Hilbert Space

} Mathematical formalisms

- QM exists in Hilbert space, a vector space $\mathcal{H}$ over the field $\mathbb{C}$.
  - ↳ commutative $\psi + \phi = \phi + \psi$
  - ↳ associative $\psi + (\phi + \chi) = (\psi + \phi) + \chi$
  - ↳ identity $\underset{\text{unique}}{\exists}!\ 0 \in \mathcal{H}$ s.t. $\psi + 0 = \psi$ (exists →)
  - ↳ scalar multiplication (distributive)
- $\mathcal{H}$ is equipped with an inner product $(\cdot, \cdot): \mathcal{H} \times \mathcal{H} \to \mathbb{C}$
  - ↳ conjugate symmetry $(\phi, \psi) = (\psi, \phi)^\dagger$
  - ↳ linear in 2^{nd} arg $(\phi, a\psi + b\chi) = a(\phi, \psi) + b(\phi, \chi)$
  - ↳ positive-definite $(\psi, \psi) \geq 0$ with equality iff $\psi = 0$
- The norm of a state is $\|\psi\| = \sqrt{(\psi, \psi)}$ and the Cauchy-Schwarz inequality holds: $|(\phi, \psi)|^2 \leq (\phi, \phi)(\psi, \psi)$
- An orthonormal set $\{\phi_1, \ldots \phi_n\}$ forms a basis of an n-dim Hilbert space if $\psi \in \mathcal{H}$ can be uniquely expressed as a LC of basis vectors: $\psi = \sum_a^n c_a \phi_a$
  - ↳ coefficients can be determined by dotting with a particular basis vector $c_m = (\phi_m, \sum c_n \phi_n)$
- Finite-dimensional Hilbert spaces are isomorphic to $\mathbb{C}^n$ and their inner product is the standard $(\underset{\sim}{u}, \underset{\sim}{v}) = \sum_{i=1}^n u_i^\dagger v_i$
- Space of square-integrable functions L^2 $\left(\int_{\mathbb{R}} |\psi|^2 dx < \infty\right)$ is an ∞-dim Hilbert space with $(\phi, \psi) = \int_{\mathbb{R}} \phi^* \psi \, dx$

Dual spaces

- The dual $\mathcal{H}^*$ of $\mathcal{H}$ is the space of linear maps (functions) from $\mathcal{H} \to \mathbb{C}$.
  - ↳ i.e $\varphi \in \mathcal{H}^*$ defines a map $\varphi: \psi \to \varphi(\psi)$ for every $\psi \in \mathcal{H}$
  - ↳ we can construct a map with the inner product. $(\phi, \cdot) \in \mathcal{H}^*$ because $(\phi, \cdot): \psi \to (\phi, \psi) \in \mathbb{C}$ for all $\psi \in \mathcal{H}$
  - ↳ in fact, any linear map $\varphi: \mathcal{H} \to \mathbb{C}$ can be written as $(\phi, \cdot)$ for some $\phi \in \mathcal{H}$
  - ↳ implies an isomorphism $\mathcal{H}^* \cong \mathcal{H}$
    i.e every linear map is also an abstract vector.
- If $\psi \in \mathcal{H}$ it is a ket $|\psi\rangle$, else if $\psi \in \mathcal{H}^*$ it is a bra $\langle\psi|$.
  - ↳ the inner product is $\langle\phi|\psi\rangle$
  - ↳ a general ket can be expanded $|\psi\rangle = \sum_a \psi_a |e_a\rangle$ given some orthonormal basis set $\{|e_a\rangle\}$
  - ↳ $\langle\chi|\psi\rangle = \sum_{ab} \chi_b^\dagger \psi_a \langle e_b|e_a\rangle = \sum_a \chi_a^\dagger \psi_a$
- Can combine Hilbert spaces for more complex systems:
  - ↳ let $\{|e_a\rangle\}$ and $\{|f_\alpha\rangle\}$ be bases for $\mathcal{H}_1, \mathcal{H}_2$
    $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \Rightarrow |\psi\rangle = \sum_{a,\alpha} c_{a\alpha} |e_a\rangle \otimes |f_\alpha\rangle$
  - ↳ the inner product is defined on basis elements intuitively.
    $(\langle e_a| \otimes \langle f_\alpha|)(|e_b\rangle \otimes |f_\beta\rangle) = \langle e_a|e_b\rangle \langle f_\alpha|f_\beta\rangle$

Continuum states

- In function space, we can have a continuum basis $|a\rangle,\ a \in \mathbb{R}$:
  - ↳ $\langle a'|a\rangle = \delta(a'-a)$
  - ↳ the expansion is $|\psi\rangle = \int \psi(a)|a\rangle\, da$
- A key example is the position basis $\{|x\rangle\},\ x \in \mathbb{R}$
  - ↳ $|\psi\rangle = \int_{\mathbb{R}} \psi(x')|x'\rangle dx'$ and the coefficients are $\langle x|\psi\rangle = \int_{\mathbb{R}} \psi(x')\langle x|x'\rangle dx' = \psi(x)$
    - ↳ i.e position-space wavefunctions are just coeffs of $|\psi\rangle$ in a particular basis.
- With this in mind, we can express $|\psi\rangle$ in a diff basis, e.g the momentum basis $|\psi\rangle = \int \tilde{\psi}(p)|p\rangle dp$
- We can now convert between bases. $\langle x|p\rangle \propto e^{ixp/\hbar}$

$$\therefore\ \psi(x) = \langle x|\psi\rangle = \int \tilde{\psi}(p)\langle x|p\rangle dp \propto \mathcal{F}^{-1}[\tilde{\psi}(p)]$$
$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int \psi(x)\langle p|x\rangle dx \propto \mathcal{F}[\psi(x)]$$

- For multiparticle continuum states, i.e combining $\{|x\rangle\}, \{|y\rangle\}$:

$$|\psi\rangle = \int_{\mathbb{R}\times\mathbb{R}} \psi(x,y)\ |x\rangle \otimes |y\rangle dx dy$$

  - ↳ the inner product is $\langle \phi|\psi\rangle = \int \chi(x,y)^{\dagger}\psi(x,y)\, d^2x$
  - ↳ as notational shorthand, for a particle in $\mathbb{R}^3$ we write $|\psi\rangle = \int \psi(\underline{x})\,|\underline{x}\rangle d^3x$, $|\underline{x}\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle$

- Even single particle systems may require larger Hilbert spaces if there is internal structure. e.g electrons have spin and are thus best described by a pair of wavefunctions $\begin{pmatrix} \psi_{\uparrow}(\underline{x}) \\ \psi_{\downarrow}(\underline{x}) \end{pmatrix}$

Operators

- A linear operator $\mathcal{H} \to \mathcal{H}$ satisfies:

$$(\alpha A + \beta B)|\psi\rangle = \alpha A|\psi\rangle + \beta B|\psi\rangle$$

  - ↳ $AB: |\psi\rangle \mapsto A(B|\psi\rangle)$ ← not necessarily commutative
- The commutator quantifies the degree of commutation:

$$[A,B] = AB - BA$$

  - ↳ antisymmetry $[A,B] = -[B,A]$
  - ↳ linearity $[\alpha A + \beta B, C] = \alpha[A,C] + \beta[B,C]$
  - ↳ Leibniz identity $[A,BC] = [A,B]C + B[A,C]$
  - ↳ Jacobi identity $[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$
- The operator A maps kets to kets. The adjoint $A^{\dagger}$ maps bras to bras: $\boxed{\langle \phi|A^{\dagger}|\psi\rangle = \langle \psi|A|\phi\rangle^*}$
  - ↳ $(A+B)^{\dagger} = A^{\dagger} + B^{\dagger}$; $(AB)^{\dagger} = B^{\dagger}A^{\dagger}$; $(A^{\dagger})^{\dagger} = A$
  - ↳ an operator is self-adjoint (Hermitian) if $A^{\dagger} = A$
- For an operator A, eigenstates/eigenvalues are defined by:

$$A|\psi\rangle = a|\psi\rangle,\quad a \in \mathbb{C}$$

  - ↳ in Dirac notation, we often label an eigenstate by its eigenvalue $A|a\rangle = a|a\rangle$ ← eigenstate

eigenvalue

↳ Hermitian operators have real eigenvalues
$q\langle q|q\rangle = \langle q|Q|q\rangle = \langle q|Q|q\rangle^* = q^*\langle q|q\rangle$

↳ eigenvectors with distinct eigenvalues are orthogonal
$(q_1-q_2)\langle q_1|q_2\rangle = 0 \Rightarrow q_1 = q_2$ or $\langle q_2|q_1\rangle = 0$

- The set of eigenstates of a Hermitian operator forms an orthonormal basis for the operator: $\boxed{Q = \sum_n q_n|n\rangle\langle n|}$

Q exists in dual space

↳ any state may be expanded in this basis: $|\Psi\rangle = \sum_n c_n|n\rangle$

↳ operating is then simple:
$Q|\Psi\rangle = \sum_n q_n|n\rangle\langle n|\left(\sum_m c_m|n\rangle\right) = \overbrace{\sum_n c_n q_n|n\rangle}^{\text{by orthonormality}}$

↳ the identity operator is $1_{\mathcal{H}} = \sum_n|n\rangle\langle n|$

↳ a function of an operator is defined by
$f(Q) = \sum_n f(q_n)|n\rangle\langle n|$

- An operator can be expressed as a matrix with elements $A_{km} = \langle k|A|m\rangle$. Operator composition is then just matrix manipulation.
- Operators on L^2 are linear differential operators.

- For composite systems, let $\{|e_a\rangle\}$ be a basis for $\mathcal{H}_1$, A and $\{|f_\alpha\rangle\}$ be a basis for $\mathcal{H}_2$, B. Define $A\otimes B$ by
$(A\otimes B)(|e_a\rangle\otimes|f_\alpha\rangle) = (A|e_a\rangle)\otimes(B|f_\alpha\rangle)$

↳ $\{|e_a\rangle\otimes|f_\alpha\rangle\}$ automatically becomes orthonormal.

↳ an operator on only one space would be $A\otimes 1_{\mathcal{H}_2}$, e.g for hydrogen $H = \frac{p_p^2}{2m_p}\otimes 1_e + 1_p\otimes\frac{p_e^2}{2m_e} - \frac{q^2}{4\pi\varepsilon_0}\frac{1}{|x_e - x_p|}$

↳ $[A\otimes 1_{\mathcal{H}_2}, 1_{\mathcal{H}_1}\otimes B] = 0$ for all A, B, because each acts on one of the Hilbert spaces only.

Postulates of QM

- The state of the system is specified by a nonzero $|\Psi\rangle\in\mathcal{H}$
- Any complete set of orthogonal states $\{|\phi_1\rangle, |\phi_2\rangle, \ldots\}$ has a 1-to-1 correspondence with the possible outcomes of some measurement

↳ the prob. of observing the outcome corresponding to $|\phi_n\rangle$ is given by the Born rule: $\boxed{P(|\Psi\rangle\to|\phi_n\rangle) = \frac{|\langle\phi_n|\Psi\rangle|^2}{\langle\phi_n|\phi_n\rangle\langle\Psi|\Psi\rangle}}$

↳ in the case of orthonormal states, this reduces to
$P(|\Psi\rangle\to|\phi_n\rangle) = |\langle\phi_n|\Psi\rangle|^2$

- Observable quantities are represented by Hermitian operators

↳ the expectation of Q in state $|\Psi\rangle$ is
$\langle Q\rangle_\Psi = \langle\Psi|Q|\Psi\rangle/\langle\Psi|\Psi\rangle$

↳ the uncertainty (rms deviation) of Q in state $|\Psi\rangle$ is:

$$\Delta_\Psi Q = \sqrt{\langle Q^2\rangle_\Psi - \langle Q\rangle_\Psi^2}$$

↳ $\Delta_\Psi Q = 0$ iff Ψ is an eigenstate

- We can define an uncertainty principle for observables A, B. Let $|\Psi_A\rangle = A|\Psi\rangle - \langle A\rangle_\Psi|\Psi\rangle$ and likewise for $|\Psi_B\rangle$
  ↳ $\|\Psi_A\| = \Delta_\Psi A$ and $\|\Psi_B\| = \Delta_\Psi B$
  ↳ $\langle\Psi_A|\Psi_B\rangle = \langle\Psi|(A-\langle A\rangle)(B-\langle B\rangle)|\Psi\rangle$
  $= \langle\Psi|AB|\Psi\rangle - \langle A\rangle_\Psi\langle B\rangle_\Psi$
  ↳ $2i\,\mathrm{Im}[\langle\Psi_A|\Psi_B\rangle] = \langle\Psi|[A,B]|\Psi\rangle$
  ↳ by Cauchy-Schwarz, $\|\Psi_A\|\|\Psi_B\| \geq |\langle\Psi_A|\Psi_B\rangle|$

$$\Rightarrow \boxed{\Delta A_\Psi \Delta B_\Psi \geq \frac{1}{2}|\langle[A,B]\rangle_\Psi|}$$

- The Copenhagen interpretation is that the state collapses to an eigenstate (corresponding to the observed eigenvalue).
  ↳ does not specify how/when collapse happens.
  ↳ applying Q to $|\Psi\rangle$ is not the same as measuring.
- The dynamical evolution of a quantum system is governed by the time-dependent Schrödinger equation (TDSE):

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle$$

  ↳ form of H depends on the system
  ↳ $\mathcal{H}$ does not involve time; $\|\Psi\|$ remains const
  ↳ TDSE does not describe wavefunction collapse

Transformations

- Consider a spatial transformation (rot/translate)
  ↳ repr. with a linear operator $U: \mathcal{H} \to \mathcal{H}$
  ↳ rot/trans forms a group G. U is a homomorphism:
  $$U(g_2 \cdot g_1) = U(g_2) \circ U(g_1), \quad \forall g_1, g_2 \in G$$
  ↳ U must be unitary, i.e $U^{-1} = U^\dagger$. This is because the system must be normalised after applying U for any $|\Psi\rangle$
  $$\langle\Psi|\Psi\rangle = \langle\Psi|U^\dagger U|\Psi\rangle = 1 \Rightarrow U^\dagger U = 1_\mathcal{H}$$
- We can instead think of the operators being transformed (not states).
  ↳ the expectation after transformation is:
  $$\langle\Psi'|A|\Psi'\rangle = \langle\Psi|U^\dagger A U|\Psi\rangle$$
  $$= \langle\Psi|A'|\Psi\rangle \quad \text{where } A' = U^{-1}AU$$
  ↳ this is known as a similarity transform
  ↳ $A'B' = U^\dagger(AB)U \Rightarrow [A',B'] = U^\dagger[A,B]U$
  ↳ similarity transforms preserve the spectrum. If $|a\rangle$ is an eigenstate $A|a\rangle = a|a\rangle$, then $U^\dagger|a\rangle$ is an eigenstate of A' with the same eigenvalue
  $$A'(U^\dagger|a\rangle) = U^\dagger A U U^\dagger = U^\dagger A|a\rangle = a(U^\dagger|a\rangle)$$
- Some transformations depend smoothly on a parameter θ
  $$\boxed{U(\delta\theta) = 1_H - i\,\delta\theta\, T + O(\delta\theta^2)}$$

↳ T is the generator of the transformation U (indep. of θ)

↳ T is Hermitian: $U^\dagger U = 1_{\mathcal{H}} \Rightarrow T = T^\dagger$ to first order.

- The infinitesimal changes in state/operator:

↳ $|\psi'\rangle = (1 - i\delta\theta T + \dots)|\psi\rangle \Rightarrow \boxed{\delta|\psi\rangle = -i\delta\theta T|\psi\rangle}$

↳ $A' = (1 + i\delta\theta T)A(1 - i\delta\theta T) + \dots \Rightarrow \boxed{\delta A = i\delta\theta[T, A]}$

deep relationship between commutator and derivative.

↳ Finite transformations by repeatedly performing infinitesimal:

$$U(\theta) = \lim_{N\to\infty}\left(1 - i\frac{\theta}{N}T\right)^N = e^{-i\theta T}$$

Translations

- Translations in $\mathbb{R}^3$, represented by $U(\underline{a})$, are simple because translations form an Abelian group:

$$U(\delta\underline{a}) = 1 - i\delta\underline{a}\cdot\underline{P}/\hbar + O(|\delta\underline{a}|^2) \Rightarrow U(\underline{a}) = e^{-i\underline{a}\cdot\underline{P}/\hbar}$$

↳ $U(\delta\underline{a})U(\delta\underline{b}) = U(\delta\underline{b})U(\delta\underline{a}) \Rightarrow [P_i, P_j] = 0.$

↳ since $U(\underline{a})$ is a translation,

$$\langle\underline{X}\rangle_{\psi'} = \langle\psi|U^\dagger(\underline{a})\,\underline{X}\,U(\underline{a})|\psi\rangle = \langle\underline{X}\rangle_\psi + \underline{a}$$

$$\Rightarrow U^\dagger(\underline{a})\,\underline{X}\,U(\underline{a}) = \underline{X} + \underline{a}$$

$$\therefore (1 + i\delta\underline{a}\cdot\underline{P}/\hbar)\,\underline{X}\,(1 - i\delta\underline{a}\cdot\underline{P}/\hbar) = \underline{X} + \delta\underline{a}$$

$$\Rightarrow [X_i, P_j] = i\hbar\,\delta_{ij}1_{\mathcal{H}}$$

- To translate a position-space wavefunction, we first consider the action on eigenstates.

$$\underline{X}\,U(\underline{a})|\underline{x}\rangle = (\underbrace{[\underline{X}, U(\underline{a})]} + U(\underline{a})\underline{X})|\underline{x}\rangle = (\underline{a} + \underline{x})U(\underline{a})|\underline{x}\rangle$$

$U^\dagger XU = X + a \Rightarrow XU = UX + Ua \Rightarrow [X, U] = U(\underline{a})\underline{a}$

↳ so $U(\underline{a})|\underline{x}\rangle = |\underline{x} + \underline{a}\rangle$

$\Rightarrow \psi_{trans}(\underline{x}) = \langle\underline{x}|U(\underline{a})|\psi\rangle = \langle\underline{x} - \underline{a}|\psi\rangle = \psi(\underline{x} - \underline{a})$

↳ we then see how $\underline{P}$ relates to spatial derivatives

$$\psi(\underline{x} - \delta\underline{a}) - \psi(\underline{x}) = -\delta\underline{a}\cdot\nabla\psi$$

$$\psi(\underline{x} - \delta\underline{a}) - \psi(\underline{x}) = \langle\underline{x}|1 - i\delta\underline{a}\cdot\underline{P}/\hbar|\psi\rangle - \langle\underline{x}|\psi\rangle$$

$$= -\frac{i}{\hbar}\langle\underline{x}|\delta\underline{a}\cdot\underline{P}|\psi\rangle$$

$$\Rightarrow \boxed{\langle\underline{x}|\underline{P}|\psi\rangle = i\hbar\nabla\psi(\underline{x})}$$

Rotations

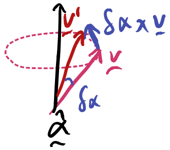
- For an ordinary vector $\underline{v} \in \mathbb{R}^3$, an anticlockwise rotation through $|\underline{\alpha}|$ around the $\hat{\underline{\alpha}}$ axis can be repr. by a rotation matrix $\underline{R}(\underline{\alpha}): \underline{v} \mapsto \underline{v}' = \underline{R}(\underline{\alpha})\underline{v}$

↳ $\det\underline{R} = 1$ so lengths are preserved

↳ but the rotation group is non-Abelian: $\underline{R}(\underline{\alpha})\underline{R}(\underline{\beta}) \neq \underline{R}(\underline{\beta})\underline{R}(\underline{\alpha})$

- For infinitesimal rotations in $\mathbb{R}^3$

$$\underline{v}' = \underline{v} + \underbrace{\delta\underline{\alpha}\times\underline{v}}_{\text{preserves length}} + O(|\delta\underline{\alpha}|^2)$$



↳ $\underline{R}(\delta\underline{\alpha})\underline{R}(\delta\underline{\beta}) = \underline{R}(\delta\underline{\alpha})(\underline{v} + \delta\underline{\beta}\times\underline{v}) + O(|\delta\underline{\beta}|^2)$

$$= \underline{v} + \delta\underline{\beta}\times\underline{v} + \delta\underline{a}\times(\underline{v} + \delta\underline{\beta}\times\underline{v}) + O(|\delta\underline{\alpha}|^2, |\delta\underline{\beta}|^2)$$

$$\Rightarrow [\underline{R}(\delta\underline{\alpha}), \underline{R}(\delta\underline{\beta})]\underline{v} = \delta\underline{\alpha}\times(\delta\underline{\beta}\times\underline{v}) - \delta\underline{\beta}\times(\delta\underline{\alpha}\times\underline{v}) + O(|\delta\underline{\alpha}|^2|\delta\underline{\beta}|^2)$$

$$= (\delta\underline{\alpha}\times\delta\underline{\beta})\times\underline{v} + O(|\delta\underline{\alpha}|^2|\delta\underline{\beta}|^2)$$

↳ i.e $[\underline{R}(\delta\underline{\alpha}), \underline{R}(\delta\underline{\beta})]\underline{v} = \underline{R}(\delta\underline{\alpha}\times\delta\underline{\beta})\underline{v} - \underline{v}$

- For the rotation operator $U(\underline{\alpha})$ on Hilbert space:

$$U(\delta\underline{a}) = 1 - i\,\delta\underline{a}\cdot\underline{J}/\hbar + \mathcal{O}(|\delta\underline{a}|^2) \quad \leftarrow \underline{J}/\hbar \text{ is the generator}$$

$$\Rightarrow U(\underline{\alpha}) = e^{-i\underline{\alpha}\cdot\underline{J}/\hbar}$$

↳ the relation in $\mathbb{R}^3$ implies: $\boxed{[U(\delta\underline{\alpha}), U(\delta\underline{\beta})] = U(\delta\underline{\alpha}\times\delta\underline{\beta}) - 1_{\mathcal{H}}}$

$$\therefore \left[1 - \tfrac{i}{\hbar}\delta\underline{a}\cdot\underline{J},\ 1 - \tfrac{i}{\hbar}\delta\underline{\beta}\cdot\underline{J}\right] = -\tfrac{i}{\hbar}(\delta\underline{a}\times\delta\underline{\beta})\cdot\underline{J}$$

$$\Rightarrow -\tfrac{1}{\hbar^2}\delta\alpha_i\,\delta\beta_j[J_i, J_j] = -\tfrac{i}{\hbar}\varepsilon_{ijk}\,\delta\alpha_i\,\delta\beta_j\,J_k$$

$$\Rightarrow \boxed{[J_i, J_j] = i\hbar\,\varepsilon_{ijk}J_k}$$

Cartesian components of the generators

↳ combining rotations and translations $[J_i, P_j] = i\hbar\varepsilon_{ijk}P_k$

- An operator V transforms under rotations as a vector if

$$U^\dagger(\underline{\alpha})\,V\,U(\underline{\alpha}) = \underline{R}(\underline{\alpha})V \iff [J_i, V_j] = i\hbar\varepsilon_{ijk}V_k$$

↳ this is true for the position operator X

↳ an operator S transforms under rotations as a scalar if

$$U^\dagger(\underline{\alpha})\,S\,U(\underline{\alpha}) = S \iff [J_i, S_j] = 0$$

Spin

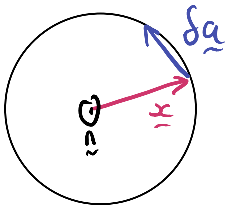
- We can alternatively think of rotation as infinitesimal translations:

$$U^\dagger(\delta\underline{a})\,\underline{X}\,U(\delta\underline{a}) = \underline{X} + \overbrace{\left(\tfrac{2\pi}{N}\right)\underline{n}\times\underline{X}}^{\delta\underline{a}}$$

$$\Rightarrow U(\delta\underline{a}) = 1 - \tfrac{i}{\hbar}\tfrac{2\pi}{N}(\underline{n}\times\underline{X})\cdot\underline{P}$$

↳ define $\underline{L} = \underline{X}\times\underline{P}$ and $\delta\underline{\alpha} = \frac{2\pi}{N}\underline{n}$

$$\therefore U(\delta\underline{a}) = 1 - \tfrac{i}{\hbar}\delta\underline{\alpha}\cdot\underline{L} + \mathcal{O}(|\delta\underline{a}|^2)$$

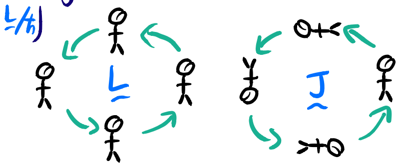


↳ this is the same expansion as for $\underline{J}$, so $\underline{L}$ and $\underline{J}$ have the same algebra.

- However, for a composite system, $\underline{J}$ is not the same as $\underline{L}$ despite them operating identically on $\mathbb{R}^3$

↳ the circular translation $(e^{-i\underline{\alpha}\cdot\underline{L}/\hbar})$ does not change orientation

↳ $\underline{J}$ is a circular rotation AND a change in orientation → spin



$$\boxed{\underline{J} = \underline{L} + \underline{S}}$$

- $\underline{S}$ does not affect the centre of mass wavefunction:

$$[S_i, X_j] = [J_i, X_j] - [L_i, X_j] = 0$$

$$[S_i, P_j] = [J_i, P_j] - [L_i, P_j] = 0$$

↳ $[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k$ implies that $\underline{S}/\hbar$ indeed generates rotations.

Parity transformations

- Parity does not depend on a continuous parameter. Parity is a unitary operator Π, where $\Pi^2 = 1_{\mathcal{H}}$. The eigenvalues are $\{+1, -1\}$: (so no generator.)

↳ $\Pi^\dagger \underline{X}\,\Pi = -\underline{X} \Rightarrow \overbrace{\Pi\underline{X} + \underline{X}\Pi}^{\text{anticommutator } \{\Pi, X\}} = 0$

↳ $\Pi^\dagger\underline{L}\,\Pi = \Pi^\dagger(X\times P)\Pi = \Pi^\dagger(X\,\Pi\Pi^\dagger)\times(\Pi P)\Pi$

$$= -\underline{X}\times-\underline{P} = \underline{L}$$

(likewise, $\Pi^\dagger\underline{J}\,\Pi = \underline{J}$)

↳ $\underline{X}$ and $\underline{P}$ are vector operators, $\underline{J}, \underline{L}$ are pseudovectors.

Time evolution

- Translations in time form an Abelian group, with time evolution operator $U(t) = \exp\left(-\frac{i}{\hbar} H t\right)$
  ↳ $H/\hbar$ is Hermitian, and will turn out to be the Hamiltonian of the system.
  ↳ since $H/\hbar$ is the generator, we can write
  $|\psi(t+\delta t)\rangle - |\psi(t)\rangle = -\frac{i}{\hbar}\delta t H|\psi(t)\rangle + O(\delta t^2)$
  $$\Rightarrow \boxed{i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle} \quad \text{TDSE.}$$
  ↳ unlike for $\underline{P}$ and $\underline{J}$, group properties do not completely constrain the form of H.
- In the Schrödinger picture, states evolve in time whilst operators have no explicit time-dependence.
  ↳ in the Heisenberg picture, the operator is evolving in time
  $$\langle\psi(t)|Q|\psi(t)\rangle = \langle\psi(0)|\underbrace{U^\dagger(t)\, Q\, U(t)}_{Q_H(t)}|\psi(0)\rangle$$
  ← H for Heisenberg
  ↳ $\frac{d}{dt}Q_H(t) = \frac{i}{\hbar}U^\dagger(t)[H, Q_S]U(t)$
  $= \frac{i}{\hbar}[H, Q_H(t)]$.
- To apply the TDSE in real life, we must specify the form of the Hamiltonian $H = H(\underline{X}, \underline{P}) \rightarrow$ the dynamical relation
  ↳ e.g $H = \underline{P}^2/2m$ is a rotationally-invariant relation between time evolution and spatial translation
  ↳ we may add a potential $V(\underline{X})$
  ↳ thus in the Heisenberg picture
  $$\frac{d\underline{X}(t)}{dt} = i\hbar[H, \underline{X}] = \frac{\underline{P}(t)}{m}$$
  $$\frac{d\underline{P}(t)}{dt} = i\hbar[H, \underline{P}] = -\nabla V(t)$$
  ← Heisenberg ops.
  ↳ only now can we associate the translation generator $\underline{P}$ with momentum.

Conserved Quantities

- Operators are conserved if they are time-independent even in the Heisenberg picture
  $$\frac{dQ_H}{dt} = 0 \Rightarrow \frac{i}{\hbar}[H, Q(t)] = U^\dagger(t)[H, Q]U(t) = 0$$
  $$\Rightarrow [H, Q] = 0$$
  ↳ conserved operators commute with the Hamiltonian
  ↳ thus systems stay in eigenstates with the same eigenvalue.
  $Q\, U(t)|q\rangle = U(t)Q|q\rangle = q\, U(t)|q\rangle$.
- Conserved quantities are generated by symmetries:
  ↳ a transformation $U(\theta) = e^{-i\theta T}$ may be applied to H: $U^\dagger(\theta)HU(\theta)$
  ↳ symmetry if H unchanged $\Rightarrow U^\dagger H U = H \Rightarrow [T, H] = 0$
  $\Rightarrow \frac{\partial T}{\partial t} = 0$ (conserved).
  ↳ translation symmetry $\Rightarrow \underline{P}$ cons; rotational symmetry $\Rightarrow \underline{J}$ cons

The Harmonic Oscillator

- Any general potential is harmonic near the minimum
- The Hamiltonian of the 1D harmonic osc is:

$$H = \frac{P^2}{2m} + \frac{m\omega^2}{2}X^2$$

↳ define the lowering and raising (ladder) operators:

$$A = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega X + iP) \qquad A^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega X - iP)$$

↳ these operators 'factorise' the Hamiltonian

$$A^\dagger A = \frac{H}{\hbar\omega} - \frac{1}{2} \implies \boxed{H = \hbar\omega(A^\dagger A + \tfrac{1}{2})}$$

- $N \equiv A^\dagger A$ is the number operator (Hermitian).

↳ $[A, A^\dagger] = 1$, $\quad [N, A^\dagger] = A^\dagger$, $\quad [N, A] = -A$

↳ let $|n\rangle$ be a normalised eigenstate of N. To find $NA^\dagger|n\rangle$, we rewrite

$$NA^\dagger = [N, A^\dagger] + A^\dagger N = A^\dagger + A^\dagger N$$

$$\implies NA^\dagger|n\rangle = (n+1)A^\dagger|n\rangle$$

and likewise $\quad NA|n\rangle = (n-1)A|n\rangle$

↳ we thus know the relationship between eigenvalues.

↳ we can further show that the eigenvals are nonneg integers:

$$n = n\langle n|n\rangle = \langle n|N|n\rangle = \langle n|A^\dagger A|n\rangle = ||A|n\rangle||^2 \geq 0$$

↳ if n were positive but not an integer, repeated lowering would violate this condition

↳ the ground state is $|0\rangle$, terminating the lowering. By definition, $A|0\rangle = 0$

$$\implies \boxed{E_n = (n + \tfrac{1}{2})\hbar\omega, \quad n \geq 0, \; n \in \mathbb{Z}}$$

- The 1D harmonic osc has non-degenerate energy levels so $A^\dagger|n\rangle = C_n|n+1\rangle$.

↳ to find C_n, note $|C_n|^2 = ||A^\dagger|n\rangle||^2 = \langle n|AA^\dagger|n\rangle = n+1$

$$\implies C_n = \sqrt{n+1}$$

↳ energy eigenstates can then be generated via

$$|n+1\rangle = \frac{1}{\sqrt{n+1}}A^\dagger|n\rangle = \frac{1}{\sqrt{(n+1)!}}(A^\dagger)^{n+1}|0\rangle$$

↳ likewise, $|n-1\rangle = \frac{1}{\sqrt{n}}A|n\rangle$ for $n \geq 1$

- Position space wavefunctions can be recovered:

↳ let $\psi_0(x) = \langle x|0\rangle$ be the ground state

↳ $\langle x|A|0\rangle = 0$

$$\implies \langle x|m\omega X + iP|0\rangle = m\omega x\psi_0(x) + \hbar\psi_0'(x) = 0$$

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

↳ 1st order ODE instead of 2nd order from TISE.

- Operator algebra can simplify expected values, e.g $\langle X^2\rangle_\psi$ in the ground state:

$$X = \sqrt{\hbar/2m\omega}\,(A + A^\dagger) \implies \langle X^2\rangle_\psi = \frac{\hbar}{2m\omega}\langle 0|(A + A^\dagger)^2|0\rangle$$

$$= \frac{\hbar}{2m\omega}\langle 0|AA^\dagger + A^\dagger A|0\rangle = 1$$

Time evolution

- In Heisenberg picture, $P(t) = P\cos\omega t - m\omega X\sin\omega t$
- Consider the ground state of the QHO translated by x_0:
  $|0;x_0\rangle = e^{-ix_0 P/\hbar}|0\rangle$.
  ↳ the state evolves over time via
  $$U(t)|0;x_0\rangle = U(t)e^{-ix_0P/\hbar}|0\rangle = U(t)e^{-ix_0P/\hbar}U^\dagger(t)U(t)|0\rangle$$
  $$= \exp\left(-i/\hbar\left(m\omega x_0 X\sin\omega t + x_0 P\cos\omega t\right)\right)e^{-i\omega t/2}|0\rangle$$
  ↳ result is Gaussian centred on $x(t) = x_0\cos\omega t$ and momentum $p(t) = -m\omega x_0\sin\omega t$.
  ↳ same as classical oscillator.

Angular Momentum

- The generators $\underline{J}$ obey algebra $[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$
  ↳ no two components commute, but $[J_i, \underline{J}^2] = 0$ so we can diagonalise J_z, $\underline{J}^2$.
  ↳ let $|\beta,m\rangle$ be an eigenstate: $\underline{J}^2|\beta,m\rangle = \beta\hbar^2|\beta,m\rangle$ and $J_z|\beta,m\rangle = \beta\hbar|\beta,m\rangle$. Eigenstates orthonormal.
- Let the angular momentum ladders be $\boxed{J_\pm = J_x \pm iJ_y}$
  ↳ $[J_z, J_\pm] = \pm\hbar J_\pm$
  ↳ $$\underline{J}^2(J_\pm|\beta,m\rangle) = ([\underline{J}^2, J_\pm] + J_\pm\underline{J}^2)|\beta,m\rangle$$
  $$= \beta\hbar^2(J_\pm|\beta,m\rangle)$$
  ↳ $J_z(J_\pm|\beta,m\rangle) = (m\pm1)\hbar(J_\pm|\beta,m\rangle)$
  ↳ $J_\pm$ can be seen as reorienting the system towards the z-axis
- To actually find the spectrum, we need to know the limits. These come from the constraint that the norm is positive.
  $$\|J_+|\beta,m\rangle\|^2 = \langle\beta,m|J_-J_+|\beta,m\rangle \geq 0$$
  $$\Rightarrow \hbar^2(\beta - m(m+1)) \geq 0$$
  ↳ J_+ increases m but β does not change, so there must be some maximal $m=j$ on which $J_+|\beta,j\rangle = |0\rangle$, and so $\beta = j(j+1)$
  ↳ likewise $\|J_-|\beta,m\rangle\|^2 \geq 0$ so $\beta = j'(j'-1)$
  ↳ $\beta = j(j+1) = j'(j'-1) \Rightarrow j' = -j$, $j \geq 0$

↳ $j - j' = 2j \in \mathbb{N}_0$ because $J_\pm$ changes in unit steps

- We now relabel the angular momentum eigenstates as $|j, m\rangle$, where j is a half-integer and $m = -j \to j$

$$\boxed{\begin{aligned} J_z |j,m\rangle &= m\hbar |j,m\rangle \\ J^2 |j,m\rangle &= j(j+1)\hbar^2 |j,m\rangle \\ J_\pm |j,m\rangle &= \sqrt{j(j+1) - m(m\pm 1)}\ |j, m\pm 1\rangle \end{aligned}}$$

- $J_x = (J_+ + J_-)/2$, $J_y = (J_+ - J_-)/2i$ so rotations around arbitrary axes preserve j.
- $|j,j\rangle$ is the state with angular momentum maximally aligned along $\hat{z}$. We can approximate the degree of alignment as $\dfrac{\langle j,j | J_x^2 + J_y^2 | j,j\rangle}{\langle j,j | J_z^2 | j,j\rangle} = \dfrac{1}{j}$
  - ↳ if we measured $\underline{J}$ along $\underline{n} = (\sin\theta, 0, \cos\theta)$, the classical result would be the projection $\hbar j \cos\theta$
  - ↳ the QM expectation agrees: $\langle j,j | \underline{n}\cdot\underline{J} | j,j\rangle = \hbar j \cos\theta$
  - ↳ but there is uncertainty
- We can model a diatomic molecule as an axisymmetric body with $I = I_x = I_y \neq I_z$ (e.g. CO )
  - ↳ $$H = \frac{J_x^2 + J_y^2}{2I} + \frac{J_z^2}{2I_z} = \frac{\underline{J}^2}{2I} + J_z^2\left(\frac{1}{2I_z} - \frac{1}{2I}\right)$$
  - ↳ $|j,m\rangle$ is thus an energy eigenstate
    $$E_{j,m} = j(j+1)\hbar^2/2I + m^2\hbar^2\left(\frac{1}{2I_z} - \frac{1}{2I}\right)$$
  - ↳ because $I_z \ll I$ for CO, the $\frac{m^2\hbar^2}{2I_z}$ term (rotation along axis) requires very high energy to excite.
- Consider a rotation of $|\psi\rangle = \sum_{m=-j}^{j} a_m |j,m\rangle$:
  - ↳ $U(\alpha\hat{z})|\psi\rangle = \sum_m a_m e^{-i\alpha J_z/\hbar}|j,m\rangle = \sum_m a_m e^{-i\alpha m}|j,m\rangle$
  - ↳ for integer j, a rotation of 2π is identity. But this is not so for half-integer j, for which $U(2\pi\hat{z}) = -1_{\mathcal{H}}$
  - ↳ nevertheless, because we are dealing with projective Hilbert spaces, this is fine.
- The Stern-Gerlach experiment showed a discrete spectrum of angular momentum.

Spin

- Same algebra as $\underline{J}$: $[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k$ $\quad [L_i, L_j] = i\hbar\varepsilon_{ijk}L_k$, so $\underline{S}$ and $\underline{L}$ have the same representation.
- Let $|s,\sigma\rangle$ be a spin eigenstate:
  - ↳ $\underline{S}^2|s,\sigma\rangle = s(s+1)\hbar^2|s,\sigma\rangle$ and $S_z|s,\sigma\rangle = \sigma\hbar|s,\sigma\rangle$
  - ↳ s is half-integer; $\sigma \in \{-s, -s+1, \dots, s-1, s\}$
- The Hilbert space of a spin-s particle is $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$:
  - ↳ unlike for J and L, the total value s cannot be changed
  - ↳ s is an intrinsic particle property.
- Spin-0 particles are called scalars (bosons). Hence there is only one state $|0,0\rangle$ which is an eigenstate of any rotation ("spherical")

• Spin-½ particles have 2 orthogonal states: $|\uparrow\rangle = |\tfrac{1}{2},\tfrac{1}{2}\rangle$, $|\downarrow\rangle = |\tfrac{1}{2},-\tfrac{1}{2}\rangle$

↳ a generic spin-½ state is $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$ with $|a|^2+|b|^2=1$

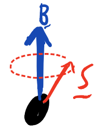
↳ matrix repr: $S_z = \begin{pmatrix} \langle\uparrow|S_z|\uparrow\rangle & \langle\uparrow|S_z|\downarrow\rangle \\ \langle\downarrow|S_z|\uparrow\rangle & \langle\downarrow|S_z|\downarrow\rangle \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

↳ likewise $S_x = (S_+ + S_-)/2$, $S_y = (S_+ - S_-)/2i$

$$\Rightarrow \quad S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

↳ we write $\underline{S} = \frac{\hbar}{2}\underline{\sigma}$ where $\underline{\sigma}$ are the Pauli spin matrices

• A spin-½ particle has a magnetic dipole moment $\underline{\mu} = \gamma\underline{S}$ where γ is the gyromagnetic ratio



↳ particle precesses in a $\underline{B}$-field with angular velocity $\underline{\omega} = -\gamma\underline{B}$ where ω is the Larmor frequency

↳ if the particle is fixed, the Hamiltonian is $H = -\gamma\underline{S}\cdot\underline{B} = -\gamma B S_z$ for a $\underline{B}$-field in the $\hat{\underline{z}}$ direction. This is the correct H because $\frac{\partial S_i}{\partial t} = \frac{1}{i\hbar}[H, S_i] = -\frac{\gamma}{i\hbar}B_j[S_j, S_i] = \underline{\mu}\times\underline{B}$ as needed.

↳ the particle may initially have its spin aligned along some axis $\underline{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$

$$\underline{n}\cdot\underline{S}|n_\uparrow\rangle = \frac{\hbar}{2}|n_\uparrow\rangle \Rightarrow |n_\uparrow\rangle = e^{-i\phi/2}\cos\tfrac{\theta}{2}|\uparrow\rangle + e^{-i\phi/2}\sin\tfrac{\theta}{2}|\uparrow\rangle$$

↳ this state evolves as $|n_\uparrow(t)\rangle = U(t)|n_\uparrow\rangle$. This recovers the classical result.

• With a rotating B-field, we can induce precession along a different axis. De-excitation produces radiation, which we can observe. This is how MRI works.

• Spin-1 particles have 3 orthogonal states:

$|+\rangle = |1,1\rangle \qquad |0\rangle = |1,0\rangle \qquad |-\rangle = |1,-1\rangle$

Orbital angular momentum

• $\underline{L}^2|l,m\rangle = l(l+1)\hbar^2|l,m\rangle \qquad L_z|l,m\rangle = m\hbar|l,m\rangle$

↳ these eigenstates may not be eigenstates of $\underline{J}$.

↳ circular translations through 2π leave the state unchanged (unlike for rotations)

$$e^{-2\pi i\hat{\underline{z}}\cdot\underline{L}/\hbar}|l,m\rangle = e^{-2\pi i m}|l,m\rangle = |l,m\rangle$$

$\Rightarrow m\in\mathbb{Z},\ l\in\mathbb{N}_0$ (no half-integer)

• In position space, $\underline{L} = \underline{X}\times\underline{P} = -i\hbar\,\underline{x}\times\nabla$

↳ $\langle\underline{x}|L_z|\psi\rangle = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi(\underline{x}) = -i\hbar\frac{\partial}{\partial\phi}\psi(\underline{x})$

↳ the eigenvalue equation is $\langle\underline{x}|L_z|l,m\rangle = m\hbar\langle\underline{x}|l,m\rangle$

$$\Rightarrow \boxed{\psi_{l,m}(\underline{x}) = K_{l,m}(r,\theta)e^{im\phi}}$$

↳ radial dependence can be derived by considering the action of L_+ on the highest weight state

$$L_\pm = L_x \pm iL_y = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_+\psi_{l,l} = 0 \Rightarrow \psi_{l,l}(\underline{x}) = R(r)\sin^l\theta\, e^{il\phi}$$

↳ other eigenstates can be constructed with L_-, giving the spherical harmonics $Y_l^m(\theta,\phi)$

↳ under parity, $Y_l^m(-\underline{x}) = (-1)^l Y_l^m(\underline{x})$ (i.e. even or odd with l)

The Isotropic Oscillator

- Consider a scalar particle in a central potential

$$H = \frac{\underline{p}^2}{2m} + V(|\underline{x}|) = \frac{p_r^2}{2m} + \frac{\underline{L}^2}{2m|\underline{x}|^2} + V(|\underline{x}|)$$

↳ $[H, \underline{L}^2] = [H, L_z] = [\underline{L}^2, L_z] = 0$ so use $|n, l, m\rangle$ as basis. n for energy eigvals, l for $\underline{L}^2$, m for L_z.

↳ energy levels must be independent of m $\because$ $[H, L_\pm] = 0$

↳ we thus expect $2l+1$ degeneracy from changing L_z

↳ in general, energies do depend on l

- Some Hamiltonians (depending on V) may have further degeneracies. If the algebra closes, i.e $[H, Q] = aH + bQ$, then we have a dynamical symmetry

- The 3D isotropic harmonic oscillator is the sum of 3 1D QHOs with the same frequency: $H = H_x + H_y + H_z$

↳ ladders same as 1D except vectors $\underline{A}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\underline{x} + i\underline{p})$

↳ $[A_i^\dagger, A_j] = \delta_{ij}$, $[A_i, A_j] = [A_i^\dagger, A_j^\dagger] = 0$

↳ $H = \hbar\omega(\underline{A}^\dagger \cdot \underline{A} + \frac{3}{2})$

↳ energy eigenstates are $|\underline{n}\rangle = |n_x, n_y, n_z\rangle = \frac{(A_x^\dagger)^{n_x}(A_y^\dagger)^{n_y}(A_z^\dagger)^{n_z}}{\sqrt{n_x!\,n_y!\,n_z!}}|0\rangle$

↳ $E_{\underline{n}} = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega$.

↳ the degeneracy is $(N+2)(N+1)/2$, i.e $\binom{N+2}{2}$ x x | x x x | x n_x n_y n_z

↳ much larger than the $2l+1$ we expect, meaning that there is more than just rotational symmetry.

- The isotropic osc has invariance of the form $A_i \to u_{ij}A_j$ where u_{ij} is a unitary matrix (not operator) that mixes the Cartesian components of $A^\dagger, A$

↳ there exists a Hermitian operator $U(\underline{u}) = 1_{\mathcal{H}} - i\varepsilon T$, and it can be shown that $\underline{T} = \underline{A}^\dagger \otimes \underline{A}$ and that T_{ij} is conserved $\frac{1}{\hbar\omega}[T_{ij}, H] = [A_i^\dagger A_j, A_k^\dagger A_k] = 0$

↳ to explicitly find symmetries, decompose T

$$T_{ij} = \underbrace{\tfrac{1}{3}\delta_{ij}\underline{A}^\dagger \cdot \underline{A}}_{\text{trace}} + \underbrace{\tfrac{1}{2}\varepsilon_{ijk}A_j^\dagger A_k}_{\text{antisymmetry}} + \underbrace{\left[\frac{A_i^\dagger A_j + A_j^\dagger A_i}{2} - \tfrac{1}{3}\delta_{ij}\underline{A}^\dagger \cdot \underline{A}\right]}_{\text{symmetry}}$$

↓ H (trivial) ↓ $\underline{L} = -i\hbar(\underline{A}^\dagger \times \underline{A})$ ↓ Symmetry mixing $\underline{x}, \underline{p}$

Isotropic oscillator in spherical coordinates

- We can analyse the isotropic osc in spherical coordinates rather than Cartesians, i.e $|n, l, m\rangle$ instead of $|n_x, n_y, n_z\rangle$.

- Let $p_r = (\hat{\underline{x}} \cdot \underline{p} + \underline{p} \cdot \hat{\underline{x}})/2$ be the radial momentum operator, $R \equiv |\underline{x}|$

$$H|n, l, m\rangle = \left(\frac{p_r^2}{2\mu} + \frac{\underline{L}^2}{2\mu|\underline{x}|^2} + \frac{1}{2}\mu\omega^2|\underline{x}|^2\right)|n, l, m\rangle$$

$$= \left(\frac{p_r^2}{2\mu} + \frac{l(l+1)\hbar^2}{2\mu R^2} + \frac{1}{2}\mu\omega^2 R^2\right)|n, l, m\rangle = H_l|n, l, m\rangle$$

↳ H_l is the radial Hamiltonian for a particular $\underline{L}^2$ eigenstate.

↳ $[R, P_r] = i\hbar$, so behaves just like standard x, p.

· Introduce ladders

$$\boxed{\begin{aligned} A_l &= \frac{1}{\sqrt{2\mu\hbar\omega}}\left(\mu\omega R + iP_r + \frac{(l+1)\hbar}{R}\right) \\ \Rightarrow H_l &= \hbar\omega\left(A_l^\dagger A_l + l + \tfrac{3}{2}\right)\end{aligned}}$$

↳ $H_{l+1}A_l = A_l(H_l - \hbar\omega) \Rightarrow H_{l+1}(A_l|E_l\rangle) = (E_l - \hbar\omega)A_l|E_l\rangle$

↳ so applying A_l to $|E_l\rangle$ creates a state with lower energy but with a radial wavefunction consistent with greater $\underline{L}^2$.

↳ but $[\underline{L}^2, A_l] = 0$ means that A_l does not change $\underline{L}^2$.

↳ considering the norm: $\frac{E_l}{\hbar\omega} - l - \frac{3}{2} = \langle E_l|A_l^\dagger A_l|E_l\rangle = \|A_l|E_l\rangle\|^2 \geq 0$

$$\Rightarrow l_{max} = n = E/\hbar\omega - 3/2$$

· The states of maximal angular momentum at a given energy has $A_{l_{max}}|E_{l_{max}}\rangle = 0$ so the radial wavefunction obeys

$$\left(\frac{d}{dr} + \frac{1}{r} + \frac{l_{max}+1}{r} + \frac{\mu\omega r}{\hbar}\right)\langle r|E_{l_{max}}\rangle = 0$$

$$\Rightarrow \langle r|E_{l_{max}}\rangle = C r^{l_{max}} e^{-r^2/4r_0^2}, \quad r_0 = \sqrt{\frac{\hbar^2}{2\mu\omega}}$$

↳ this is the quantum equivalent of a circular orbit, but it still has nonzero radial KE

↳ can obtain eccentric orbits by acting with $A_l^\dagger$.

Coulomb potential

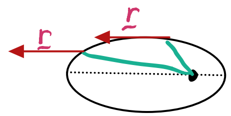
· In $\mathbb{R}^3$ only the isotropic osc and Coulomb potential have dynamical symmetries.

↳ $H = \frac{p^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0|\underline{x}|}$, $E_{n,l,m} = -R/n^2$

↳ for fixed energy, $l \in \{0, \dots, n-1\}$ so degeneracy is $\sum_0^{n-1}(2l+1) = n^2$.

↳ this extra degeneracy exists classically also.

· In a closed kepler orbit, constant $\underline{L}$ confines the orbit to a plane, but it is the conserved Runge-Lenz vector that closes the orbit. $\underline{r} = \frac{1}{\mu}\underline{p} \times \underline{L} - \kappa\frac{\underline{x}}{|\underline{x}|}$



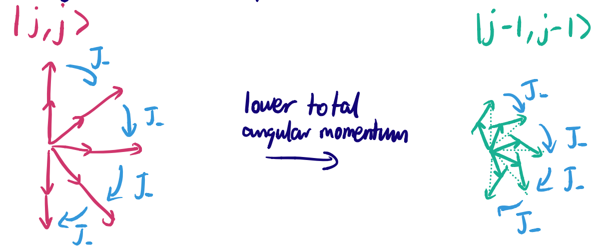
↳ $|\underline{r}|^2 = \kappa^2 + \frac{2E}{\mu}|\underline{L}|^2$ and $e = \frac{|\underline{r}|}{\kappa}$

↳ in QM we define $\underline{R} = \frac{1}{2\mu}(\underline{p} \times \underline{L} - \underline{L} \times \underline{p}) - \kappa\frac{\underline{x}}{|\underline{x}|}$

Addition of Angular Momenta

- Classically, angular momenta combine as $\underline{j}_{tot} = \underline{j}_1 + \underline{j}_2$:
  $$|\underline{j}_1| - |\underline{j}_2| \le |\underline{j}_{tot}| \le |\underline{j}_1| + |\underline{j}_2|$$
- Consider a 2-particle quantum system; particles have momenta j_1, j_2 and eigenstates $\{|j_1, m_1\rangle\}$, $\{|j_2, m_2\rangle\}$
  - ↳ a basis of the composite system is $\{|j_1, m_1\rangle \otimes |j_2, m_2\rangle\}$
  - ↳ we want to better understand the total angula momentum.
  - We define the composite angular momentum operator as:
    $$\underline{J} = \underline{J}_1 + \underline{J}_2 \quad , \quad \underline{J}^2 = \underline{J}_1^2 + \underline{J}_2^2 + 2\,\underline{J}_1 \cdot \underline{J}_2$$
  - ↳ $\underline{J}_1 \cdot \underline{J}_2 = J_{1x}J_{2x} + J_{1y}J_{2y} + J_{1z}J_{2z}$, rewrite with ladders
    $$\Rightarrow \quad \underline{J}^2 = \underline{J}_1^2 + \underline{J}_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2\,J_{1z}J_{2z}$$
- Consider the state $|j_1, j_1\rangle|j_2, j_2\rangle$, i.e both subsystems max aligned to $\hat{\underline{z}}$
  - ↳ $J_z\left(|j_1,j_1\rangle|j_2,j_2\rangle\right) = (j_1+j_2)\hbar\,|j_1,j_1\rangle|j_2,j_2\rangle$
  - ↳ $\underline{J}^2\left(|j_1,j_1\rangle|j_2,j_2\rangle\right) = (j_1+j_2)(j_1+j_2+1)\hbar^2\,|j_1,j_1\rangle|j_2,j_2\rangle$
  - ↳ hence $|j_1,j_1\rangle|j_2,j_2\rangle \equiv |j,j\rangle$ is the max j eigenstate of the total system with eigenvalue $j = j_1 + j_2$
- Other eigenstates can be generated with the total ladder $J_- = J_{1-} + J_{2-}$
  - ↳ $J_-|j,j\rangle = \sqrt{2j}\,\hbar\,|j,j-1\rangle$
  - ↳ we can equivalently expand as $J_-|j,j\rangle = (J_{1-}+J_{2-})(|j_1,j_1\rangle|j_2,j_2\rangle)$
  - ↳ all of these eigenstates have $j = j_1 + j_2$, so momenta are still maximally aligned, just not along $\hat{\underline{z}}$.

- There are also states with imperfectly aligned subsystems, e.g $|j-1, j-1\rangle$
  - ↳ $J_z|j-1,j-1\rangle = (j_1 + j_2 - 1)\hbar\,|j-1,j-1\rangle$
  - ↳ can find $|j-1,j-1\rangle$ by writing as a LC of basis states,
    $$|j-1,j-1\rangle = a|j_1,j_1-1\rangle|j_2,j_2\rangle + b|j_1,j_1\rangle|j_2,j_2-1\rangle$$
  - ↳ a, b can be found by orthogonality: $\langle j,j-1|j-1,j-1\rangle = 0$
- Can be depicted graphically as rotation around semicircles, with radius determined by the total angular mom j.



- The Clebsch-Gordan coefficients give the prob amplitudes that, when the total system is in state $|j,m\rangle$, the subsystems are in $|j_1,m_1\rangle$, $|j_2,m_2\rangle$.
  $$\boxed{C_{j,m}(j_1,m_1;\,j_2,m_2) = \langle j,m|\left(|j_1,m_1\rangle \otimes |j_2,m_2\rangle\right)}$$

Hydrogen

- In the ground state, no orbital angular mom $\therefore j_1 = j_2 = 1/2$
- Maximally aligned state is $|1,1\rangle = |\uparrow\rangle_e|\uparrow\rangle_p$
  - ↳ $|1,0\rangle = J_-|1,1\rangle = \frac{1}{\sqrt{2}}\left(|\downarrow\rangle_e|\uparrow\rangle_p + |\uparrow\rangle_e|\downarrow\rangle_p\right)$
  - ↳ $|1,-1\rangle = J_-|1,0\rangle = |\downarrow\rangle_e|\downarrow\rangle_p$
  - ↳ all states are exchange-symmetric if we swap $p \leftrightarrow e$

- $|0,0\rangle$ determined by orthogonality: $\langle 1,0|0,0\rangle = 0$

  $\Rightarrow |0,0\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle_e|\uparrow\rangle_p - |\uparrow\rangle_e|\downarrow\rangle_p)$

  ↳ state now antisymmetric under exchange.

  ↳ state annihalated by J_z, J_x, J_y

Comparison with the classical limit

- Classically, we expect j to range from $|j_1 - j_2| \to j_1 + j_2$.

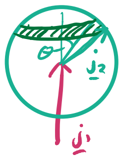
  ↳ the total number of states is $\sum_{j=|j_1-j_2|}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1)$

  ↳ this agrees with the dimensionality of $\mathcal{H}_1 \otimes \mathcal{H}_2$

- Classically, $|\underline{j}|^2 = j_1^2 + j_2^2 + 2\underline{j}_1 \cdot \underline{j}_2$

  ↳ pdf of alignments from area of band

  $dP = \frac{2\pi|j_2|\sin\theta d\theta}{4\pi|j_2|^2} = \frac{|\underline{j}|d|\underline{j}|}{2|\underline{j}_1||\underline{j}_2|}$



  ↳ in QM, the fraction of states with some amount j of angular momentum is $\frac{2j+1}{(2j_1+1)(2j_2+1)} \approx \frac{j}{2j_1 j_2}$ if $j_1, j_2 \gg 1$

  ↳ agrees with classical.

Identical Particles

- For a 2-particle system, $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ with basis $|\alpha_1\rangle|\alpha_2\rangle$

  ↳ for indistinguishable particles, exchanging $1 \leftrightarrow 2$ can only lead to a difference in scaling $|\alpha_2, \alpha_1\rangle = \lambda|\alpha_1, \alpha_2\rangle$

  ↳ exchanging twice gives $|\alpha_1, \alpha_2\rangle = \lambda^2 |\alpha_1, \alpha_2\rangle$.

  ↳ $\lambda = +1$ describes bosons (exchange-symmetric)

  ↳ $\lambda = -1$ describes fermions (exchange-antisymmetric).

  } exchange All quantum numbers

- Pauli's exclusion principle: no two fermions can be in the same state:

  $|\Psi\rangle = \frac{|\alpha_1, \alpha_2\rangle - |\alpha_2, \alpha_1\rangle}{2}$ $\therefore$ $\alpha_1 = \alpha_2 \Rightarrow |\Psi\rangle = 0$

- The Spin-Statistics theorem relates spin to exchange symmetry:

  ↳ bosons have integer spin

  ↳ fermions have half-integer spin.

Degeneracy pressure

- Free fermions in a box are described by $H = \sum_{a=1}^{N} \frac{p_a^2}{2m}$
- If the box has size L, the wavevector is $\underline{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$
- The Pauli exclusion principle prevents all N particles from sitting in the ground state.

  ↳ the Fermi energy is the highest filled energy level $E_F = \frac{\hbar^2 \underline{k}_F^2}{2m}$

  ↳ each electron occupies a box in k-space with volume $\left(\frac{2\pi}{L}\right)^3$

  ↳ for $N_e \gg 1$, this fills up as a sphere $\frac{4}{3}\pi|\underline{k}_F|^3 = \left(\frac{2\pi}{L}\right)^3 N_e$

- The total energy in the box can be found by integrating in k-space: $E_{tot} = \int_0^{|k_F|} \frac{\hbar^2 k^2}{2m_e} \cdot \frac{4\pi k^2}{(2\pi/L)^3} \, dk$
  - ↳ reduction in box volume is opposed by degeneracy pressure

$$\boxed{P_{deg} = \frac{-\partial E_{tot}}{\partial V}}$$

  - ↳ can be used to model a star, where $E_{tot} = -\frac{3}{5}\frac{GM^2}{R}$

Exchange and parity

- A 2-particle wavefunction can be described in CoM-relative coordinates: $X_{com} = \frac{1}{2}(X_1 + X_2)$ $\quad P_{com} = P_1 + P_2$

$$X_{rel} = X_1 - X_2 \qquad P_{rel} = \frac{1}{2}(P_1 - P_2)$$

  - ↳ exchange leaves CoM unchanged, but parity transforms rel (can think of as inverting through CoM).
- Because $Y_l^m \to (-1)^l Y_l^m$ under parity (and exchange is equivalent to parity on the relative component), the symmetry of exchange depends on l.

Time-Independent Perturbation Theory

- We may not be able to analyse the true Hamiltonian H, so we can write it in terms of a simpler model Hamiltonian H_0.
- For $\lambda \in [0,1]$, define $H_\lambda = H_0 + \lambda\underbrace{(H - H_0)}_{\equiv \Delta H}$
  - ↳ $\lambda = 0$ gives the simple model; $\lambda = 1$ recovers true Hamiltonian.
  - ↳ to find eigenstates $|E_\lambda\rangle$ of H_λ, we assume that the eigenstates and eigenvalues are analytic in λ:

$$|E_\lambda\rangle = |\alpha\rangle + \lambda|\beta\rangle + \lambda^2|\gamma\rangle + \dots$$
$$E(\lambda) = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \dots$$

  - ↳ sub into $H_\lambda|E_\lambda\rangle = E(\lambda)|E_\lambda\rangle$ and compare coeffs:

e.g
(0) $H_0|\alpha\rangle = E^{(0)}|\alpha\rangle$
(1) $H_0|\beta\rangle + \Delta H|\alpha\rangle = E^{(0)}|\beta\rangle + E^{(1)}|\alpha\rangle$
(2) $H_0|\gamma\rangle + \Delta H|\beta\rangle = E^{(0)}|\gamma\rangle + E^{(1)}|\beta\rangle + E^{(2)}|\alpha\rangle$

- The zeroth order equation (0) is the eigenvalue eq for our simple system, which we know obeys $H_0|E_n\rangle = E_n|E_n\rangle$, so we relabel $|\alpha\rangle \equiv |n\rangle$, $E^{(0)} \equiv E_n$. Can thus explore how different order corrections affect the nth eigenstate of H_0.
- (1) becomes $H_0|\beta_n\rangle + \Delta H|n\rangle = E_n|\beta_n\rangle + E_n^{(1)}|n\rangle$
  - ↳ contract with $\langle n|$ to give $E_n^{(1)} = \langle n|\Delta H|n\rangle$
  - ↳ contract with $\langle m| \neq \langle n|$ to give $\langle m|\Delta H|n\rangle = (E_n - E_m)\langle m|\beta_n\rangle$.

    Expand $|\beta_n\rangle = \sum b_k|k\rangle$ so for a non-degenerate H_0:

$$b_m = \frac{\langle m|\Delta H|n\rangle}{E_n - E_m} \Rightarrow |\beta_n\rangle = \sum_{m\neq n} \frac{\langle m|\Delta H|n\rangle}{E_n - E_m}|m\rangle$$

- ② gives $H_0|\gamma_n\rangle + \Delta H|\beta_n\rangle = E_n|\gamma_n\rangle + E_n^{(1)}|\beta_n\rangle + E_n^{(2)}|n\rangle$
  - ↳ $E_n^{(2)} = \langle n|\Delta H|\beta\rangle = \sum_{m\neq n} \frac{|\langle n|\Delta H|m\rangle|^2}{E_n - E_m}$
    - ↳ $|\langle n|\Delta H|m\rangle|$ represents a mixing between $|m\rangle$ and $|n\rangle$. Assuming this mixing is similar for many $|m\rangle$, the closest energy levels (smallest $E_n - E_m$) contributes most to the perturbation.
  - ↳ in the limiting case, degeneracies are lifted.
- Provided there is no degeneracy:

$$\boxed{\begin{aligned} |n(\lambda)\rangle &= |n\rangle + \lambda \sum_{m\neq n} \frac{\langle m|\Delta H|n\rangle}{E_n - E_m}|m\rangle + O(\lambda^2) \\ E_n(\lambda) &= E_n + \lambda\langle n|\Delta H|n\rangle + \lambda^2 \sum_{m\neq n}\frac{|\langle m|\Delta H|n\rangle|^2}{E_n - E_m} + O(\lambda^3) \end{aligned}}$$

Fine structure of Hydrogen

- The gross structure is a result of the Coulomb potential
  - ↳ $E_n = -\frac{1}{2}\mu c^2 \cdot \frac{\alpha^2}{n^2}$, where μ is the reduced mass and $\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}$ is the fine structure constant
  - ↳ the gross structure is independent of l, m
- To understand the fine structure of H, we make corrections:
  - ↳ relativistic correction to energy
  - ↳ magnetic field
  - ↳ Darwin term – 'smearing' of the potential near the nucleus.
- Using the relativistic expression for energy:

$$E = \sqrt{\mu^2 c^4 + p^2c^2} = \mu c^2 + \frac{p^2}{2\mu} - \frac{p^4}{8\mu^3 c^2}$$

  - ↳ we thus have a perturbation $\Delta H_{kin} = -\frac{(p^2)^2}{8\mu^3c^2}$ around the Coulomb Hamiltonian
  - ↳ ΔH_{kin} is rotationally invariant so does not mix degenerate states, so we can use non-degenerate perturbation theory to show that: $E_{nlm}^{(1)} = \langle nlm|\Delta H_{kin}|nlm\rangle$
- Evaluate the correction by writing in terms of H_0, V:

$$E_{nlm}^{(1)} = \langle H_{kin}\rangle_{nlm} = -\frac{1}{2\mu c^2}\langle (H_0 - V)^2\rangle_{nlm} = -\frac{E_n^2 - 2E_n\langle V\rangle_{nlm} + \langle V^2\rangle_{nlm}}{2\mu c^2}$$

  - ↳ from the virial theorem, $2\langle K\rangle + \langle V\rangle = 0 \Rightarrow E_n = \langle V\rangle/2$
  - ↳ $\frac{\langle V^2\rangle}{2\mu c^2} = \frac{\hbar^2}{2\mu}\langle \frac{\alpha^2}{r^2}\rangle$. This could be incorporated into the effective potential: $V_{eff}(r) = \frac{\hbar^2}{2\mu}\left[\frac{l(l+1)}{r^2} + \frac{\alpha^2}{r^2}\right] - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$
$$= \frac{\hbar^2}{2\mu}\frac{l'(l'+1)}{r^2} - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$$
  - ↳ $E_n(l') = -\frac{1}{2}\mu\alpha^2c^2\frac{1}{(l'+1)^2} \Rightarrow E_n(l+\delta l) = -\frac{1}{2}\mu\alpha^2c^2\left[\frac{1}{(l+1)^2} - \frac{2\delta l}{(l+1)^3}\right]$,
    but $\delta l(2l+1) = \alpha^2 \Rightarrow E_n(l+\delta l) = E_n + \frac{1}{2}\mu c^2\frac{\alpha^4}{n^3(l+1/2)}$
  - ↳ collecting terms, $E_{nl}^{(1)} = -\frac{1}{2}\mu c^2\left(\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right)\frac{\alpha^4}{n^4}$

- A charged particle in the Coulomb field experiences a B-field

$$B = \frac{\gamma_v}{c^2}\underline{v}\times\underline{E} = \frac{1}{\mu c^2}\underline{p}\times\left(\frac{e}{4\pi\varepsilon_0}\frac{\hat{\underline{x}}}{|\underline{x}|^2}\right) = -\frac{e}{4\pi\varepsilon_0\mu c^2}\frac{\underline{L}}{|\underline{x}|^3} \quad (\text{using } \underline{p} = \gamma\mu\underline{v})$$

  - ↳ the electron has magnetic dipole moment $-\frac{e}{2\mu}\underline{S}$, which couples to the B-field leading to a spin-orbit coupling correction:
$$\Delta H_{so} = -\frac{e}{2\mu}\underline{S}\cdot\underline{B} = \frac{e^2}{8\pi\varepsilon_0\mu c^2}\frac{\underline{L}\cdot\underline{S}}{|\underline{x}|^3}$$
  - ↳ $\underline{L}\cdot\underline{S} = \frac{1}{2}(\underline{J}^2 - \underline{L}^2 - \underline{S}^2) \Rightarrow \underline{L}\cdot\underline{S}|n,j,m_j,l\rangle = \frac{\hbar^2}{2}\left(j(j+1) - l(l+1) - \frac{3}{4}\right)|n,j,m_j,l\rangle$
  - ↳ $E_{njl}^{(1)} = \langle njl|\Delta H_{so}|njl\rangle = -\frac{1}{4\mu^2c^2}\frac{e^2\hbar^2}{4\pi\varepsilon_0}\left\{\begin{matrix} l \\ -(l+1)\end{matrix}\right\}\left\langle\frac{1}{|\underline{x}|^3}\right\rangle_{njl}$

↳ we know $[p_r, H_L] = -i\hbar\left(-\frac{\hbar^2 L(L+1)}{\mu R^3} + \frac{e^2}{4\pi\epsilon_0 R^2}\right)$ and $\langle [p_r, H_L]\rangle_{nlm} = 0$

↳ this gives an expr for $\langle \frac{1}{|x|^3}\rangle_{njl}$ given we know $\langle \frac{1}{|x|^2}\rangle_{njl}$

• Combining kinetic and spin-orbit corrections gives

$$E_{njl} = -\frac{1}{2}\mu\alpha^2 c^2\left[\frac{1}{n^2} - \frac{\alpha^2}{n^3}\left(\frac{3}{4n} - \frac{1}{j+\frac{1}{2}}\right) + \dots\right]$$

↳ Formula holds for $j = l \pm 1/2$

↳ Darwin term means it holds for $l=0$ also

↳ For heavier atoms, relativistic corrections become more impt:

$$E_{n,l+\frac{1}{2},l} - E_{n,l-\frac{1}{2},l} = \frac{1}{2}\mu c^2 \cdot \frac{1}{n^3}\frac{Z^4\alpha^4}{l(l+1)}$$

Helium

• Gross structure described by:

$$H = \frac{p_1^2}{2m_e} + \frac{p_2^2}{2m_e} - \frac{2e^2}{4\pi\epsilon_0}\left(\frac{1}{|x_1|} + \frac{1}{|x_2|}\right) + \underbrace{\frac{e^2}{4\pi\epsilon_0}\frac{1}{|x_1 - x_2|}}_{e^- \text{ repulsion}}$$

• We treat the electron repulsion as the perturbation:

↳ unperturbed single-electron states have $E_n = -\frac{1}{2}m_e Z^2\alpha^2 c^2\frac{1}{n^2} = -2m_e\alpha^2c^2\frac{1}{n^2}$

↳ ground state is $|\Psi_0\rangle = |1,0,0\rangle \otimes |1,0,0\rangle \otimes \left(\frac{|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle}{\sqrt{2}}\right)$, with energy $E_0 = 2\times(4\times -13.6\text{eV}) = -108.8\text{eV}$

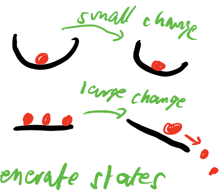
• The first order correction in the ground state is

$$E_0^{(1)} = \langle\Psi|\Delta H|\Psi\rangle = \frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{|x_1 - x_2|}\right\rangle_{\Psi_0}$$

↳ this expectation must be explicitly integrated to give:

$$E_1(Z) = -4\alpha^2 m_e c^2\left(1 - \frac{5}{16}\frac{1}{Z} + \dots\right)$$

Degenerate perturbation theory



• Perturbing a state with degeneracy can lead to large changes in the eigenstates. Imagine tilting a bowl vs tabletop.

$$|n_\lambda\rangle = |n\rangle + \lambda\sum_{m\neq n}\frac{\langle m|\Delta H|n\rangle}{E_n - E_m}|m\rangle$$

$E_n - E_m \to 0$ for degenerate states

• Consider a subspace $W \subset \mathcal{H}$ spanned by degenerate states of a particular energy w.r.t H_0, ie $\forall|\psi\rangle \in W$, $H_0|\psi\rangle = E_W|\psi\rangle$

↳ let $\{|r\rangle\}_{r=1}^{N}$ be an orthonormal basis for W and define the projection operator $P_W : \mathcal{H} \to W$, $P_W \equiv \sum_{r=1}^{N}|r\rangle\langle r|$

↳ also define an orthogonal complement to W as

$$W_\perp = \{|\chi\rangle \in \mathcal{H} : \langle\psi|\chi\rangle = 0,\ \forall|\psi\rangle \in W\},$$

along with a projector $P_\perp = 1 - P_W$

↳ projectors obey the intuitive relations: $P^2 = P$, $P_W P_\perp = P_\perp P_W$

↳ since W defined by H_0, also have $[H_0, P_W] = [H_0, P_\perp] = 0$

• Consider an eigenstate of the perturbed Hamiltonian and insert $1_{\mathcal{H}} = P_\perp + P_W$: $H_\lambda|\psi_\lambda\rangle = E(\lambda)|\psi_\lambda\rangle$

$$\Rightarrow (H_0 + \lambda\Delta H - E(\lambda))(P_\perp + P_W)|\psi_\lambda\rangle = 0$$

$$\Rightarrow (E_W - E(\lambda) + \lambda\Delta H)P_W|\psi_\lambda\rangle + (H_0 + \lambda\Delta H - E(\lambda))P_\perp|\psi_\lambda\rangle = 0$$

↳ apply P_W and $P_\perp$ to the left to get 2 simpler eqs

$$(E_W - E(\lambda) + \lambda P_W\Delta H)P_W|\psi_\lambda\rangle + \lambda P_W\Delta H P_\perp|\psi_\lambda\rangle = 0$$

$$(H_0 + \lambda P_\perp\Delta H - E(\lambda))P_\perp|\psi_\lambda\rangle + \lambda P_\perp\Delta H P_W|\psi_\lambda\rangle = 0$$

↳ now expand $|\psi_\lambda\rangle = |\alpha\rangle + \lambda|\beta\rangle + \lambda^2|\gamma\rangle + \dots$ and $E(\lambda) = E^{(0)} + \lambda E^{(1)} + \dots$

For a zeroth order eigenstate $|\alpha\rangle \in W$ with eigenvalue $E^{(0)} = E_W$.

↳ First order: $(P_W\Delta H P_W)|\alpha\rangle = E^{(1)}|\alpha\rangle$

- We must therefore choose $|\alpha\rangle$ to also be an eigenstate of $P_W \Delta H P_W$, i.e. an eigenstate of ΔH within the subspace W
  - ↳ in practice, easier to diagonalise in subspace.
  - ↳ finding an eigenbasis $\{|r\rangle\}_1^N$ of W, we recover the non-degenerate expression $E_r^{(1)} = \langle r|P_W \Delta H P_W|r\rangle = \langle r|\Delta H|r\rangle$
  - ↳ perturbations thus break degeneracy because degenerate states of H_0 may not be degenerate states of ΔH.

Stark effect

- H atom in constant E field (arbitrarily along $\underline{\hat{z}}$); model as a perturbation $\Delta H = e|\underline{E}|z$
- The ground state unaffected to first order:

$$\langle \Delta H\rangle_{\psi_1} = \langle 1,0,0|z|1,0,0\rangle = 0 \text{ by parity}$$

- The $n=2$ level has degeneracy 4:

$$W = \text{span}(|2,0,0\rangle, |2,1,1\rangle, |2,1,0\rangle, |2,1,-1\rangle)$$

  - ↳ parity implies $\langle 2,l',m'|z|2,l,m\rangle = 0$ unless $|l-l'|$ odd
  - ↳ $[L_z, z] = 0 \Rightarrow \langle 2,0,0|z|2,1,\pm1\rangle = 0$
  - ↳ so within the degenerate subspace W, the matrix elements of z simplify to: $\Delta H = e|\underline{E}|\begin{pmatrix} 0 & 0 & a & 0 \\ 0 & 0 & 0 & 0 \\ \bar{a} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$, $a = \langle 2,0,0|z|2,1,0\rangle = -3a_0$
- The perturbation has eigenstates and eigenvalues as follows:

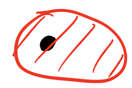
$$3e|\underline{E}|a_0, \quad 0, \quad 0, \quad -3e|\underline{E}|a_0$$

$$\tfrac{1}{\sqrt{2}}(|2,0,0\rangle - |2,1,0\rangle), \quad |2,1,1\rangle, \quad |2,1,-1\rangle, \quad \tfrac{1}{\sqrt{2}}(|2,0,0\rangle - |2,1,0\rangle)$$

  - ↳ the degeneracy between $|2,1,1\rangle$ and $|2,1,-1\rangle$ has not been lifted because the perturbation has (axi)symmetry.
  - ↳ the other states represent deformed orbits due to the field. A tiny field is sufficient to deform orbits and lift this perturbation.
  - ↳ the $|2,0,0\rangle$ state is normally metastable because two photons must be emitted to get $|1,0,0\rangle$ (to keep L constant). In the presence of an E field, it becomes much less stable because of the mixing with $|2,1,0\rangle$ (can decay with one photon).
- The ground state is nondegenerate with $E_{n=1}^{(1)} = 0$, but the state is perturbed (quadratic Stark effect)

$$|\psi\rangle = |1,0,0\rangle + e|\underline{E}|\sum_{n=2}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l}\frac{\langle n,l,m|z|1,0,0\rangle}{E_1 - E_n}|n,l,m\rangle$$

  - ↳ only states with $l=1, m=0$ survive
  - ↳ the perturbation of the ground state is interpreted as a polarisation – the field induces an electric dipole moment $\underline{D} = e\langle \underline{x}\rangle_\psi = \alpha\underline{E}$ with polarisability α



$$\alpha = -2e^2\sum_{n=2}^{\infty}\frac{|\langle n,1,0|z|1,0,0\rangle|^2}{E_1 - E_n} = \frac{9}{2}a_0^3$$

  - ↳ this dipole causes a 2nd order energy shift $E_{n=1}^{(2)} = -\frac{1}{2}\underline{E}\cdot\underline{D} = -\frac{9}{4}|\underline{E}|^2 a_0^3$

Time-dependent Perturbation Theory

- In the time-dependent case, we want to know how fast a quantum system changes in response to a perturbation
- $H(t) = H_0 + \Delta(t)$, where H_0 is the model Hamiltonian and Δ is the time-dependent perturbation
- Use the eigenstates of H_0 as a basis:
  - ↳ a general state is then $|\Psi(t)\rangle = \sum_n e^{-iE_n t/\hbar} a_n(t)|n\rangle$
  - ↳ coefficients a_n have time-dependence due to the perturbation
  - ↳ from the TDSE, $i\hbar\, \partial|\Psi(t)\rangle/\partial t = H(t)|\Psi(t)\rangle$

$$\Rightarrow \sum_n (a_n E_n + i\hbar \dot{a}_n) e^{-iE_n t/\hbar}|n\rangle = \sum_n (a_n E_n + \Delta(t)) e^{-iE_n t/\hbar}|n\rangle$$

  - ↳ contract with $\langle k|$

$$\Rightarrow i\hbar \dot{a}_k(t) = \sum_n a_n(t) e^{i(E_k - E_n)t/\hbar}\langle k|\Delta(t)|n\rangle$$

$$\Rightarrow a_k(t) = a_k(t_0) + \frac{1}{i\hbar}\int_{t_0}^{t}\sum_n a_n(t') e^{i(E_k - E_n)t'/\hbar}\langle k|\Delta(t')|n\rangle\, dt'$$

- $\dot{a}_n \neq 0$ only because of $\Delta(t)$, so we can approx $a_n(t') \approx a_n(t_0)$ (= const) in the integral
  - ↳ define $\omega_{kn} = (E_k - E_n)/\hbar$, then the first-order approx is:

$$\boxed{a_k(t) \approx a_k(t_0) + \frac{1}{i\hbar}\int_{t_0}^{t}\sum_n a_n(t_0) e^{i\omega_{kn}t'}\langle k|\Delta(t')|n\rangle\, dt'}$$

  - ↳ if we start in an eigenstate $|m\rangle$, $a_k(t_0) = \delta_{km}$

- Consider a QHO with some force $F_0 X e^{-t^2/\tau^2}$. If it was in state $|0\rangle$, $t \to -\infty$, what will its state be as $t \to \infty$?
  - ↳ $\lim_{t\to\infty} a_k(t) = -\frac{F_0}{i\hbar}\int_{-\infty}^{\infty} e^{ik\omega t'} e^{-t'^2/\tau^2}\langle k|X|0\rangle\, dt'$

$$= i\,\delta_{k1} F_0 \sqrt{\frac{\pi\hbar}{2m\omega}}\,\tau\, e^{-\omega^2\tau^2/4}$$

  - ↳ to first order, the state can only have transitioned to $|1\rangle$ with amplitude $\sim \frac{\tau^2}{\omega} e^{-\omega^2\tau^2/2}$.
- A common example is a time-independent perturbation $\Delta(X, P, \ldots)$ switched on at $t=0$, i.e. $\Delta(t) = \begin{cases} 0, & t \leq 0 \\ \Delta(X,P), & t > 0 \end{cases}$
  - ↳ if the system starts in eigenstate $|m\rangle$

$$a_k(t) \approx \delta_{km} + \frac{1}{i\hbar}\int_0^t e^{i\omega_{km}t}\langle k|\Delta|m\rangle\, dt'$$

  - ↳ the prob. of finding the system in state $|k\rangle$ at time t:

$$|a_k(t)|^2 = \frac{4}{\hbar^2}|\langle k|\Delta|m\rangle|^2\, \frac{\sin^2(\omega_{km}t/2)}{\omega_{km}^2}$$

- Define the transition rate $\boxed{\Gamma(|m\rangle \to |k\rangle) = \lim_{t\to\infty}\frac{\partial}{\partial t}|a_k(t)|^2}$
  - ↳ $\lim_{t\to\infty}\left(\sin^2(\omega_{km}t/2)/\omega_{km}^2 t\right) = \frac{\pi}{2}\delta(\omega_{km})$, so for the 'step function' perturbation, $\Gamma(|m\rangle \to |k\rangle) = \frac{2\pi}{\hbar}|\langle k|\Delta|m\rangle|^2\delta(E_k - E_m)$
  - ↳ so to first order, this type of perturbation will only cause transitions between states degenerate with $|m\rangle$

Fermi's Golden Rules

- An important special case is monochromatic perturbation
$$\Delta(t) = \Delta e^{-i\omega t} + \Delta^{+} e^{i\omega t}, \quad t \geq 0$$
  ↳ as before, start in $|m\rangle$
$$a_k(t) = \frac{\langle k|\Delta|m\rangle}{\hbar(\omega_{km}-\omega)}\left(e^{i(\omega_{km}-\omega)t}-1\right) + \frac{\langle k|\Delta^{+}|m\rangle}{\hbar(\omega_{km}+\omega)}\left(e^{i(\omega_{km}+\omega)t}-1\right)$$
  ↳ as $t \to \infty$, there will be transitions to states $|k\rangle$
  when either $E_k \approx E_m + \hbar\omega$ absorption
  $E_k \approx E_m - \hbar\omega$ stimulated emission
  ↳ the transition rate is then:
$$\Gamma(|m\rangle \to |k\rangle) = \frac{2\pi}{\hbar}|\langle k|\Delta|m\rangle|^2 \, \delta(E_k - E_m \mp \hbar\omega)$$
  Fermi's Golden rules
- In reality, the transition rate does not include perfect delta functions (else you would need infinitely precise ω). Nevertheless, monochromatic light does not cause appreciable transitions.
- In an isotropic radiation bath, there will be a range of frequencies from all directions
  ↳ use the dipole approx: $E(t)$ constant in space over the atomic lengthscale $\Rightarrow H = H_{atom} + e\,\underline{E}(t)\cdot\underline{X}$
  ↳ because of isotropy, $\overline{\underline{E}(t)} = 0$ and:
$$\overline{E_i(t_1)E_j(t_2)} = \delta_{ij}\cdot\frac{1}{6\varepsilon_0}\int_{-\infty}^{\infty}\rho(\omega)\,e^{-i\omega(t_1-t_2)}\,d\omega$$
  ↳ $\rho(\omega)$ is the energy density, $\varepsilon_0 \overline{\underline{E}^2(t)} = \int_0^{\infty}\rho(\omega)\,d\omega$

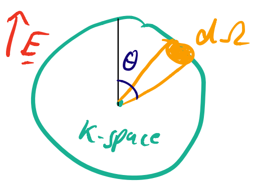
↳ treating $e\,\underline{E}(t)\cdot\underline{X}$ as a perturbation:
$$a_k(t) = -\frac{ie}{\hbar}\int_0^t e^{i\omega_{km}t'}\langle k|\underline{E}(t')\cdot\underline{X}|m\rangle\,dt'$$
$$\Rightarrow \overline{|a_k(t)|^2} = \frac{e^2}{\hbar^2}\int_0^t\int_0^t \overline{E_i(t_1)E_j(t_2)}\,e^{i\omega_{km}(t_1-t_2)}|\langle k|\underline{X}|m\rangle|^2\,dt_1\,dt_2$$
$$= \frac{4e^2|\langle k|\underline{X}|m\rangle|^2}{6\varepsilon_0\hbar^2}\int_{-\infty}^{\infty}\rho(\omega)\,\Big|\underbrace{\int_0^t e^{i(\omega_{km}-\omega)t'}\,dt'}_{\frac{\pi t}{2}\delta(\omega_{km}-\omega)}\Big|^2\,d\omega$$
↳ the transition rate thus depends on the energy density of the field at a particular freq:
$$\Gamma(|m\rangle \to |k\rangle) = \frac{\pi e^2\langle k|\underline{X}|m\rangle\cdot\langle m|\underline{X}|k\rangle}{3\varepsilon_0\hbar^2}\,\rho(\omega_{km})$$

- The absorption rate is equal to the stimulated emission rate because $\rho(\omega_{km})$ is an even function
  ↳ even isolated atoms may spontaneously decay due to random fluctuations in the vacuum
  ↳ Einstein showed this with a thermodynamical argument.
  $\Gamma_{m\to k} = \rho(\omega)\,B_{m\to k}(\omega_{km})$
  $\Gamma_{k\to m} = \rho(\omega)\,B_{k\to m}(\omega_{km})$
  $A_{k\to m}$ for spontaneous emission
  ↳ in equilibrium, $n_k[A_{k\to m} + \rho B_{k\to m}] = n_m \rho B_{m\to k}$
  and $\frac{n_m}{n_k} = \exp(\hbar\omega_{km}/k_BT)$, $\rho(\omega) = \frac{\hbar\omega^3}{\pi^2c^3}(e^{\hbar\omega/k_BT}-1)^{-1}$
  ↳ $A_{k\to n}$ must be independent of temp (as it is intrinsic)
$$\Rightarrow A_{k\to n}(\omega_{km}) = \frac{\hbar\omega_{km}^3}{\pi^2c^3}B_{m\to k}(\omega_{km})$$

Ionisation

- Sufficiently energetic radiation can ionise the atom, moving the electron into a continuum state.
- Consider the probability that H atom transitions from its ground state to a state in which the electron is a plane wave: $\langle \underline{x} | 100 \rangle = e^{-r/a} \sqrt{\pi/a^3} \to \langle \underline{x} | \underline{k} \rangle = e^{i\underline{k}\cdot\underline{x}} / (2\pi\hbar)^{3/2}$
  - ↳ neglect Coulomb potential for the free particle
  - ↳ in the dipole approximation:
    $$\Delta(t) = e\,(E_z z e^{-i\omega t} + E_z^* z e^{i\omega t})$$
  - ↳ the transition probability is then $|\langle \underline{k} | z | 100 \rangle|^2$
- Ionisation absorbs energy:
  $$\Gamma(|100\rangle \to |\underline{k}\rangle) = \frac{2\pi}{\hbar^2} e^2 \underline{E}^2 |\langle \underline{k} | z | 100 \rangle|^2 \delta(E_{\underline{k}} - E_{100} - \hbar\omega)$$
- The differential ionisation rate describes the rate of ionisation to momenta in range $(\underline{k}, \underline{k} + d\underline{k})$

$$\frac{d\Gamma(|100\rangle \to |\underline{k}\rangle)}{d\Omega} = \frac{256 e^2 \underline{E}^2 m_e \cos^2\theta}{\pi \hbar^3 |\underline{k}|^9 a^5}$$



  - ↳ valid for wavelengths much larger than the Bohr radius so we can apply Dipole approx
  - ↳ but λ small enough (freq high enough) so that we can neglect the binding energy E_{100}.

Interpreting QM

- We may not know what state the system is in, because real systems are never completely isolated.
- Suppose we think the system could be in one of the states $\{|\alpha\rangle\}$ with classical probabilities p_α for each
  - ↳ the density operator is $\rho = \sum_\alpha p_\alpha |\alpha\rangle\langle\alpha|$
  - ↳ ρ projects a state onto $|\alpha\rangle$ with probability p_α
  - ↳ $\{|\alpha\rangle\}$ do not need to be complete or orthogonal
- The density operator is defined by the properties:
  - ↳ $\rho = \rho^\dagger$
  - ↳ $\langle\phi|\rho|\phi\rangle \geq 0 \quad \forall |\phi\rangle \in \mathcal{H}$
  - ↳ $tr_{\mathcal{H}}(\rho) = 1$

  $\Longleftrightarrow$ probabilities are real, positive, sum to one.
- A system is pure if there is some $|\chi\rangle \in \mathcal{H}$ for which $\rho = |\chi\rangle\langle\chi|$, e.g. one $p_\alpha = 1$, rest are zero.
  - ↳ otherwise the state is impure/mixed.
  - ↳ for a pure state $\rho^2 = \rho$ so eigenvalues are 0 or 1.
- $\rho(t) = U(t)\rho(0)U^\dagger(t)$, so there is an extra minus sign in the Heisenberg equation of motion: $\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H, \rho(t)]$
- ☆ For a system described by ρ, the average value of some observable Q is $\boxed{tr(\rho Q) = \sum_\alpha p_\alpha \langle\alpha|Q|\alpha\rangle}$
  - ↳ combination of quantum and classical expectations
  - ↳ we thus never need to know the states $|\alpha\rangle$; just take trace

- A qubit is a 2-state system with basis $\{|\uparrow\rangle, |\downarrow\rangle\}$
  - ↳ any 2-state system in $\mathbb{C}^2$ can be written as an LC of identity and the Pauli matrices
    $$\rho = \frac{1}{2}(1_{\mathcal{H}} + \underline{b}\cdot\underline{\sigma}) = \frac{1}{2}\begin{pmatrix} 1+b_z & b_x - ib_y \\ b_x + ib_y & 1-b_z \end{pmatrix}$$
  - ↳ for both eigenvalues to be nonnegative, we need
    $$\det\rho = \frac{1}{4}(1-\underline{b}\cdot\underline{b}) \geq 0 \implies |\underline{b}| \leq 1$$
  - ↳ this defines the Bloch sphere
  - ↳ ρ is pure iff $|\underline{b}| = 1$
  - ↳ if $\underline{b} = \underline{0}$, $\rho = \frac{1}{2}1_{\mathcal{H}}$ so we are maximally ignorant
- We may want to copy a system so that we can measure different aspects of it without disturbing others
  - ↳ no cloning theorem: this is impossible
  - ↳ consider some unitary copying operator which copies a state $|\psi\rangle \in \mathcal{H}_1$ onto a state $|e\rangle \in \mathcal{H}_2$ (with some arbitrary phase)
    $$C: |\psi\rangle \otimes |e\rangle \mapsto e^{-i\alpha(\psi,e)}|\psi\rangle \otimes |\psi\rangle$$
  - ↳ $(\langle\phi|\langle e|)(|\psi\rangle|e\rangle) = (\langle\phi|\langle e|)C^\dagger C(|\psi\rangle|e\rangle) = e^{i(\alpha(\phi,e)-\alpha(\psi,e))}\langle\phi|\psi\rangle^2$
    $$\implies |\langle\phi|\psi\rangle| = |\langle\phi|\psi\rangle|^2 \implies |\langle\phi|\psi\rangle| = 0 \text{ or } 1$$
  - ↳ cannot be true for all $|\phi\rangle, |\psi\rangle \in \mathcal{H}_1$, so C cannot exist.
- To measure the impurity of a system we can use the von Neumann entropy: $S(\rho) = -\mathrm{tr}_{\mathcal{H}}(\rho\ln\rho)$
  - ↳ ρ eigenvalues $\in[0,1]$, so $S(\rho)\geq 0$ with equality iff ρ pure
  - ↳ S concave: entropy of combined subsystems always $\geq$ sum of subsystem entropies: $S(\sum_i \lambda_i\rho_i) \geq \sum_i \lambda_i S(\rho_i)$
- The density operator with maximum ignorance can be found with Lagrange multipliers. Extremise $S(\rho) - \lambda(1-\mathrm{tr}_{\mathcal{H}}\rho)$:
  $$-\mathrm{tr}_{\mathcal{H}}(\delta\rho\ln\rho + \rho\rho^{-1}\delta\rho - \lambda\delta\rho) = 0 \quad (1)$$
  $$\delta\lambda(\mathrm{tr}_{\mathcal{H}}\rho - 1) = 0 \quad (2)$$
  - ↳ (1) $\implies \ln\rho + 1 - \lambda = 0 \implies \rho = e^{\lambda-1}1_{\mathcal{H}}$
  - ↳ (2) fixes the constant $e^{\lambda-1}$
  - ↳ $\rho_{max} = \frac{1}{\dim(\mathcal{H})}1_{\mathcal{H}}$, $S(\rho_{max}) = \ln\dim(\mathcal{H})$

Entanglement

- For some Hilbert space $\mathcal{H} \cong \mathcal{H}_A\otimes\mathcal{H}_B$ describing a system and its surroundings, a state $|\Psi\rangle\in\mathcal{H}$ is entangled if it cannot be written as a simple product $|\Psi\rangle = |\phi\rangle\otimes|\psi\rangle$
  - ↳ e.g for a qubit $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)|\downarrow\rangle$ is not entangled; $|EPR\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$ is entangled
  - ↳ entanglement means that subsystem states are correlated.
- The reduced density operator for subsystem A is given by $\rho_A = \mathrm{tr}_{\mathcal{H}_B}(\rho_{AB})$, i.e 'sum over' B.
  - ↳ an observable which only depends on A has the form $Q = Q_A\otimes 1_B$ and has expectation $\mathrm{tr}_{\mathcal{H}_A\otimes\mathcal{H}_B}(\rho_{AB}(Q_A\otimes 1_B)) = \mathrm{tr}_{\mathcal{H}_A}(\rho_A Q_A)$
  - ↳ this agrees with the result for an isolated system.
- The entanglement entropy quantifies the entanglement. It is the Von Neumann entropy of the reduced density:
  $$S_A = -\mathrm{tr}_{\mathcal{H}_A}(\rho_A\ln\rho_A)$$

↳ if ρ_{AB} is pure and unentangled, $S_A = 0$

↳ if ρ_{AB} is pure but entangled, $S_A > 0$ even though $S_{A\cup B} = 0$

↳ so tracing over B also loses info about A

- If the total system is pure, the entanglement entropy is symmetric, i.e $S_A = S_B$.
- Unlike Von Neumann entropy, entanglement entropy is subadditive: whole is at most the sum of parts. $S_{A\cup B} \leq S_A + S_B$

  ↳ in fact strongly subadditive: $S_{A\cup B\cup C} \leq S_{A\cup B} + S_{B\cup C} - S_B$

Decoherence

- Suppose the whole universe were in a pure and unentangled state at $t=0$, with $\rho(0) = |\Psi_0\rangle\langle\Psi_0|$ for $|\Psi_0\rangle = |\phi\rangle \otimes |\psi\rangle$ where $|\phi\rangle \in \mathcal{H}_A$, $|\psi\rangle \in \mathcal{H}_B$
- Under time evolution, $\rho(t) = U_{AB}(t)\,\rho(0)\,U_{AB}^\dagger(t)$
- If A starts off as pure and doesn't interact with B, then it remains in a pure state

  ↳ i.e $H_{AB} = H_A + H_B$ $\quad [H_A, H_B] = 0 \Rightarrow U_{AB}(t) = U_A(t) \otimes U_B(t)$

  ↳ then $\rho_A(t) = tr_{\mathcal{H}_B}\, \rho_{AB}(t) = |\phi(t)\rangle\langle\phi(t)|$
- Generally, there will be some coupling, so:

$$\rho_A(t) = tr_{\mathcal{H}_B}\left(U_{AB}(t)\,|\Psi_0\rangle\langle\Psi_0|\,U_{AB}^\dagger(t)\right)$$

  ↳ can think of this in terms of matrix elements $M_\beta(t) = \langle\beta|U_{AB}(t)|\chi\rangle$ between the original states evolved in time and basis states $\{|\beta\rangle\}$ of $\mathcal{H}_B$ $\quad \Rightarrow \rho_A(t) = \sum_\beta M_\beta(t)\,\rho_A(0)\,M_\beta^\dagger(t)$

  ↳ $M_\beta(t)$ is a unitary operator on $\mathcal{H}_A$

  ↳ interactions then cause a pure $\rho(0)$ to become entangled.

- Consider system A as a qubit, with system B being some measuring apparatus with basis $\{|0\rangle, |1\rangle, |2\rangle\}$

  ↳ B initially in state $|0\rangle$; ideally, will change to $|1\rangle$ or $|2\rangle$ depending on A being $|\uparrow\rangle$ or $|\downarrow\rangle$ without changing A.

  ↳ this will happen with some probability:

$$U(|\uparrow\rangle \otimes |0\rangle) = |\uparrow\rangle\left(\sqrt{1-p}\,|0\rangle + \sqrt{p}\,|1\rangle\right)$$
$$U(|\downarrow\rangle \otimes |0\rangle) = |\downarrow\rangle\left(\sqrt{1-p}\,|0\rangle + \sqrt{p}\,|2\rangle\right)$$

  ↳ for this evolution, $M_\beta = \langle\beta|U|0\rangle$:

$$M_0 = \langle 0|U|0\rangle = \sqrt{1-p}\,\mathbb{1}_A$$
$$M_1 = \langle 1|U|0\rangle = \sqrt{p}\,|\uparrow\rangle\langle\uparrow|, \quad M_2 = \langle 2|U|0\rangle = \sqrt{p}\,|\downarrow\rangle\langle\downarrow|$$

  ↳ combining these, ρ_A evolves as

$$\begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix} \longrightarrow \begin{pmatrix} \rho_{\uparrow\uparrow} & (1-p)\rho_{\uparrow\downarrow} \\ (1-p)\rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix}$$

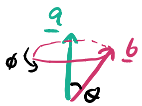
  ↳ or if we define a probability rate $\Gamma = p/\delta t$,

$$\lim_{t\to\infty} \rho_A(t) = \lim_{t\to\infty}\begin{pmatrix} |a|^2 & e^{-\Gamma t}\bar{a}b \\ e^{-\Gamma t}\bar{b}a & |b|^2 \end{pmatrix} = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}$$

- Hence even if A is initially in some quantum superposition, entanglement results in phase damping: system is a classical superposition (still probabilistic, but not quantum).

The EPR Gedankenexperiment ← thought experiment

- Measuring the properties of one particle entangled with another violates locality: spooky action
- Consider e^-e^+ pair in the state $|EPR\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$, give e^- to Alice and e^+ to Bob
  - ↳ A measures the spin along axis $\underline{a}$ of her choice. In the Copenhagen interpretation, if A measures $+\hbar/2$, we know the state collapsed to $|EPR\rangle = |\uparrow_a\rangle|\downarrow_a\rangle$
  - ↳ B measures spin of e^+ along $\underline{b}$



$$|\uparrow_b\rangle = \cos\left(\tfrac{\theta}{2}\right)e^{-i\phi/2}|\uparrow_a\rangle + \sin\left(\tfrac{\theta}{2}\right)e^{i\phi/2}|\downarrow_a\rangle$$

  - ↳ because A found e^- in $|\uparrow_a\rangle$, B finds e^+ in $|\uparrow_b\rangle$ with prob $|\langle\uparrow_b|\downarrow_a\rangle|^2 = \sin^2\left(\tfrac{\theta}{2}\right)$
- Einstein objects that this means A can affect B instantaneously
  - ↳ proposed that when e^-e^+ was created, some hidden variable $\underline{v} \in \mathbb{R}^N$ was fixed, which completely determines the result of a spin measurement along $\underline{a}$
  - ↳ this would mean A, B measurements are correlated so no spooky action
  - ↳ i.e. spin is a function $S_e(\underline{a},\underline{v})$ that deterministically gives $\{+\frac{\hbar}{2}, -\frac{\hbar}{2}\}$. Uncertain because we don't know $\underline{v}$
- If Hidden variable theory is true, let $\underline{v}$ have some classical prob dist. We are then interested in the quantity

$$\langle S_e(\underline{a})\, S_p(\underline{b})\rangle = \int_{\mathbb{R}^n} S_e(\underline{a},\underline{v})\, S_p(\underline{b},\underline{v})\, \rho(\underline{v})\, d^n v$$

Bell's inequality

- Bell explored the consequences of Hidden variable theory.
- $\langle S_e(\underline{a})S_p(\underline{b})\rangle$ hard to compute. Bob could choose to measure along $\underline{b}'$ instead, so consider

$$\langle S_e(\underline{a})S_p(\underline{b})\rangle - \langle S_e(\underline{a})S_p(\underline{b}')\rangle = \int_{\mathbb{R}^n} S_e(\underline{a},\underline{v})[S_p(\underline{b},\underline{v}) - S_p(\underline{b}',\underline{v})]\rho(\underline{v})d^n v$$

  - ↳ cons angular momentum $\Rightarrow S_e(\underline{a},\underline{v}) + S_p(\underline{a},\underline{v}) = 0$, and $S_p(\underline{b},\underline{v})^2 = \frac{\hbar^2}{4}$ always:

$$LHS = -\int_{\mathbb{R}^n} \underbrace{S_p(\underline{a},\underline{v})\, S_p(\underline{b},\underline{v})}_{\text{fluctuates between } \pm\hbar^2/4}\left[1 - \frac{4}{\hbar^2}S_p(\underline{b},\underline{v})S_p(\underline{b}',\underline{v})\right]\rho(\underline{v})d^n v$$

  - ↳ result is Bell's inequality:

$$|\langle S_p(\underline{a})S_p(\underline{b})\rangle - \langle S_p(\underline{a})S_p(\underline{b}')\rangle| \le \frac{\hbar^2}{4} - \langle S_p(\underline{b})S_p(\underline{b}')\rangle$$

☆ · $\boxed{\text{QM violates Bell's inequality}}$

  - ↳ cons angular momentum: $(\underline{S}_e \otimes 1_p + 1_e \otimes \underline{S}_p)|EPR\rangle = 0$
  - ↳ measuring e^- along $\underline{a}$ and e^+ along $\underline{b}$:

$$(\underline{a}\cdot\underline{S}_e \otimes 1_p)(1_e \otimes \underline{b}\cdot\underline{S}_p)|EPR\rangle = -1_e \otimes ((\underline{a}\cdot\underline{S}_p)(\underline{b}\cdot\underline{S}_p))|EPR\rangle$$

$$\Rightarrow \langle(\underline{a}\cdot\underline{S}_p)(\underline{b}\cdot\underline{S}_p)\rangle_{EPR} = \hbar^2\, \underline{a}\cdot\underline{b}/4$$

  - ↳ LHS of Bell's ineq: $\frac{\hbar^2}{4}|\underline{a}\cdot(\underline{b}-\underline{b}')|$
  - ↳ RHS of Bell's ineq: $\frac{\hbar^2}{4}(1-\underline{b}\cdot\underline{b}')$
  - ↳ RHS can be < LHS, violating Bell's inequality
- Hence QM is inconsistent with Hidden variable theory, so we just need to test which is correct.
- However, Bell's inequality is hard to test experimentally

CHSH inequality

- The Clauser-Horne-Shimony-Holt inequality is similar to Bell's inequality but easier to test:
  - ↳ WLOG, Alice and Bob measure either $\{+1, -1\}$ depending on some hidden var $\underline{v} \in \mathbb{R}^n$
  - ↳ define the LC $C = (a_1 + a_2)b_1 + (a_1 - a_2)b_2$
  - ↳ depending on $\underline{v}$, either $a_1(\underline{v}) + a_2(\underline{v}) = \pm 2$ & $a_1(\underline{v}) - a_2(\underline{v}) = 0$
    OR $a_1(\underline{v}) + a_2(\underline{v}) = 0$ & $a_1(\underline{v}) - a_2(\underline{v}) = \pm 2$
  - ↳ so the CHSH ineq is $-2 \leq \langle C \rangle \leq 2$
- In QM, replace measurements a, b with commuting operators A, B with eigenvalues ± 1
  - ↳ $A_i^2 = B_j^2 = \pm 1 \quad \therefore \; C^2 = 4 - [A_1, A_2][B_1, B_2]$
  - ↳ $|\langle [A_1, A_2] \rangle| \leq |\langle A_1 A_2 \rangle| + |\langle A_2 A_1 \rangle| \leq 2$ and $\langle Q^2 \rangle \geq \langle Q \rangle^2$ for any Hermitian Q
  - ↳ these combine to give the Tsirelson bound $-2\sqrt{2} \leq \langle C \rangle \leq 2\sqrt{2}$, which can violate CHSH
- Experiment shows $\langle C \rangle > 2$, so Hidden var theory is <u>wrong</u>.