

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = H\Psi(\vec{r}, t) \quad (1)$$

Energy eigenstates: $H = \vec{p}^2/2m + V(\vec{r})$

$$H\psi(\vec{r}) = E\psi(\vec{r}), \quad \Psi(\vec{r}, t) = \psi(\vec{r}) e^{-iEt/\hbar} \quad (2)$$

Differential operators corresponding to momentum and energy:

$$\vec{p} \rightarrow -i\hbar \vec{\nabla} \quad E \rightarrow i\hbar \frac{\partial}{\partial t} \quad (3)$$

Harmonic oscillator in 1 dimension:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \quad H|n\rangle = E_n|n\rangle, \quad E_n = \hbar\omega(n + 1/2) \quad (4)$$

Raising and lowering operators:

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad (5)$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \quad p_x = -i\sqrt{\frac{m\omega\hbar}{2}}(a - a^\dagger) \quad (6)$$

Harmonic oscillator in 3 dimensions (isotropic), $H = \vec{p}^2/2m + m\omega^2 \vec{r}^2/2 = H_x + H_y + H_z$: spatial wavefunctions are just the products of the solutions of the 1-dim harmonic oscillator.

$$H|n_1 n_2 n_3\rangle = E_{n_1 n_2 n_3}|n_1 n_2 n_3\rangle, \quad E_{n_1 n_2 n_3} = \hbar\omega(n_1 + n_2 + n_3 + 3/2); \quad (7)$$

the wavefunctions can also be written in terms of the spherical harmonics,

$$\langle \vec{r} | n_r \ell m \rangle = R_{n_r \ell}(r) Y_{\ell m}(\theta, \phi), \quad E_{n_r \ell m} = \hbar\omega(2n_r + \ell + 3/2). \quad (8)$$

Particle in a box (infinite square well), 1 dimensional:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, \quad 0 \leq x \leq L, \quad E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \quad (9)$$

Particle in a box, 3 dimensional, $L \times L \times L$, one corner at the origin:

$$\psi(x, y, z) = \left(\frac{2}{L}\right)^{3/2} \sin \frac{n_1 \pi x}{L} \sin \frac{n_2 \pi y}{L} \sin \frac{n_3 \pi z}{L}, \quad E = \frac{\hbar^2 \pi^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) \quad (10)$$

Angular momentum:

$$L^2|\ell, m\rangle = \hbar^2 \ell(\ell + 1)|\ell, m\rangle, \quad L_z|\ell, m\rangle = \hbar m|\ell, m\rangle, \quad m_{\max} = \ell \quad (11)$$

$$L_\pm = L_x \pm iL_y, \quad [L^2, L_\pm] = 0, \quad L_\pm|\ell, m\rangle = C_\pm(\ell, m)|\ell, m \pm 1\rangle \quad (12)$$

$$C_+(\ell, m) = \hbar\sqrt{(\ell - m)(\ell + m + 1)}, \quad C_-(\ell, m) = \hbar\sqrt{(\ell + m)(\ell - m + 1)} \quad (13)$$

$$\vec{L} = \vec{r} \times \vec{p} \quad \text{so, e.g., } L_z = xp_y - yp_x. \quad (14)$$

Addition of angular momentum: when $\vec{J} = \vec{L} + \vec{S}$,

$$j = \ell + s, \dots, |\ell - s|, \quad J_z = L_z + S_z, \quad J_\pm = L_\pm + S_\pm \quad (15)$$

Spherical harmonics, up to $\ell = 2$:

$$\begin{aligned}
Y_{00} &= \frac{1}{\sqrt{4\pi}} & Y_{\ell m}(-\hat{r}) &= (-1)^\ell Y_{\ell m}(\hat{r}) \\
Y_{11} &= -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi} & Y_{10} &= \sqrt{\frac{3}{4\pi}} \cos \theta & Y_{1,-1} &= \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi} \\
Y_{22} &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{2i\phi} & Y_{21} &= -\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{i\phi} & Y_{20} &= \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1) \\
Y_{2,-1} &= \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{-i\phi} & Y_{2,-2} &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{-2i\phi}
\end{aligned} \tag{16}$$

Pauli principle: under the exchange of any two identical particles, multi-particle wavefunctions are symmetric for bosons (integer spin), antisymmetric for fermions (half-odd-integer spin).

Time-independent perturbation theory:

$$H = H_0 + \lambda H_1, \quad H_0|\phi_n\rangle = E_n^{(0)}|\phi_n\rangle, \quad H|\psi_n\rangle = E_n|\psi_n\rangle \tag{17}$$

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots \tag{18}$$

$$E_n^{(1)} = \langle \phi_n | \lambda H_1 | \phi_n \rangle \quad E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_n | \lambda H_1 | \phi_k \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \tag{19}$$

$$|\psi_n\rangle = |\phi_n\rangle + \sum_{k \neq n} \frac{\langle \phi_k | \lambda H_1 | \phi_n \rangle}{E_n^{(0)} - E_k^{(0)}} |\phi_k\rangle + \mathcal{O}(\lambda^2) \tag{20}$$

Degenerate perturbation theory: first find the combinations of states that diagonalize the matrix $\langle \phi_i | \lambda H_1 | \phi_j \rangle$ made up of states degenerate at zeroth order. The eigenvalues of this matrix are $E_n^{(1)}$.

Time-dependent perturbation theory:

$$H_0|\phi_n\rangle = E_n^{(0)}|\phi_n\rangle, \quad i\hbar \frac{d}{dt} |\psi(t)\rangle = (H_0 + \lambda V(t)) |\psi(t)\rangle \tag{21}$$

$$|\psi(t)\rangle = \sum_n c_n(t) e^{-iE_n^{(0)}t/\hbar} |\phi_n\rangle \tag{22}$$

For $c_k(0) = 1$ and all other $c_n(0) = 0$, to first order in λ the coefficients are

$$c_m(t) = \frac{1}{i\hbar} \int_0^t dt' e^{i\omega_{mk}t'} \langle \phi_m | \lambda V(t') | \phi_k \rangle \tag{23}$$

where $\omega_{mk} = (E_m^{(0)} - E_k^{(0)})/\hbar$. The transition probability is $P_{k \rightarrow m}(t) = |c_m(t)|^2$.

Variational principle: for *any* wavefunction $|\Psi\rangle$, $\langle \Psi | H | \Psi \rangle \geq E_0 =$ ground state energy of H .

Some math:

Taylor series about $x = 0$:

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left. \frac{d^n f}{dx^n} \right|_{x=0} x^n \tag{24}$$

Eigenvalues of a matrix M (I is the unit matrix; solve for λ):

$$\det(M - \lambda \cdot I) = 0 \tag{25}$$

Electron interacting with EM fields:

$$H = \frac{1}{2m_e} (\vec{p} + e\vec{A}(\vec{r}, t))^2 - e\phi(\vec{r}, t) \quad (26)$$

where $\vec{B} = \vec{\nabla} \times \vec{A}$ and $\vec{E} = -\vec{\nabla}\phi$.

Gauge transformation (ψ = electron wavefunction):

$$\vec{A}'(\vec{r}, t) = \vec{A}(\vec{r}, t) - \vec{\nabla}g(\vec{r}, t), \quad \phi'(\vec{r}, t) = \phi(\vec{r}, t) + \frac{\partial g(\vec{r}, t)}{\partial t}, \quad \psi'(\vec{r}, t) = e^{ieg(\vec{r}, t)/\hbar}\psi(\vec{r}, t). \quad (27)$$

Transition rate for radiative decays:

$$\Gamma_{n \rightarrow m} = \frac{2\pi}{\hbar} |\langle \phi_m | V | \phi_n \rangle|^2 \rho(E), \quad (28)$$

where $\rho(E)$ is the density of (final) states (the last expression uses $p = E/c$ for photons),

$$\rho(E) = \frac{V}{(2\pi\hbar)^3} p^2 \frac{dp}{dE} d\Omega = \frac{V}{(2\pi\hbar)^3} \frac{\hbar^2 \omega^2}{c^3} d\Omega. \quad (29)$$

Matrix element $\langle \phi_m | V | \phi_n \rangle$ involves

$$V = \frac{e}{m_e} \vec{A} \cdot \vec{p} = \frac{e}{m_e} \sqrt{\frac{\hbar}{2\epsilon_0 \omega V}} e^{-i\vec{k} \cdot \vec{r}} \vec{\epsilon}^{(\lambda)} \cdot \vec{p}. \quad (30)$$

Electric dipole approximation: $e^{-i\vec{k} \cdot \vec{r}} \simeq 1$.

Photon is transverse: $\vec{\epsilon}^{(\lambda)} \cdot \vec{k} = 0$.

Handy trick for evaluating matrix elements of \vec{p} : use

$$\vec{p} = m_e \frac{d\vec{r}}{dt} = m_e \frac{-i}{\hbar} [H_0, \vec{r}]. \quad (31)$$

Scattering theory

Elastic scattering cross section $d\sigma = |f(\theta)|^2 d\Omega$ (k = wavenumber of beam):

$$f(\theta) = \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{S_{\ell}(k) - 1}{2ik} P_{\ell}(\cos \theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) e^{i\delta_{\ell}(k)} \sin \delta_{\ell}(k) P_{\ell}(\cos \theta), \quad (32)$$

where $S_{\ell}(k) = e^{2i\delta_{\ell}(k)}$ is the phase shift. Total cross section is

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_{\ell}(k). \quad (33)$$

Inelastic scattering: $S_{\ell}(k) = e^{2i\delta_{\ell}(k)} \rightarrow \eta_{\ell}(k) e^{2i\delta_{\ell}(k)}$, $0 \leq \eta_{\ell}(k) \leq 1$.

Elastic, inelastic, and total cross sections:

$$\sigma_{\text{el}} = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \frac{1 + \eta_{\ell}^2 - 2\eta_{\ell} \cos 2\delta_{\ell}}{4} \quad (34)$$

$$\sigma_{\text{inel}} = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \frac{1 - \eta_{\ell}^2}{4} \quad (35)$$

$$\sigma_{\text{tot}} = \sigma_{\text{el}} + \sigma_{\text{inel}} = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \frac{1 - \eta_{\ell} \cos 2\delta_{\ell}}{2} \quad (36)$$

Born approximation: scattering rate:

$$R_{i \rightarrow f} = \frac{2\pi}{\hbar} \int \frac{V}{(2\pi\hbar)^3} d^3 p_f |M_{fi}|^2 \delta(E_f - E_i) = \frac{1}{4\pi^2 \hbar^4 V} \int d\Omega p_f m_f |\tilde{V}(\vec{\Delta})|^2 \quad (37)$$

where $\vec{\Delta} = (\vec{p}_f - \vec{p}_i)/\hbar$ and

$$M_{fi} = \langle \psi_f | V(\vec{r}) | \psi_i \rangle = \int d^3 r \frac{1}{\sqrt{V}} e^{-i\vec{p}_f \cdot \vec{r}/\hbar} V(\vec{r}) \frac{1}{\sqrt{V}} e^{i\vec{p}_i \cdot \vec{r}/\hbar} = \frac{1}{V} \int d^3 r e^{-i\vec{\Delta} \cdot \vec{r}} V(\vec{r}) \equiv \frac{1}{V} \tilde{V}(\vec{\Delta}). \quad (38)$$

Cross section: divide scattering rate by incoming flux = $|v_{\text{rel}}|/V$ (with $|v_{\text{rel}}| = p_i/m_i$):

$$d\sigma = \frac{1}{4\pi^2 \hbar^4} \frac{1}{|v_{\text{rel}}|} p_f m_f |\tilde{V}(\vec{\Delta})|^2 d\Omega. \quad (39)$$

Identical particles:

$$\frac{d\sigma}{d\Omega} = |f(\theta) \pm f(\pi - \theta)|^2 \quad (40)$$

with the \pm sign chosen according to whether the spatial part of the wavefunction should be even or odd under interchange of the two particles.

Unpolarized cross section: average over initial spins, sum over final spins.

40. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over every coefficient, e.g., for $-8/15$ read $-\sqrt{8/15}$.

Notation:

J	J	...
M	M	...

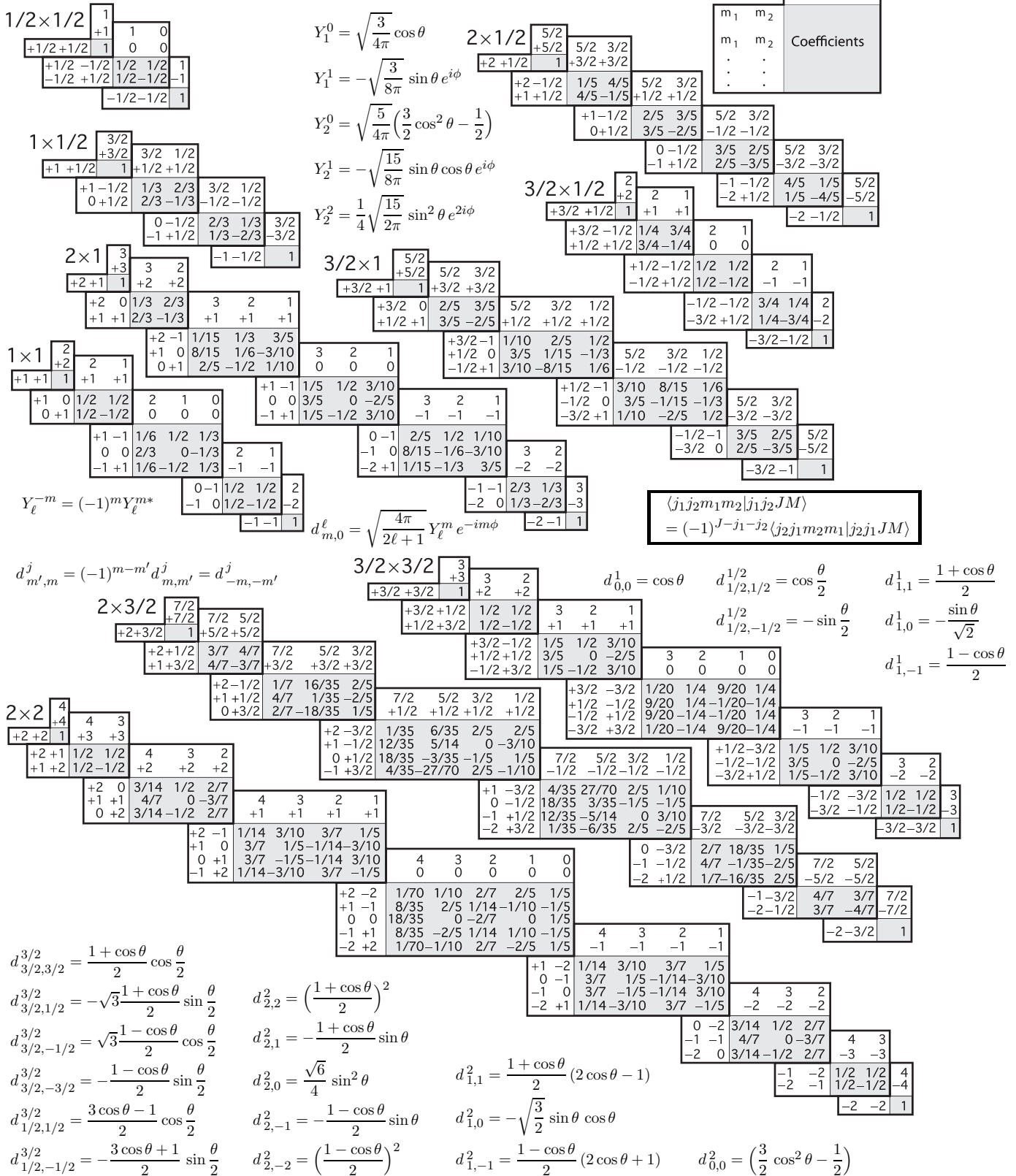


Figure 40.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974).