delta_{ij}$$

$$\hat{\vec{L}}=\hat{\vec{r}}\times\hat{\vec{p}},\qquad \hat{L}_i=\epsilon_{ijk}\hat{x}_j\hat{p}_k\ \ \textbf{(Hermitian, no ordering issue)}$$

$$[\hat{L}_x,\hat{L}_y]=i\hbar\hat{L}_z\ (\text{+cyclic}),\quad [\hat{L}_i,\hat{L}_j]=i\hbar\epsilon_{ijk}\hat{L}_k$$

$$[\hat{L}_i,\hat{x}_j]=i\hbar\epsilon_{ijk}\hat{x}_k,\quad [\hat{L}_i,\hat{p}_j]=i\hbar\epsilon_{ijk}\hat{p}_k,\quad [\hat{L}_i,\hat{\vec{L}}^2]=0$$

- $\vec{r}^2$, $\vec{p}^2$, $\vec{r}\cdot\vec{p}$ are scalars: commute with every $\hat{L}_i$. Central $V(r)\Rightarrow[\hat{H},\hat{L}_i]=0$, $[\hat{H},\hat{L}^2]=0$.
- $\hat{L}_x,\hat{L}_y,\hat{L}_z$ mutually incompatible ⇒ choose CSCO $\{\hat{H},\hat{L}^2,\hat{L}_z\}$.
- $\hat{L}_i$ generate rotations (as $\hat{p}$ generates translations).

$$\hat{L}_z=\frac{\hbar}{i}\frac{\partial}{\partial\phi},\quad \hat{L}^2=-\hbar^2\left[\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta)+\frac{1}{\sin^2\theta}\partial_\phi^2\right]$$

$$\nabla^2=\frac{1}{r}\frac{\partial^2}{\partial r^2}r-\frac{\hat{L}^2}{\hbar^2r^2}$$

$$\hat{L}^2Y_{\ell m}=\hbar^2\ell(\ell+1)Y_{\ell m},\quad \hat{L}_zY_{\ell m}=\hbar mY_{\ell m}$$

$\ell=0,1,2,\ldots$; $m=-\ell,\ldots,\ell$ ($2\ell+1$ values); $Y_{\ell m}\propto e^{im\phi}P_\ell^m(\cos\theta)$; $\int Y^*_{\ell'm'}Y_{\ell m}d\Omega=\delta_{\ell\ell'}\delta_{mm'}$.

$Y_{\ell m}$	
Y_{00}	$\frac{1}{\sqrt{4\pi}}$
Y_{10}	$\sqrt{\frac{3}{4\pi}}\cos\theta$
$Y_{1,\pm1}$	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta\,e^{\pm i\phi}$

Cartesian ↔ ℓ: $\ell=1\leftrightarrow x,y,z$: $z\propto rY_{10}$, $x\pm iy\propto rY_{1,\pm1}$. Single-valuedness in $\phi\Rightarrow m\in\mathbb{Z}$.

Radial equation

$$\psi_{E\ell m}=\frac{u_{E\ell}(r)}{r}Y_{\ell m}(\theta,\phi),\qquad -\frac{\hbar^2}{2m}u''+V_{\text{eff}}(r)\,u=E\,u$$

$$V_{\text{eff}}=V(r)+\frac{\hbar^2\,\ell(\ell+1)}{2mr^2},\qquad \int_0^\infty|u|^2dr=1$$

$$u(0)=0,\qquad u\sim r^{\ell+1}\ \ (r\to 0,\ V\text{ less singular than }1/r^2)$$

- A 1D problem on the half-line $r>0$ with a hard wall at 0 — 1D results apply (no degeneracy for fixed ℓ; node counting).
- Label states by (n,ℓ); each has $2\ell+1$ degeneracy from m. For fixed ℓ, energy increases with # radial nodes. For fixed n_r, E increases with ℓ (centrifugal barrier).
- Large r with $V\to 0$, $E<0$: $u\sim e^{-\kappa r}$.
- 3D isotropic SHO: $E=\hbar\omega(N+\frac{3}{2})$, deg. $\frac{1}{2}(N+1)(N+2)$; $\ell=N,N-2,\ldots$
- Infinite spherical well (radius a), $\ell=0$: $u=\sin kr$, $E=\frac{n^2\pi^2\hbar^2}{2ma^2}$. Finite spherical well, $\ell=0$ ↔ odd states of 1D well ⇒ bound state needs $z_0>\pi/2$.

17 · Hydrogen atom L21–22 · Ch 11

Two-body → one-body: $\vec{P}=\vec{p}_p+\vec{p}_e$, $\vec{R}=\frac{m_p\vec{x}_p+m_e\vec{x}_e}{M}$; relative $\vec{x}=\vec{x}_e-\vec{x}_p$, $\vec{p}=\frac{m_p\vec{p}_e-m_e\vec{p}_p}{M}$. $[x_i,p_j]=[X_i,P_j]=i\hbar\delta_{ij}$, cross commutators vanish. $\hat{H}=\frac{\hat{P}^2}{2M}+\frac{\hat{p}^2}{2\mu}+V(r)$, $\mu=\frac{m_em_p}{m_e+m_p}\approx m_e$. CM moves freely.

$V=-\frac{e^2}{r}$ (Gaussian; $e^2\to\frac{q^2}{4\pi\epsilon_0}$ in SI)

$$a_0=\frac{\hbar^2}{me^2}\approx 0.529\,\text{Å},\qquad \alpha=\frac{e^2}{\hbar c}\approx\frac{1}{137}$$

$$E_n=-\frac{e^2}{2a_0}\frac{1}{n^2}=-\frac{\alpha^2mc^2}{2n^2}=-\frac{13.6\,\text{eV}}{n^2}$$

$$n=N+\ell+1,\quad \ell=0,1,\ldots,n-1,$$

$$\textbf{degeneracy}=\textstyle\sum_{\ell=0}^{n-1}(2\ell+1)=n^2$$

N = number of radial nodes. Accidental degeneracy in ℓ (hidden symmetry: Runge–Lenz vector). $u\sim r^{\ell+1}e^{-r/na_0}\times$ polynomial of degree N.

$n\ell$	$R_{n\ell}(r)$ ($\psi = RY_{\ell m}$, $R = u/r$)
1s	$2a_0^{-3/2}e^{-r/a_0} \to \psi_{100} = \frac{e^{-r/a_0}}{\sqrt{\pi a_0^3}}$
2s	$\frac{1}{\sqrt{2}}a_0^{-3/2}\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}$
2p	$\frac{1}{2\sqrt{6}}a_0^{-3/2}\frac{r}{a_0}e^{-r/2a_0}$

- Ground state: $\langle r\rangle = \frac{3}{2}a_0$, most probable $r = a_0$; $\langle V\rangle = 2E_1$, $\langle T\rangle = -E_1$ (virial for $1/r$).
- Spectral lines: $\frac{1}{\lambda} = R_\infty\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$, $R_\infty \approx 1.097\times10^7\ \mathrm{m}^{-1}$. Lyman ($n_f = 1$, UV), Balmer ($n_f = 2$, visible).
- Unit-free radial: $\rho = r/a_0$, energy $E = -\frac{e^2}{2a_0}\frac{1}{\nu^2}$; series terminates iff $\nu = n \in \mathbb{Z}$.
- **Orbits & degeneracy:** for fixed n, $\ell = n-1$ ↔ circular orbit ($u \propto r^n e^{-r/na_0}$, peak at n^2a_0); small ℓ ↔ eccentric orbits. $\langle r\rangle_{n\ell} = \frac{a_0}{2}\left[3n^2 - \ell(\ell+1)\right]$.
- **Rydberg atoms** ($n \gg 1$): size $\sim n^2a_0$; spacing $E_{n+1} - E_n \simeq \frac{2\,\mathrm{Ry}}{n^3}$, which equals $\hbar\times$ the classical orbital frequency (correspondence principle).

18 · Math toolkit

$$\int_{-\infty}^{\infty} e^{-ax^2+bx}dx = \sqrt{\frac{\pi}{a}}\,e^{b^2/4a}, \qquad \int x^2e^{-ax^2}dx = \frac{\sqrt{\pi}}{2a^{3/2}}$$

$$\int_0^\infty x^n e^{-x/a}dx = n!\,a^{n+1}, \qquad \int_0^a \sin^2\frac{n\pi x}{a}dx = \frac{a}{2}$$

$$\delta(x) = \frac{1}{2\pi}\int e^{ikx}dk, \quad \delta(ax) = \frac{\delta(x)}{|a|}, \quad \int f(x)\delta(x-x_0)dx = f(x_0)$$

Commutators: $[\hat A, \hat B\hat C] = [\hat A,\hat B]\hat C + \hat B[\hat A,\hat C]$; $[\hat x, f(\hat p)] = i\hbar f'(\hat p)$; $[\hat p, f(\hat x)] = -i\hbar f'(\hat x)$; $[\hat x,\hat p^2] = 2i\hbar\hat p$; $(\hat A\hat B)^\dagger = \hat B^\dagger\hat A^\dagger$; $e^{\hat A}\hat B e^{-\hat A} = \hat B + [\hat A,\hat B] + \frac{1}{2!}[\hat A,[\hat A,\hat B]] + \dots$

Hermitian checks: $\hat Q$, $\hat R$ Hermitian ⇒ $i[\hat Q,\hat R]$ Hermitian; $\hat Q\hat R$ Hermitian iff they commute; $\hat A^\dagger\hat A$ has $\langle\cdot\rangle \ge 0$.

Trig/hyp: $\cot(A+B) = \frac{\cot A\cot B - 1}{\cot A + \cot B}$; $\sinh^2 + 1 = \cosh^2$; $\tan^{-1}$ jumps by π across a pole.

19 · Constants & scales

$\hbar$	1.055×10^{-34} J·s $= 6.58\times10^{-16}$ eV·s
hc / $\hbar c$	**1240** eV·nm / **197.3** MeV·fm $=$ **1973** eV·Å
m_ec^2 / m_pc^2	**0.511** MeV / **938.3** MeV
a_0, α	**0.529** Å, $1/137.036$
e^2 (Gaussian)	$\alpha\hbar c = 14.4$ eV·Å
Ry	**13.6** eV $= \frac{1}{2}\alpha^2m_ec^2$
k_BT (300 K)	$\approx \frac{1}{40}$ eV
1 eV	1.602×10^{-19} J

20 · Problem-solving playbook

Bound-state problem: (1) sketch V, mark E & turning points; (2) write ψ in each region ($e^{\pm ikx}$ or $e^{\pm\kappa x}$), kill growing exponentials; (3) use parity if V even; (4) match ψ, ψ' (or the δ-jump) at boundaries; (5) get transcendental eq. → unit-free variables (z_0, ξ, η); (6) count nodes to label states.

Scattering problem: incident Ae^{ikx} + reflected Be^{-ikx} on left, only $Ce^{ik'x}$ on right; match; $R = |B/A|^2$, $T = \frac{k'}{k}|C/A|^2$; check $R+T=1$. Phases → time delays via $\Delta t = 2\hbar\,d\delta/dE$.

Time evolution: expand $\Psi(x,0) = \sum c_n\psi_n$, attach $e^{-iE_nt/\hbar}$. For free particles, go through $\Phi(k)$. Probabilities of energies are $|c_n|^2$ — time-independent.

Sanity checks: units; $\hbar\to0$ classical limit; $R,T\in[0,1]$; $E_{\text{ground}} > V_{\min}$; nodes = $n-1$; $\Delta x\Delta p \ge \hbar/2$; normalization $\int|\psi|^2 = 1$ (3D: $\int|u|^2dr = 1$).

Common mistakes: forgetting $1/r$ in $\psi = u/r$ or r^2 in $d^3x = r^2dr\,d\Omega$; using $|C/A|^2$ for T; assuming $\langle V'(x)\rangle = V'(\langle x\rangle)$; normalizing with a time phase still attached to only some terms; treating $\hat L_x$ & $\hat L_z$ as simultaneously measurable; wrong sign in δ-function jump.