

Ph12b Book Notes
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Chapter 1

General Notes

1. Rayleigh-Jeans approximation: $u(\nu) = \frac{8\pi\nu^2}{c^3} k_B T$. Where $u(\nu)$ is the energy per frequency interval per unit volume. Total energy per unit volume is $U = \int_0^\infty u(\nu) d\nu$.

2. Planck's equation:

$$u(\nu) = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{h\nu/k_B T} - 1}$$

3. Bohr radius: $r_n = \frac{n^2 \hbar^2}{m e^2}$.

4. Rydberg constant: $\frac{m e^4}{2 \hbar^2} = 13.6 eV$.

5. Schrodinger's Equation (Time-dependent):

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

6. Gaussian (square of the Gaussian wave function):

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

7. Solution to initial value problem:

$$\psi(\vec{r}, t) = \exp\left(\frac{-it\hat{H}}{\hbar}\right) \psi(\vec{r}, 0) = \hat{U} \psi(\vec{r}, 0)$$

Note that the eigenvalue equation for this unitary operator is:

$$\exp\left(\frac{-i\hat{H}t}{\hbar}\right) \psi_n = \exp\left(\frac{-iE_n t}{\hbar}\right) \psi_n$$

8. Position displacement operator:

$$\hat{D}[f(x)] = \exp\left(\frac{idxp_x}{\hbar}\right) f(x) = f(x + dx)$$

9. Angular displacement operator:

$$\hat{R}_{\Delta\phi} = \exp\left(\frac{i\Delta\vec{\phi} \cdot \hat{L}}{\hbar}\right)$$

where \hat{L} is the vector operator for the total angular momentum of the system.

10. Schrodinger's Equation (time-independent)

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

11. Expectation Value

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

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \Psi^* Q(x, p) \Psi dx$$

12. Standard Deviation

$$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$$

$$\sigma^2 = \langle (\hat{Q} - \langle Q \rangle)^2 \rangle$$

13. Momentum

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

14. Position

$$\langle x \rangle = \int_{-\infty}^{\infty} \Phi^* \left(\frac{-\hbar}{i} \frac{\partial}{\partial p} \right) \Phi dp$$

where $\Phi(p, t)$ is the momentum space wave function.

15. Velocity:

$$v_p = \frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{p}{2m} = \frac{v_{cl}}{2}$$

$$v_g = \frac{\partial\omega}{\partial k} = \frac{p}{m} = v_{cl}$$

16. Position and Momentum space correspondence:

Position space: $\hat{Q}(x, p) \rightarrow \hat{Q} \left(x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right)$

k-space: $\hat{Q}(x, p) \rightarrow \hat{Q} \left(-i \frac{\partial}{\partial k}, \hbar k \right)$

Momentum space: $\hat{Q}(x, p) \rightarrow \left(\frac{-\hbar}{i} \frac{\partial}{\partial p}, p \right)$

17. Hamiltonian Operator

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

18. Hamilton's Equations:

$$\frac{\partial H}{\partial x} = -\dot{p}_x \quad \frac{\partial H}{\partial p_x} = \dot{x}$$

$$\frac{\partial H}{\partial y} = -\dot{p}_y \quad \frac{\partial H}{\partial p_y} = \dot{y}$$

$$\frac{\partial H}{\partial z} = -\dot{p}_z \quad \frac{\partial H}{\partial p_z} = \dot{z}$$

$$\frac{\partial H}{\partial \theta} = -\dot{p}_\theta \quad \frac{\partial H}{\partial p_\theta} = \dot{\theta}$$

$$\frac{\partial H}{\partial \phi} = -\dot{p}_\phi \quad \frac{\partial H}{\partial p_\phi} = \dot{\phi}$$

$$\frac{\partial H}{\partial r} = -\dot{p}_r \quad \frac{\partial H}{\partial p_r} = \dot{r}$$

In general:

$$\frac{\partial H}{\partial q_l} = -\dot{p}_l, \quad \frac{\partial H}{\partial p_l} = \dot{q}_l, \quad l = 1, 2, \dots, N$$

19. General solution to TISE:

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

20. Infinite square well: Boundary conditions: $\psi(0) = \psi(a) = 0$. Energy: $E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{\hbar^2 k_n^2}{2m}$, $k_n = \frac{n\pi}{a}$. One solution:

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

21. Orthonormality: $\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$.

22. Delta function orthogonality:

$$\langle \psi_k | \psi_{k'} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ix(k'-k)} dx = \delta(k' - k)$$

23. Fourier decomposition. Given $f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$, obtain $c_n = \int \psi_n(x)^* f(x) dx$.

24. General solution to stationary states:

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

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

25. Energy expectation value: $\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$.

26. TISE for harmonic oscillator:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi \implies \frac{1}{2m} [p^2 + (m\omega x)^2] \psi = E \psi$$

27. Canonical commutation relation: $[x, p] = i\hbar$

28. Ground state of harmonic oscillator:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}, E_0 = \frac{1}{2}\hbar\omega$$

29. Energy expectation values:

$$\langle T \rangle = \frac{\langle p^2 \rangle}{2m}$$

$$\langle V \rangle = \frac{1}{2} m \omega^2 \langle x^2 \rangle$$

30. Normalised stationary states for harmonic oscillator:

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

31. Hermite polynomials:

$$H_0 = 1$$

$$H_1 = 2\xi$$

$$H_2 = 4\xi^2 - 2$$

$$\text{Rodrigues formula: } H_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2} \implies H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi)$$

$$\frac{dH_n}{d\xi} = 2n H_{n-1}(\xi)$$

$$\text{Generating function: } e^{-z^2 + 2z\xi} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(\xi)$$

32. Plancherel's theorem:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)e^{ikx} dk \iff F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{-ikx} dx$$

Say that $F(k)$ is the Fourier transform of $f(x)$ and that $f(x)$ is the inverse Fourier transform of $F(k)$.

33. The Fourier transform of a Gaussian is also a Gaussian. A Gaussian in space with width Δx will be a Gaussian in wavenumber with width $\Delta k = \frac{1}{2\Delta x}$.

34. Wave packet solution to Free Particle system:

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

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

35. Delta function well bound state: Given $V(x) = -\alpha\delta(x)$, $\alpha > 0$,

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

36. Reflection and Transmission coefficients (relative probability that a particle will be reflected/transmitted):

$$R = \frac{1}{1 + 2\hbar^2 E/m\alpha^2}$$

$$T = \frac{1}{1 + m\alpha^2/2\hbar^2 E}$$

37. Strategies for solving potential distributions:

- (a) Make solution guess in each region (complex exponentials or trigo functions)
- (b) Impose boundary conditions (wavefunction vanishes at infinity, continuity of wavefunction across boundaries, continuity of derivative across boundaries), no incoming wave from the other side for scattering states)
- (c) Normalisation (or infinite superposition for scattering states)

38. Hilbert Space: A (real or complex) complete inner product space. Complete: every Cauchy sequence of functions converges to a function that is also in the space.

39. Inner product of two functions: $\langle f|g \rangle = \int_a^b f(x)^*g(x)dx$.

40. Conjugate of inner product (skew symmetry): $\langle g|f \rangle = \langle f|g \rangle^*$

41. Inner product is positive semidefinite: $\langle f|f \rangle \geq 0$, $\langle f|f \rangle = 0 \iff f(x) = 0$.

42. Inner product is antilinear in first element: $\langle ax_1 + bx_2|y \rangle = a^*\langle x_1|y \rangle + b^*\langle x_2|y \rangle$.

43. Inner product is linear in the second element: $\langle x|ay_1 + by_2 \rangle = a\langle x|y_1 \rangle + b\langle x|y_2 \rangle$.

44. Integral Schwarz inequality: $\left| \int_a^b f(x)^*g(x)dx \right| \leq \sqrt{\int_a^b |f(x)|^2 dx \int_a^b |g(x)|^2 dx}$.

45. Expectation value: $\langle Q \rangle = \int \Psi^* \hat{Q} \Psi dx = \langle \Psi | \hat{Q} \Psi \rangle = \sum_i \langle \Psi | \omega_i \rangle \langle \omega_i | \Psi \rangle \omega_i = \sum_i |\langle \omega_i | \Psi \rangle|^2 \omega_i$.

46. Operators representing observables must give a real expectation value $\langle Q \rangle = \langle Q \rangle^*$ and hence must be Hermitian: $\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle, \forall f(x)$.

47. The product of two Hermitian operators is Hermitian iff they commute.

48. If Ω and Λ are two commuting Hermitian operators, there exists a basis of common eigenvectors that diagonalises them both.

49. Matrix Representation of Operators:

$$\begin{aligned}\Omega_{ji} &= \langle j|\Omega|i\rangle \\ \Omega|V\rangle &= \Omega \sum_i v_i|i\rangle = \sum_i v_i\Omega|i\rangle = \sum_i v'_i|i\rangle = |V'\rangle \\ v'_i &= \sum_j \Omega_{ij}v_j \\ \begin{pmatrix} v'_1 \\ v'_2 \\ \vdots \\ v'_n \end{pmatrix} &= \begin{pmatrix} \langle 1|\Omega|1\rangle & \langle 1|\Omega|2\rangle & \cdots & \langle 1|\Omega|n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle n|\Omega|1\rangle & \langle n|\Omega|2\rangle & \cdots & \langle n|\Omega|n\rangle \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}\end{aligned}$$

The columns are the components of the transformed basis vector under Ω in the given basis.

50. Projection Operator:

- Note the completeness relation $|V\rangle = (\sum_{i=1}^n |i\rangle\langle i|)|V\rangle$.
- Hence $|i\rangle\langle i|$ is the projection operator \mathbb{P}_i for the ket $|i\rangle$.
- On kets, $\mathbb{P}_i|V\rangle = |i\rangle\langle i|V\rangle = |i\rangle v_i$.
- On bras: $\langle V|\mathbb{P}_i = \langle V|i\rangle\langle i| = v_i^*\langle i|$.
- The identity operator: $\mathbb{I} = \sum_{i=1}^n \mathbb{P}_i$. In infinity dimensions, $\mathbb{I} = \int |x'\rangle\langle x'|dx'$.
- Product: $\mathbb{P}_i\mathbb{P}_j = \delta_{ij}\mathbb{P}_j$.

51. Matrix product (prove by writing the identity in between the operators and noting the identity can be written as a sum of projection operators):

$$(\Omega\Lambda)_{ij} = \langle i|\Omega\Lambda|j\rangle = \sum_k \Omega_{ik}\Lambda_{kj}$$

52. Anticommutator: $\{A, B\} = AB + BA$.

53. Commutation identities:

- \hat{A} commutes with any function $f(\hat{A})$.

$$\begin{aligned}[A, BC] &= B[A, C] + [A, B]C \\ [AB, C] &= A[B, C] + [A, C]B\end{aligned}$$

- $[A + B, C] = [A, C] + [B, C]$
- $[A, BC] = [A, B]C + B[A, C]$
- $[A, BCD] = [A, B]CD + B[A, C]D + BC[A, D]$
- $[A, BCDE] = [A, B]CDE + B[A, C]DE + BC[A, D]E + BCD[A, E]$
- $[AB, C] = A[B, C] + [A, C]B$
- $[ABC, D] = AB[C, D] + A[B, D]C + [A, D]BC$
- $[ABCD, E] = ABC[D, E] + AB[C, E]D + A[B, E]CD + [A, E]BCD$
- $[AB, CD] = A[B, CD] + [A, CD]B = A[B, C]D + AC[B, D] + [A, C]DB + C[A, D]B$
- $[[[A, B], C], D] + [[[B, C], D], A] + [[[C, D], A], B] + [[[D, A], B], C] = [[A, C], [B, D]]$
- $[AB, C] = A\{B, C\} - \{A, C\}B$, where $\{A, B\} = AB + BA$ is the anticommutator defined above.

54. Hermitian conjugate (adjoint): The adjoint of an operator \hat{Q} is the operator \hat{Q}^\dagger such that $\langle f|\hat{Q}g\rangle = \langle \hat{Q}^\dagger f|g\rangle$ for all f and g . A Hermitian operators is its own Hermitian conjugat.

55. General rule for taking adjoint of a product: Reverse the order of all factors, replace everything with the adjoint: $\Omega \leftrightarrow \Omega^\dagger, |V\rangle \leftrightarrow \langle V|, a \leftrightarrow a^*$.

56. The eigenvalues of a Hermitian operator are real. Also, all Hermitian operators are diagonalisable and has an orthonormal eigenbasis.

57. Every operator can be written as a sum of a Hermitian and an Antihermitian operator:

$$\Omega = \frac{\Omega + \Omega^\dagger}{2} + \frac{\Omega - \Omega^\dagger}{2}$$

58. Unitary operator: $UU^\dagger = I$. Unitary operators preserve the inner product: $\langle V_2|V_1' \rangle = \langle UV_2|UV_1 \rangle = \langle V_2|V_1 \rangle$. For real vector spaces, we have the orthogonality condition: $U^{-1} = U^T$.

59. Determinate states have $\sigma^2 = 0$, which only occur when $\hat{Q}\Psi = q\Psi$, where q is the value that the measurement returns. Hence q is an eigenvalue of the operator \hat{Q} with eigenfunction Ψ . The zero function cannot be an eigenfunction.

60. Degenerate spectrum: When two or more linearly independent eigenfunctions share the same eigenvalue.

61. Types of eigenfunctions:

- Discrete eigenvalues: Eigenfunction lies in Hilbert space and constitute physically realizable states. Eigenvalues are real if the operator is Hermitian. Eigenfunctions belonging to distinct eigenvalues are orthogonal $\langle f|g \rangle = 0$.
- Continuous eigenvalues: Eigenfunctions are not normalizable, but linear combinations may be normalizable.

62. Axiom on completeness: The eigenfunctions of an observable operator are complete: Any function in Hilbert space can be expressed as a linear combination of them.

63. Dirac Delta function from integral: $\delta(p - p') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(p-p')x} dx$.

64. Dirac orthonormality for continuous spectra: $\langle f_{p'}|f_p \rangle = \delta(p - p')$.

65. Completeness of eigenfunctions for continuous spectra: Any function can be written as $f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p)e^{ipx/\hbar} dp$ with the coefficient function calculated using $\langle f_{p'}|f \rangle = \int_{-\infty}^{\infty} c(p)\delta(p - p')dp = c(p')$.

66. Statistical Interpretation:

- If the particle is in a state $|\psi\rangle$, measurement of the variable corresponding to Ω will yield one of the eigenvalues ω with probability $P(\omega) = \frac{|\langle \omega|\psi \rangle|^2}{\langle \psi|\psi \rangle}$. The denominator is 1 if the state was normalised. The state of the system after the measurement is then the eigenstate $|\omega\rangle$ after the measurement.
- Discrete spectra: $\Psi(x, t) = \sum_n c_n f_n(x) \implies \langle Q \rangle = \sum_n q_n |c_n|^2, \sum_n |c_n|^2 = 1$.

67. Momentum space wave function: $\Phi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x, t) dx$. Note that this is the inverse Fourier transform of the position space wave function. Hence we also have $\Psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \Phi(p, t) dp$.

68. Generalized uncertainty principle: $\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle\right)^2$.

- Commutator of two Hermitian operators is anti-Hermitian: $\hat{Q}^\dagger = -\hat{Q}$ and hence has imaginary expectation value.

69. Commutator identity: $[AB, C] = A[B, C] + [A, C]B$.

70. Minimum uncertainty: The necessary and sufficient condition for minimum uncertainty is that $g(x) = ia f(x), a \in \mathbb{R}$. For position-momentum uncertainty, the general solution is a Gaussian.

71. Common Uncertainty Principles:

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$$\Delta t \Delta E \geq \frac{\hbar}{2}$$

Δt is the amount of time it takes for the expectation value of Q to change by one standard deviation:

$$\sigma_Q = \left| \frac{d\langle Q \rangle}{dt} \right| \Delta t$$

72. Time derivative of operator expectation value:

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

obtained using product rule on LHS and using TDSE. If operator does not depend explicitly on time (typical), third term $\left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle$ vanishes, and hence if the operator commutes with the Hamiltonian, then $\langle Q \rangle$ is a constant, and hence is a conserved quantity.

73. Special Case: Ehrenfest's Theorem:

$$\frac{d\langle p \rangle}{dt} = - \left\langle \frac{\partial V}{\partial x} \right\rangle$$

in 3D:

$$\begin{aligned} \frac{d}{dt} \langle \mathbf{r} \rangle &= \frac{1}{m} \langle \mathbf{p} \rangle \\ \frac{d}{dt} \langle \mathbf{p} \rangle &= \langle -\nabla V \rangle \end{aligned}$$

74. Harmonic Oscillator Operators:

$$\begin{aligned} \text{Lowering: } \hat{a} &= \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega_0} \right) \\ \text{Raising: } \hat{a}^\dagger &= \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{m\omega_0} \right) \\ \hat{x} &= \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a}) \\ \hat{p} &= i\sqrt{\frac{\hbar m\omega}{2}} (\hat{a}^\dagger - \hat{a}) \\ [\hat{a}, \hat{a}^\dagger] &= 1 \\ \hat{N}\phi_n &= \hat{a}^\dagger\phi_n = n\phi_n \end{aligned}$$

75. Correspondence principle: Classical harmonic oscillator probability density: $P = \frac{1}{\pi\sqrt{x_0^2 - x^2}}$ such that $\int_{-x_0}^{x_0} P(x)dx = 1$ where $\pm x_0$ are the classical turning points.

76. Dirac Notation

- Operators are linear transformations $|\beta\rangle = \hat{Q}|\alpha\rangle$.
- Vectors can be represented in any basis by their components: $|\alpha\rangle = \sum_n a_n |e_n\rangle$ with $a_n = \langle e_n | \alpha \rangle$.
- Operators can be represented by their matrix elements: $\langle e_m | \hat{Q} | e_n \rangle \equiv Q_{mn}$.
 - $\langle x | X | x' \rangle = x\delta(x - x')$
 - $\langle x | P | x' \rangle = -i\hbar\delta'(x - x')$.
- Bra: $\langle f | = \int f^*[\dots]dx$. In finite-dimensional vector space, it is the Hermitian conjugate of the Ket.
- Projection operator: $\hat{P} = |\alpha\rangle\langle\alpha|$ picks out the portion of any other vector that "lies along" $|\alpha\rangle$.
- Orthonormal basis: $\langle e_m | e_n \rangle = \delta_{mn}$ and the sum of the projects along all the finite dimensions is clearly the identity: $\sum_n |e_n\rangle\langle e_n| = I$.
- Dirac orthonormal continuous basis: $\langle e_z | e_{z'} \rangle = \delta(z - z')$ with analogous integral over the basis: $\int |e_z\rangle\langle e_z| dz = 1$.
- Spectral decomposition: For an operator \hat{Q} with a complete set of orthonormal eigenvectors $\hat{Q}|e_n\rangle = q_n|e_n\rangle$, $n = 1, 2, 3, \dots$, we can write the operator as:

$$\hat{Q} = \sum_n q_n |e_n\rangle\langle e_n|$$

77. Virial Theorem:

$$\begin{aligned} \frac{d}{dt} \langle xp \rangle &= 2\langle T \rangle - \left\langle x \frac{dV}{dx} \right\rangle \\ 2\langle T \rangle &= \left\langle x \frac{dV}{dx} \right\rangle \end{aligned}$$

78. Dealing with the matrix Hamiltonian.

- Find the eigenvalues and eigenvectors of the matrix Hamiltonian.
- Consider the initial conditions (t=0) to find the coefficients of each of the eigenvectors to describe the system.

- Tack on the time-dependence (since the eigenvalues obtained are the energies) to each of the eigenvector terms to obtain the time-evolution of the system.

79. Equations in 3D:

- Momentum operator: $\mathbf{p} \rightarrow \frac{\hbar}{i} \nabla$
- TDSE: $i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V\Psi$
- TISE: $\frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$.
- Solution to TDSE: $\Psi(\mathbf{r}, t) = \sum_n c_n \psi_n(\mathbf{r}) e^{-iE_n t/\hbar}$

80. Canonical commutation relations: Let $\mathbf{r} = (r_1, r_2, r_3)$ and $\mathbf{p} = (p_1, p_2, p_3)$. Then:

$$\begin{aligned} [r_i, p_j] &= -[p_i, r_j] = i\hbar \delta_{ij} \\ [r_i, r_j] &= [p_i, p_j] = 0 \end{aligned}$$

81. Spherical coordinates

- Laplacian:

$$\nabla^2 f = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2}$$

- Separation of variables: Write $\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$.
- Solution for azimuthal angle:

$$\Phi(\phi) = e^{im\phi}, m = 0, \pm 1, \pm 2, \dots$$

- Solution for polar angle:

$$\Theta(\theta) = AP_l^m(\cos \theta)$$

- Legendre function:

$$P_l^m(x) \equiv (1-x^2)^{|m|/2} \left(\frac{d}{dx} \right)^{|m|} P_l(x) = P_l^{-m}(x)$$

- Legendre polynomial (using Rodrigues formula):

$$P_l(x) \equiv \frac{1}{2^l l!} \left(\frac{d}{dx} \right)^l (x^2 - 1)^l$$

requires that l is a non-negative integer. Note also that if $|m| > l$, then $P_l^m = 0$. Hence for any l there are $2l + 1$ possible values of $m : -l, -l + 1, \dots, -1, 0, 1, \dots, l$.

- Legendre polynomials are orthonormal:

$$\int_{-1}^1 P_l(x) P_{l'}(x) dx = \left(\frac{2}{2l+1} \right) \delta_{ll'}$$

- Call l the azimuthal quantum number and m the magnetic quantum number.
- Normalized angular wavefunction:

$$\begin{aligned} Y_l^m(\theta, \phi) &= \epsilon \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P_l^m(\cos \theta) \\ \epsilon &= \begin{cases} (-1)^m, m \geq 0 \\ 1, m \leq 0 \end{cases} \end{aligned}$$

- Radial Equation:

$$\begin{aligned} u(r) &\equiv rR(r) \\ \frac{-\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[V + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] u &= Eu \end{aligned}$$

- Effective potential

$$V_{eff} = V + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$

tends to throw the particle away from the origin.

- General solution to radial equation in infinite spherical well: $u(r) = Arj_l(kr) + Brn_l(kr)$, where $j_l(x)$ is the spherical Bessel function of order l and $n_l(x)$ is the spherical Neumann function of order l :

$$j_l(x) \equiv (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\sin x}{x}$$

$$n_l(x) \equiv -(-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\cos x}{x}$$

$B = 0$ because Neumann functions blow up at the origin.

- Energies in infinite spherical well:

$$E_{nl} = \frac{\hbar^2}{2ma^2} \beta_{nl}^2$$

where β_{nl} is the n th zero of the l th spherical Bessel function.

82. Hydrogen Atom

- Bohr formula:

$$E_n = - \left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2}$$

- Bohr radius

$$a = \frac{4\pi\epsilon_0\hbar^2}{me^2} \approx 0.529 \times 10^{-10} m$$

- Ground state of hydrogen ($n = 1, l = 0, m = 0$):

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

- See page 145 onwards for all the formulae for the hydrogen atom.

83. Angular Momentum operators and commutation relations:

$$\mathbf{L} = \frac{\hbar}{i} (\mathbf{r} \times \nabla)$$

$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$

$$[L_x, L_y] = i\hbar L_z$$

$$[L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y$$

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$[L^2, \mathbf{L}] = 0$$

$$[L_z, L^2] = 0$$

$$[L_z, x] = i\hbar y, \quad [L_z, y] = -i\hbar x, \quad [L_z, z] = 0$$

$$[L_z, p_x] = i\hbar p_y, \quad [L_z, p_y] = -i\hbar p_x, \quad [L_z, p_z] = 0$$

Note that only one of the three Cartesian components of the angular momentum may be known at one time.

84. Angular momentum stuff in spherical coordinates:

$$\begin{aligned}\hat{L}^2 &= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \\ \hat{L}_x &= i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right) \\ \hat{L}_y &= i\hbar \left(-\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right) \\ \hat{L}_z &= -i\hbar \frac{\partial}{\partial \phi} \\ \hat{L}_+ &= \hbar e^{i\phi} \left(i \cot \theta \frac{\partial}{\partial \phi} + \frac{\partial}{\partial \theta} \right) \\ \hat{L}_- &= \hbar e^{-i\phi} \left(i \cot \theta \frac{\partial}{\partial \phi} - \frac{\partial}{\partial \theta} \right)\end{aligned}$$

85. Angular momentum ladder operators (increases or decreases the value of m by 1):

$$\begin{aligned}L_{\pm} &= L_x \pm iL_y \\ L_z(L_{\pm}f) &= (\mu \pm \hbar)(L_{\pm}f) \\ [L^2, L_{\pm}] &= 0 \\ [L_z, L_{\pm}] &= \pm \hbar L_{\pm} \\ L^2 &= L_{\mp}L_{\pm} + L_z^2 \pm \hbar L_z\end{aligned}$$

86. Angular momentum eigenvalue equations:

$$\begin{aligned}\hat{L}^2 \phi_{lm} &= \hbar^2 l(l+1) \phi_{lm}, l = 0, 1, 2, \dots \\ \hat{L} \phi_{lm} &= \hbar \sqrt{l(l+1)} \phi_{lm} \\ \hat{L}_z \phi_{lm} &= \hbar m \phi_{lm}, m = -l, \dots, 0, \dots, l\end{aligned}$$

87. Solid angle $dS = r^2 d\Omega = r^2 \sin \theta d\theta d\phi$.

88. Two body problem: If the interaction potential only depends on the separation between particles $\vec{r} = \vec{r}_1 - \vec{r}_2$, then we define the position of the centre of mass $\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}$ such that $\vec{r}_1 = \vec{R} - \frac{\mu}{m_1} \vec{r}$, $\vec{r}_2 = \vec{R} - \frac{\mu}{m_2} \vec{r}$. Differentiation with respect to particle 1 and 2 positions can then be written as:

$$\begin{aligned}\nabla_1 &= \frac{\mu}{m_2} \nabla_R + \nabla_r \\ \nabla_2 &= \frac{\mu}{m_1} \nabla_R - \nabla_r\end{aligned}$$

where $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$ is the reduced mass, and the time independent Schrodinger equation becomes:

$$\frac{-\hbar^2}{2(m_1 + m_2)} \nabla_R^2 \Psi - \frac{\hbar^2}{2\mu} \nabla_r^2 \Psi + V(\vec{r}) \Psi = E \Psi$$

Alternatively, define the weighted momentum $\mathbf{p} = \frac{m_1 \mathbf{p}_2 - m_2 \mathbf{p}_1}{m_1 + m_2}$ and the total momentum $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$ and write the Hamiltonian as:

$$H = \frac{P^2}{2M} + \left[\frac{p^2}{2\mu} + V(r) \right] = H_{CM} + H_{rel}$$

89. Composite wavefunction for indistinguishable particles: $\psi_{\pm}(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_a(x_1)\psi_b(x_2) \pm \psi_b(x_1)\psi_a(x_2)]$. If the particles are distinguishable, then $\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$. Plus sign for bosons, minus sign for fermions.

90. Symmetrization requirement. For two identical particles, $\psi(\vec{r}_1, \vec{r}_2) = \pm\psi(\vec{r}_2, \vec{r}_1)$, plus sign for bosons, minus sign for fermions.
91. Exchange force: Non-trivial. See page 208.
92. Probability Current Density:

$$\mathbf{J} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

with dimensions per area per second.

93. Transmission and Reflection. Given:

$$\begin{aligned}\psi_{inc} &= Ae^{i(k_1x - \omega_1t)} \\ \psi_{ref} &= Be^{i(k_1x + \omega_1t)} \\ \psi_{trans} &= Ce^{i(k_2x - \omega_2t)}\end{aligned}$$

The reflection and transmission coefficients are:

$$\begin{aligned}T &= \left| \frac{\mathbf{J}_{trans}}{\mathbf{J}_{inc}} \right| = \left| \frac{C}{A} \right|^2 \frac{k_2}{k_1} \\ R &= \left| \frac{\mathbf{J}_{refl}}{\mathbf{J}_{inc}} \right| = \left| \frac{B}{A} \right|^2\end{aligned}$$

94. Finite rectangular barrier:

$$\begin{aligned}\frac{1}{T} &= 1 + \frac{V^2}{4E(E-V)} \sin^2(2k_2a), \quad k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}, E > V \\ \frac{1}{T} &= 1 + \frac{V^2}{4E(E-V)} \sinh^2(2k_2a), \quad k_2 = \frac{\sqrt{2m(V-E)}}{\hbar}, E < V\end{aligned}$$

95. Potential step:

$$\begin{aligned}T &= \frac{4k_2/k_1}{(1 + (k_2/k_1))^2}, E > V \\ \frac{k_2^2}{k_1^2} &= 1 - \frac{V}{E}\end{aligned}$$

Transmission is zero if $E < V$, so that the kinetic energy in the entire step region is negative.

96. Scattering off a finite potential well

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

97. Double potential step:

$$T = \frac{4k_1k_3k_2^2}{k_2^2(k_1 + k_3)^2 + (k_3^2 - k_2^2)(k_1^2 - k_2^2) \sin^2(k_2a)}, \quad k_1 \geq k_2 \geq k_3$$

98. Delay from reflection and transmission. Let X be the centre of the incident wavepacket at $t = 0$, which moves with group velocity $\frac{\hbar k_0}{m}$.

$$\begin{aligned}\text{Incident packet: } x &= \frac{\hbar k_0}{m}t - X \\ \text{Reflected packet: } x &= \frac{-\hbar k_0}{m}t + X + \left(\frac{\partial \phi_R}{\partial k} \right)_{k_0} \\ \text{Transmitted packet: } x &= \frac{\hbar k_0}{m}t - X - \left(\frac{\partial \phi_T}{\partial k} \right)_{k_0}\end{aligned}$$

where the wave functions are:

$$\begin{aligned}\psi_{inc} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{ikX} e^{i(kx-\omega t)} dk \\ \psi_{refl} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sqrt{R} e^{i\phi_R} b(k) e^{ikX} e^{-i(kx+\omega t)} dk \\ \psi_{trans} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sqrt{T} e^{i\phi_T} b(k) e^{ikX} e^{i(kx-\omega t)} dk\end{aligned}$$

99. Plane wave solution to 3D Schrodinger equation (free particle in 3D):

$$\psi_{\mathbf{k}}(\mathbf{r}, t) = A e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}, \quad \hbar\omega = E_{\mathbf{k}}$$

100. 3D Dirac Delta:

$$\begin{aligned}\delta(\mathbf{r} - \mathbf{r}') &= \delta(x - x')\delta(y - y')\delta(z - z') \\ \delta(\mathbf{r} - \mathbf{r}') &= \frac{1}{(2\pi)^3} \iiint e^{i(\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}'))} d\mathbf{k} \\ d\mathbf{k} &= dk_x dk_y dk_z \\ \psi_{\mathbf{k}} &= \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} \iff \iiint \psi_{\mathbf{k}}^* \psi_{\mathbf{k}'} dx dy dz = \delta(\mathbf{k} - \mathbf{k}')\end{aligned}$$

101. 3D Wavepacket:

$$\begin{aligned}\psi(\mathbf{r}, t) &= \frac{1}{(2\pi)^{3/2}} \iiint b(\mathbf{k}, t) e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} d\mathbf{k} \\ b(\mathbf{k}, t) &= \frac{1}{(2\pi)^{3/2}} \iiint \psi(\mathbf{r}, t) e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} d\mathbf{r}\end{aligned}$$

102. Radial and Angular momentum:

$$\hat{H} = \frac{p^2}{2m} = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2}, \quad p_r = \frac{\hbar}{i} \frac{1}{r} \frac{\partial}{\partial r} = \frac{1}{2} \left(\frac{1}{r} \mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r} \frac{1}{r} \right)$$

p_r is not just simplify $\frac{\mathbf{r}\cdot\mathbf{p}}{r}$ because this is not Hermitian.

103. Central potential radial equation. Write $\phi = R(r)Y_l^m(\theta, \phi)$. Then $R(r)$ satisfies:

$$\left[\frac{p_r^2}{2\mu} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r) \right] R(r) = ER(r)$$

where the second term is the angular momentum barrier.