General Facts

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

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

For some basis $\{|i\rangle\}$. For operators with continuious 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 $e^{-i\hat{A}\cdot a/\hbar}$ is Unitary

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

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

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

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

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

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 $\hat{U}$.

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

The uncertianty principle regarding two operators $\hat{A}$ and $\hat{B}$ is given by

$$\sigma_A^2\sigma_B^2 \geq \langle [A, B]\rangle \qquad \sigma_A^2 = \langle A^2\rangle - \langle A\rangle^2.$$

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

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

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

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

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

Harmonic Oscillator

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

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

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

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

$$\left\langle \hat{x}^2\right\rangle = \frac{\hbar}{2m\omega} \quad \left\langle \hat{p}^2\right\rangle = \frac{\hbar m\omega}{2}$$

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

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

$$\langle x'|0\rangle = \frac{1}{\sqrt{x_0\sqrt{\pi}}}\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

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

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

From this, we can see that $\hat{P}^\dagger\hat{p}\hat{P} = -\hat{p}$ An operator $\hat{O}$ has is 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

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

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, $|\theta, E\rangle = \sum_n e^{in\theta}\left|n, E\right\rangle$

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

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

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

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

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

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

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

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

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

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

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

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

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 inegration to get the correct expression.

Trig Identities for WKB

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

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

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

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

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

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

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

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.

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

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

Propagators and Path integrals

The propogator 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

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

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

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

Then, the path integral for

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

where

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

Gauge Symmetry

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

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

In the Heisenberg picture, we have that

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

Furthermore, we see that our wavefunction transforms as

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

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;

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

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

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

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

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 $2J_1 \bullet J_2 = J^2 - J_2^2 - J_1^2$.

Clebsch Gordan Coefficients

The Clebsch–Gordan coefficients are change of basis matrix elements to transform between two CSCO's which are $\{\hat{J}^2, \hat{J}_z\hat{J}_1^2, \hat{J}_2^2\}$ and $\{\hat{J}_1^2, \hat{J}_2^2\hat{J}_{1z}, \hat{J}_{2z}\}$. A table of coefficients has been appended to this document. The components are represented as the overlap of an eigenstate of one CSCO with an eigenstate of the other CSCO. $\langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m\rangle$

Tensor Products and Direct Sums

Let A and B be matrices with matrix elements a_{ij} and b_{ij}. Let us define $\vec{a}$ and $\vec{b}$ as vectors which can be operated on by A and B respectively. In block form,

$$A\oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \quad \vec{a}\oplus\vec{b} = \begin{pmatrix} \vec{a} \\ \vec{b} \end{pmatrix} \quad (A_1\oplus A_2)(B_1\oplus B_2) = A_1B_1\oplus A_2B_2$$

Tensor products have similar arithmetic rules.

$$A\otimes B = \begin{pmatrix} A_{11}B & A_{12}B & A_{13}B & \dots \\ A_{21}B & A_{22}B & A_{23}B & \dots \\ A_{31}B & A_{32}B & A_{33}B & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Tensors and More Angular Momentum

From a nasty and obscure derivation using the Wigner D matrix, we have the identity that

$$\int d\Omega Y^*_{lm} Y_{l_1m_1} Y_{l_2m_2} = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \langle l_1, l_2; 00 | l_1, l_2; l_0\rangle \times \langle l_1, l_2; m_1, m_2 | l_1, l_2; l, m\rangle.$$

If $\hat{T}^{(k)}_q$ is a spherical tensor of rank k, then

$\langle \alpha', l', m' | \hat{T}^{(k)}_q | \alpha, l, m\rangle = 0$ unless $m' = m+q$ and $|j-k| \leq j' \leq j+k$.

Cartesian vector operators satisfy the commutation relation

$$[V_i, J_j] = i\hbar\epsilon_{ijk}V_k \text{ so } V^{(1)}_{\pm1} = \mp\frac{1}{\sqrt{2}}(V_x \pm iV_y) \quad V^{(1)}_0 = V_z.$$

Spherical tensors obey the equations (which suffices as a definition)

$$[\hat{J}_z, T^{(k)}_q] = \hbar q T^{(k)}_q \quad [\hat{J}_\pm, T^{(k)}_q] = \hbar\sqrt{(k\mp q)(k\pm q+1)}T^{(k)}_{q\pm1}$$

Any rank 2 Cartesian tensor can be decomposed as $T_{ij} = E\delta_{ij} + A_{ij} + S_{ij}$ where

$$E = \frac{1}{3}\sum_i T_{ii} \quad A_{ij} = \frac{1}{2}(T_{ij} - T_{ji})$$

$$S_{ij} = \frac{1}{2}(T_{ij} + T_{ji}) - \frac{1}{3}\delta_{ij}\sum_k T_{kk}$$

Then, the components of the spherical tensors are

$$T^{(0)}_0 = E, \quad T^{(1)}_0 = A_{xy}, \quad T^{(1)}_{\pm_1} = \mp\frac{1}{\sqrt{2}}(A_{yz} \pm iA_{zx}), \quad T^{(2)}_0 = \sqrt{3/2}S_{zz},$$

$$T^{(2)}_{\pm1} = \mp(S_zx \pm iS_zy), \quad T^{(2)}_{\pm2} = \frac{1}{2}(S_{xx} - S_{yy} \pm 2iS_{xy})$$

If $X^{(k_1)}_{q_1}$ and $Z^{(k_2)}_{q_2}$ are spherical tensors then

$$T^{(k)}_q = \sum_{q_1,q_2} \langle k_1, k_2; q_1, q_2 | k_1, k_2; k, q\rangle X^{(k_1)}_{q_1} Z^{(k_2)}_{q_2}.$$

is also a spherical tensor. This is inverted by

$$X^{(k_1)}_{q_1} Z^{(k_2)}_{q_2} = \sum_{k=|k_1-k_2|}^{k_1+k_2} \sum_{q=-k}^{k} \langle k_1, k_2; k, q | k_1, k_2; q_1, q_2\rangle.$$

Explicitly, for combining two rank one spherical tensors, U and V then,

$$T^{(2)}_{\pm2} = U^{(1)}_{\pm1}V^{(1)}_{\pm1} \quad T^{(2)}_{\pm1} = \frac{1}{\sqrt{2}}(U^{(1)}_{\pm1}V^{(1)}_0 + U^{(1)}_0V^{(1)}_{\pm1})$$
$$T^{(2)}_0 = \frac{1}{\sqrt{6}}(U^{(1)}_1V^{(1)}_{-1} + 2U^{(1)}_0V^{(1)}_0 + U^{(1)}_{-1}V^{(1)}_1).$$

The Wigner–Eckhart Theorem and Corollaries

The Wigner–Eckhart Theorem says that, if $T^{(k)}_q$ is a spherical tensor,

$$\langle \alpha', l\, m | T^{(k)}_q | \alpha, l, m\rangle = \langle j, k; m, q | j, k; j', m'\rangle \frac{\langle \alpha', j' || T^{(k)} || \alpha, j\rangle}{\sqrt{2j'+1}}.$$

The Wigner–3j symbols are written as

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}.$$

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = (-1)^{j_1+j_2+j}\sqrt{2j+1}\begin{pmatrix} j_2 & j_1 & j \\ m_1 & m_2 & -m \end{pmatrix}$$
$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \begin{pmatrix} j & j_1 & j_2 \\ m & m_1 & m_2 \end{pmatrix} = (-1)^{j_1+j_2+j}\begin{pmatrix} j_2 & j_1 & j \\ m_2 & m_1 & m \end{pmatrix}$$
$$\begin{pmatrix} j_1 & j_2 & j \\ -m_1 & -m_2 & -m \end{pmatrix} = (-1)^{j_1+j_2+j}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix}.$$
$$(-1)^{1-j-m}\frac{m}{\sqrt{j(j+1)(2j+1)}} = \begin{pmatrix} j & 1 & j \\ m & 0 & -m \end{pmatrix}$$

The Projection theorem states that if $J^{(1)}_q$ is an angular momentum operator and $V^{(1)}_q$ is a rank one spherical tensor,

$$\langle \alpha', j, m' | V_q | \alpha, j, m\rangle = \frac{\langle \alpha', j, m' | J \bullet V | \alpha, j, m\rangle}{\hbar^2 j(j+1)} \langle j, m' | J_q | j, m\rangle$$

where

$$J\bullet V = J^{(1)}_0V^{(1)}_0 - J^{(1)}_1V^{(1)}_{-1} - J^{(1)}_{-1}V^{(1)}_1.$$