

General Facts

Suppose \hat{A} is either Hermitan or unitary. Then \hat{A} admits a spectral decomposition. That is

$$\hat{A} = \sum_i \lambda_i |i\rangle \langle i|.$$

For some basis $\{|i\rangle\}$. For operators with continuous spectrum, this sum is replaced by an integral. Hermitan operators have real eigenvalues and unitary operators have eigenvalues which lie on the complex unit circle. If two operators \hat{A} and \hat{B} commute, then it is possible to find a basis $\{|i\rangle\}$ where $|i\rangle$ is a simultaneous eigenket of both \hat{A} and \hat{B} . If \hat{A} is Hermitan, then $e^{-i\hat{A}a/\hbar}$ is Unitary

The projector from one basis $\{|a_i\rangle\}$ to another basis $\{|b_i\rangle\}$ is a unitary operator

$$\hat{U} = \sum_i |b_i\rangle \langle a_i|.$$

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \quad \hat{x} = x \quad \hat{U} = e^{-i\hat{H}t/\hbar}$$

$$[\hat{p}, \hat{x}^n] = -i n \hbar \hat{x}^{n-1} \quad [\hat{x}, \hat{p}^n] = i n \hbar \hat{p}^{n-1}$$

$$[\hat{x}, F(\hat{p})] = i\hbar \frac{\partial F}{\partial p} \quad [\hat{p}, F(\hat{x})] = -i\hbar \frac{\partial F}{\partial x}$$

For some operator \hat{O} in the Schrodinger picture, the corresponding operator in the Heisenberg picture is $\hat{U}^\dagger \hat{O} \hat{U}$. And time dependence in the Schrodinger picture is carried by \hat{U} .

$$i\hbar \frac{\partial}{\partial t} |\varphi\rangle = \hat{H} |\varphi\rangle \iff \frac{d\hat{A}}{dt} = \frac{1}{i\hbar} [\hat{A}, \hat{H}] + \frac{\partial \hat{A}}{\partial t}$$

Two State Systems

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$[\sigma_i, \sigma_j] = \delta_{ab} I + i\epsilon_{ijk} \sigma_k \quad S_i = \frac{\hbar}{2} \sigma_i$$

The arbitrary 2-state Hamiltonian can be expressed as a linear combination of the σ matrices and the identity matrix. This is sometimes written as an inner product as below.

$$\hat{H} = A \bullet S + c \mathbb{I}.$$

For a charge in a magnetic field, with components B_x , B_y , and B_z the Hamiltonian is

$$\hat{H} = \frac{\hbar}{2} \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}.$$

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \lambda_\uparrow = \frac{\hbar}{2} \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \lambda_\downarrow = -\frac{\hbar}{2}.$$

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \lambda_+ = \frac{\hbar}{2}$$

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \lambda_- = -\frac{\hbar}{2}.$$

Harmonic Oscillator

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

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a}) \quad \hat{p} = i\sqrt{\hbar m\omega/2} (\hat{a}^\dagger - \hat{a}) \quad \hat{H} = \hbar\omega (\hat{a}^\dagger \hat{a} + \frac{1}{2})$$

$$\hat{N} = \hat{a}^\dagger \hat{a} \quad \hat{N} |n\rangle = n |n\rangle.$$

$$[\hat{a}, \hat{a}^\dagger] = 1 \quad \hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle$$

$$\hat{a}(t) = e^{-i\omega t} \hat{a}(0) \quad \hat{p}(t) = -m\omega \hat{x}(0) \sin(\omega t) + \hat{p}(0) \cos(\omega t)$$

$$\hat{x}(t) = \hat{x}(0) \cos(\omega t) + \frac{\hat{p}(0)}{m\omega} \sin(\omega t)$$

Parity and Symmetry

The parity operator \hat{P} is defined by its action on the position operator, that is $\hat{P}^\dagger \hat{x} \hat{P} = -\hat{x}$. Therefore it is also the case that

$$\hat{P} |x\rangle = |-x\rangle \quad \hat{P} |p\rangle = |-p\rangle.$$

From this, we can see that $\hat{P}^\dagger \hat{p} \hat{P} = -\hat{p}$. An operator \hat{O} has a symmetry of \hat{A} if $[\hat{A}, \hat{O}] = 0$ and \hat{O} preserves probabilities in general. Symmetries must be unitary. In the position basis, even functions are of even parity and odd functions are of odd parity.

If \hat{H} is a Hamiltonian which has a potential with periodicity a . Then

$$\hat{\tau}(a) = e^{-\frac{ia \cdot \hat{p}}{\hbar}}.$$

Is a symmetry of the Hamiltonian. If \hat{U} is a symmetry of some Hamiltonian generated by \hat{Q} . Then $[\hat{H}, \hat{Q}] = 0 \implies \frac{d\hat{Q}}{dt} = 0$

Translation and Bloch's Theorem

$$\hat{\tau}(a) |x\rangle = |x+a\rangle.$$

Momentum is the generator of translation. If \hat{H} is a Hamiltonian with potential that has period a and some (potentially infinite) number of disconnected wells, we may label the eigenstates of \hat{H} as $|n, E\rangle$ where n corresponds to the localization of the state, and E is the eigenvalue of \hat{H} corresponding to $|n, E\rangle$. We can find a linear combination of these states, $|\theta, E\rangle = \sum_n e^{in\theta} |n, E\rangle$

$$\hat{\tau}(a) |\theta, E\rangle = e^{-i\theta} |\theta, E\rangle.$$

When the number of wells is finite, this quantizes θ . The **Tight Binding Approximation** is the assumption that

$$\langle n, E | \hat{H} | n+m, E \rangle = 0 \quad : \quad |m| > 1.$$

Bloch's Theorem says that, in such a system,

$$\langle x | \theta \rangle = e^{i\theta x/a} u_k(x) \quad : \quad u_k(x+a) = u_k(x).$$

The **Brillioun Zone** associated with a potential is The set of physically distinct values of k for which energy is defined in terms of k .

Scattering and Wave mechanics

$$V(x) = \begin{cases} 0 & x < a_1 \\ V(x) & a_1 \leq x \leq a_2 \\ 0 & x > a_2 \end{cases} \implies$$

$$\varphi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < a_1 \\ \text{garbage} & a_1 \leq x \leq a_2 \\ Fe^{ikx} + Ge^{-ikx} & x > a_2 \end{cases}.$$

$$T = \left| \frac{F}{A} \right|^2 \quad R = \left| \frac{B}{A} \right|^2.$$

The S matrix is defined by the relation.

$$\begin{pmatrix} F \\ B \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}.$$

Which is unitary.

The WKB Approximation

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2} (V(x) - E)} \quad k(x) = \sqrt{\frac{2m}{\hbar^2} E - V(x)}.$$

$$\varphi(x) = \begin{cases} \frac{1}{\sqrt{k(x)}} \exp[\pm i \int^x k(x) dx] & E > V(x) \\ \frac{1}{\sqrt{\kappa(x)}} \exp[\pm \int^x \kappa(x) dx] & E < V(x) \end{cases}.$$

If $\frac{dV}{dx}|_{x=a} > 0$

$$\frac{A}{\sqrt{\kappa(x)}} \exp \left[- \int_a^x \kappa(x') dx' \right] + \frac{B}{\sqrt{\kappa(x)}} \exp \left[\int_a^x \kappa(x) dx' \right] =$$

$$\frac{2A}{\sqrt{k(x)}} \cos \left[\int_x^a k(x') dx' - \frac{\pi}{4} \right] - \frac{B}{\sqrt{k(x)}} \sin \left[\int_x^a k(x') dx' - \frac{\pi}{4} \right].$$

If the derivative at a flips sign, you just flip all limits of integration to get the correct expression.

Trig Identities for WKB

$$\sin\left(\theta \pm \frac{\pi}{2}\right) = \pm \cos(\theta) \quad \cos\left(\theta \pm \frac{\pi}{2}\right) = \mp \sin(\theta).$$

$$\sin(\alpha \pm \beta) = \sin(\alpha) \cos(\beta) \pm \cos(\alpha) \sin(\beta).$$

$$\cos(\alpha \pm \beta) = \cos(\alpha) \cos(\beta) \mp \sin(\alpha) \sin(\beta).$$

$$2 \cos(\theta) \cos(\varphi) = \cos(\theta - \varphi) + \cos(\theta + \varphi).$$

$$2 \sin(\theta) \sin(\varphi) = \cos(\theta - \varphi) - \cos(\theta + \varphi).$$

$$2 \sin(\theta) \cos(\varphi) = \sin(\theta + \varphi) + \sin(\theta - \varphi).$$

$$2 \sin(\theta) \sin(\varphi) = \sin(\theta + \varphi) - \sin(\theta - \varphi).$$

Spherically Symmetric Potentials

If a particle is subjected to a purely radial potential, its wavefunction is given by $\varphi_{nlm} = R_{nl} Y_l^m$ where R_{lm} satisfies.

$$\frac{d^2 R_{nl}}{d\rho^2} + \frac{2}{\rho} \frac{dR_{nl}}{d\rho} + \left(1 - \frac{l(l+1)}{\rho^2}\right) R_{nl} = 0 \quad \rho = r \sqrt{2m(E - V)/\hbar^2}.$$

$$u_{nl} = r R_{nl} \quad -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} u_{nl} + \left(\frac{l(l+1)\hbar^2}{2mr^2} + V \right) u_{nl} = E u_{nl}.$$

Propagators and Path integrals

The propagator of a particle subject to a Hamiltonian \hat{H} is given by

$$K(x', t; x, t_0) = \langle x' | e^{-i\hat{H}(t-t_0)/\hbar} | x \rangle = \sum_a \langle x' | a \rangle \langle a | x \rangle e^{-iE_a(t-t_0)/\hbar}.$$

And note further that such propagators compose as

$$K(x'', t''; x, t_0) = \int K(x'', t''; x', t') \times K(x', t'; x, t_0) d^3 x'.$$

Now, let the action of the classical analogue of a quantum system be given by

$$S = \int_{t_1}^{t_N} dt \mathcal{L}(x, \dot{x}) \quad \text{and} \quad \delta t = \frac{t_N - t_1}{N - 1}.$$

Then, the path integral for

$$\lim_{\delta t \rightarrow 0} \langle x_N, t_N | x_1, t_1 \rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)] e^{iS(x, \dot{x})/\hbar}$$

where

$$\int_{x_1}^{x_N} \mathcal{D}[x(t)] = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \delta t} \right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1.$$

Gauge Symmetry

Classically, electromagnetic fields are invariant under a gauge transformation of the form $\phi \rightarrow \phi + \lambda$ and $A \rightarrow A + \nabla \lambda$. Where A is a vector potential (I neglect to place vector arrows). The Hamiltonian for a charged particle subject to such a potential is

$$\hat{H} = \frac{1}{2m} \hat{\Pi}^2 + e\phi \quad \text{with} \quad \hat{\Pi} = p - \frac{e}{c} A.$$

In the Heisenberg picture, we have that

$$m \frac{d\hat{x}}{dt} = \hat{\Pi} \quad \text{and} \quad [\hat{\Pi}_i, \hat{\Pi}_j] = \frac{i\hbar e}{c} \epsilon_{ijk} B_k.$$

Furthermore, we see that our wavefunction transforms as

$$|\varphi\rangle \rightarrow e^{ie\Lambda/\hbar c} |\varphi\rangle.$$

Note that the kinematical momentum $\hat{\Pi}$ is invariant under gauge transformations by construction.

Angular Momentum

We denote the angular momentum operator as \hat{J} , and the components of this operator as \hat{J}_i . Angular momentum is the generator of rotations;

$$\hat{R}(x_i, \theta) = \exp \left[-i \hat{J}_i \theta / \hbar \right].$$

$$\hat{J}_{\pm} = \hat{J}_x \pm i \hat{J}_y \quad [\hat{J}_i, \hat{J}_j] = i\hbar \epsilon_{ijk} J_k \quad [\hat{J}_z, \hat{J}_{\pm}] = \pm \hbar \hat{J}_{\pm} \quad [\hat{J}_+, \hat{J}_-] = 2\hbar \hat{J}_z$$

$$(\hat{J}^2, \hat{J}_z) |j, m\rangle = (\hbar^2 j(j+1), \hbar m) |j, m\rangle$$

$$\hat{J}_{\pm} |j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)} |j, m \pm 1\rangle \quad \hat{J}_z = -i\hbar \frac{\partial}{\partial \phi}.$$

Suppose now that we have two different particles with angular momentum operators \hat{J}_1 and \hat{J}_2 so that $\hat{J} = \hat{J}_1 + \hat{J}_2$. Then $2J_1 \bullet J_2 = J^2 - J_2^2 - J_1^2$.

34. 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 $-\sqrt{8/15}$.

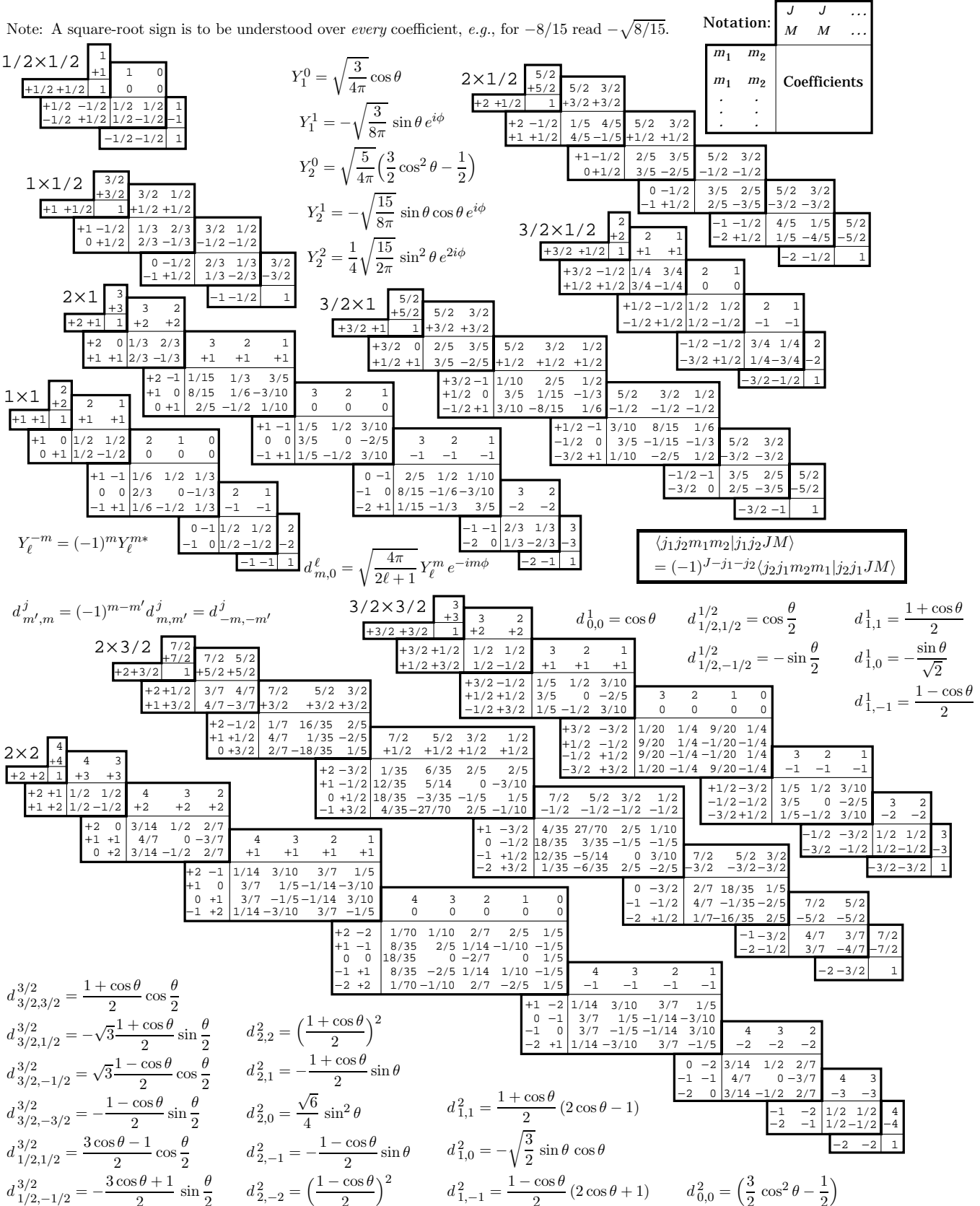


Figure 34.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.