II Principles of Quantum Mechanics

Aims: • provide systematic study of QM from the abstract Dirac framework
- ground formalism with physical intuition
- understand role of symmetries, representations in QM
- perturb systems to reach realistic description (see AQM)
- discuss QM interpretations, the measurement problem

Def^n of Hilbert Space Vector space $\mathcal{H}$ over $\mathbb{C}$, with an inner product $(\,,\,)$ making $\mathcal{H}$ complete.

$(\phi,\psi) = \overline{(\psi,\phi)}$, $(\phi, a\psi) = (\phi,\psi)a$, $(\phi,\phi) \geq 0$ equal iff $\phi = 0$

Note anti-linear in first argument (physics convention)

Obtain norm $\|\psi\| = \sqrt{(\psi,\psi)}$, have C-S $|(\phi,\psi)| \leq \|\phi\|\|\psi\|$

Completeness $\Rightarrow$ $\sum_{n=1}^{\infty} \phi_n$ converges if $\sum_{n=1}^{\infty} \|\phi_n\| < \infty$

Some Rmks VECTOR SPACES ∴ but ∞-dim subtlety

blah, blah, VS in physics are very nice

Weirdness of superposing states, $\frac{1}{\sqrt{2}}|$  $\rangle + \frac{1}{\sqrt{2}}|$  $\rangle$

Suspicious vector spaces, linear approximations ∴, but QM so linear

Examples Finite dimension $\mathbb{C}^n$ with $(\underline{v},\underline{u}) = \sum_{i=1}^{n} \overline{v_i} u_i$

In QM, these arise as
- toy model, illustrate general phenomenon
- approximation (maybe only low energy relevant)
- subspace of larger space { fixed energy / fixed ang momentum

Simple generalisation ℓ^2, space of sequences $\underline{u} = (u_1, u_2, \ldots)$ s.t. $\|\underline{u}\|^2 = \sum |u_i|^2 < \infty$, with $(\underline{v},\underline{u}) = \sum \overline{v_i} u_i$

By C-S have $(\underline{v},\underline{u}) < \infty$

These could arise as
- wavefunctions of particle on a circle, $\psi(\theta) = \sum_{n\in\mathbb{Z}} a_n e^{in\theta}$

  $\|\psi\|^2 = \int_0^{2\pi} |\psi|^2 d\theta = 2\pi \sum_n |a_n|^2$ ~ Parseval
- bound states of a potential, e.g. harmonic oscillator

  $\psi(x) = \sum_n a_n H_n(x) e^{-\alpha x^2}$, $H_n(x)$ Hermite poly, $\|\psi\|^2 = \sum_n |a_n|^2$

Important example $L^2(\mathbb{R}, dx)$

Inner product is $(\phi, \psi) = \int_{\mathbb{R}} \overline{\phi(x)}\, \psi(x)\, dx$, converges by C-S

These describe wavefunctions of particle on $\mathbb{R}$.

In general, ψ need not be smooth, diff or even cts

⌜ $L^2(\mathbb{R}, dx)$ is really an equiv class of functions with agree almost every

Suppose $\phi(x) = \mathbb{1}_{\mathbb{Z}}(x)$. Then $\|\phi\|^2 = 0$. So ϕ ought to be zero ⌟

Dual Spaces

The dual $\mathcal{H}^*$ of a Hilbert space $\mathcal{H}$ is the space of lin maps $f: \mathcal{H} \to \mathbb{C}$

- Can use inner product to construte these, e.g. for $\phi \in \mathcal{H}$, $(\phi, \cdot) \in \mathcal{H}^*$
  - > When $\dim(\mathcal{H}) < \infty$, showed all elts of $\mathcal{H}^*$ like this, so $\mathcal{H} \cong \mathcal{H}^*$
  - > $\mathcal{H}^*$ inherits an IP from that on $\mathcal{H}$, and $\|f_\phi\|_{\mathcal{H}^*} = \|\phi\|_{\mathcal{H}}$
- Reisz rep thm says this also holds for ∞-dim $\mathcal{H}$

⌜ Technically, look at space of <u>continuous</u> functionals on $\mathcal{H}$

E.g. Dirac delta gives functional, but not continuous ⌟

Dirac Notation

- If $\psi \in \mathcal{H}$, place it within a ket, $|\psi\rangle$
- If $\chi \in \mathcal{H}^*$, place within a bra, $\langle \chi|$

Then IP between $|\psi\rangle, |\phi\rangle$ is written as $\langle \phi | \psi \rangle$, bra-ket

Continuum States

Suppose $\mathcal{H} \cong \mathbb{C}^n$ or ℓ^2. Then can expand in orthonormal basis $|\psi\rangle = \sum a_n |\phi_n\rangle$

Extend to $L^2(\mathbb{R}, dx)$ via continuum states

- For $x \in \mathbb{R}$, have a continuum state $|x\rangle$ such that $\langle x'|x\rangle = \delta(x - x')$
- Expand $|\psi\rangle = \int_{\mathbb{R}} \psi(x')\, |x'\rangle\, dx'$. Coeffs are the wavefunction in the position basis, $\langle x|\psi\rangle = \int_{\mathbb{R}} \psi(x') \langle x|x'\rangle\, dx' = \psi(x)$.
- Normalisation ensures

$$\langle \phi|\psi\rangle = \int \overline{\phi(x')}\, \psi(x) \langle x'|x\rangle\, dx' dx = \int \overline{\phi(x)}\, \psi(x)\, dx$$

but also implies $\langle x|x\rangle = \delta(0)$?? so continuum states not in $L^2(\mathbb{R}, dx)$

Different bases

- Can equally well expand in momentum basis $\{|p\rangle\}$

$$|\psi\rangle = \int \psi(x)|x\rangle\, dx = \int \tilde{\psi}(p)|p\rangle\, dp$$

where new exp^n coeffs $\tilde{\psi}(p)$ are the wavef^n in the momentum basis

- We'll show later that $\langle x|p\rangle = e^{ixp/\hbar}/\sqrt{2\pi\hbar}$. Using this

$$\psi(x) = \langle x|\psi\rangle = \int \tilde{\psi}(p)\langle x|p\rangle\, dp = \int e^{ixp/\hbar}\tilde{\psi}(p)\frac{dp}{\sqrt{2\pi\hbar}}$$

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int \psi(x)\langle p|x\rangle\, dx = \int e^{-ixp/\hbar}\psi(x)\frac{dx}{\sqrt{2\pi\hbar}}$$

so momentum, space wavefunctions related by a Fourier transform.

Tensor products

To build complicated systems use tensor product

- Suppose $\dim(\mathcal{H}_1), \dim(\mathcal{H}_2) < \infty$; let $\{|e_a\rangle\}, \{|f_\alpha\rangle\}$ be orthonormal bases for $\mathcal{H}_1, \mathcal{H}_2$. Then

$$\mathcal{H}_1 \otimes \mathcal{H}_2 \ni |\psi\rangle = \sum_{a,\alpha} c_{a\alpha}|e_a\rangle \otimes |f_\alpha\rangle$$

$\{|e_a\rangle \otimes |f_\alpha\rangle\}$ are basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$

- The inner product to make basis orthonormal
- If $\{|x\rangle\}$ and $\{|y\rangle\}$ are continuum states for particles moving in the x and y directions, then a particle in $\mathbb{R}^2$ is described by

$$|\psi\rangle = \int_{\mathbb{R}^2} \psi(x,y)|x\rangle \otimes |y\rangle\, dx\, dy$$

Again, inner product $\langle\phi|\psi\rangle = \int \overline{\chi(x',y')}\,\psi(x,y)\langle x'|x\rangle\langle y'|y\rangle\, d^2x\, d^2x'$

[Technically, need to take completion of tensor product]

We'll often use shorthand

$$|\psi\rangle = \int \psi(\underline{x})|\underline{x}\rangle\, d^3x \quad \text{where } \psi(\underline{x}) = \psi(x,y,z) \text{ and } |\underline{x}\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle$$

Quantum systems with internal structure

- Hydrogen atom with e^-, p so described by

$$|\underline{\Psi}\rangle = \int \underline{\Psi}(\underline{x}_e, \underline{x}_p)|\underline{x}_e\rangle \otimes |\underline{x}_p\rangle\, d^3x_e\, d^3x_p \in L^2(\mathbb{R}^6, d^3x_e d^3x_p)$$

> Can also introduce $\underline{x}_{rel} = \underline{x}_e - \underline{x}_p$ and $\underline{x}_{cm} = \frac{m_e\underline{x}_e + m_p\underline{x}_p}{m_e + m_p}$ and do

$$|\underline{\Psi}\rangle = \int \underline{\Psi}'(\underline{x}_{cm}, \underline{x}_{rel})|\underline{x}_{rel}\rangle \otimes |\underline{x}_{cm}\rangle\, d^3x_{cm}\, d^3x_{rel}$$

This is often more convenient, usually only care about simple states wrt this basis, e.g. $\underline{\Psi}'(\underline{x}_{cm}, \underline{x}_{rel}) = e^{i\underline{k}\cdot\underline{x}_{cm}}\psi(\underline{x}_{rel})$

- More generally, wavefn of N-particle system lives in
$L^2(\mathbb{R}^{3N}, d^{3N}x) \cong L^2(\mathbb{R}^3, d^3x_1) \hat{\otimes} \cdots \hat{\otimes} L^2(\mathbb{R}^3, d^3x_N)$
- Spin means electrons are actually described by a pair of wavefn's
$|\Psi\rangle \in L^2(\mathbb{R}^3, d^3x) \otimes \mathbb{C}^2$ with $\Psi(\underline{x}) = \begin{pmatrix} \psi_\uparrow(\underline{x}) \\ \psi_\downarrow(\underline{x}) \end{pmatrix}$

TLDW Quantum systems described by $|\psi\rangle \in \mathcal{H}$, Hilbert space
Choice of $\mathcal{H}$ depends of system under study; variable dimension
In Dirac notation, IP is $\langle\chi|\psi\rangle$ e.g. in $L^2(\mathbb{R}, dx)$ is $\int \overline{\chi(x)}\psi(x)\,dx$
Physical information contained in abstract vector $|\psi\rangle \in \mathcal{H}$ not wrt basis

Linear Operators

In finite dimensions, a lin operator is a lin map $A: \mathcal{H} \to \mathcal{H}$

- Operators form an associative but not commutative algebra over $\mathbb{C}$
  - $(\alpha A + \beta B) : |\psi\rangle \mapsto \alpha A|\psi\rangle + \beta B|\psi\rangle \quad \forall \alpha, \beta \in \mathbb{C}, |\psi\rangle \in \mathcal{H}$
  - product via $AB : |\psi\rangle \mapsto A(B|\psi\rangle)$
- We define the commutator of A and B via $[A,B] = AB - BA$. Then
  - antisymm, > linear, > Leibniz rule $[A,BC] = B[A,C] + [A,B]C$
  - > Jacobi identity $[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$
- The inner product allows def^n of the adjoint $A^\dagger$ of an operator A by $\langle\phi|A^\dagger|\psi\rangle = \overline{\langle\psi|A|\phi\rangle}$ for all $|\psi\rangle, |\phi\rangle \in \mathcal{H}$
  - $(A+B)^\dagger = A^\dagger + B^\dagger$, $(AB)^\dagger = B^\dagger A^\dagger$, $(A^\dagger)^\dagger = A$
  - An operator is self-adjoint or Hermitian if $A^\dagger = A$

Eigenstates, eigenvalues

State $|\psi\rangle$ is eigenstate of op A if $A|\psi\rangle = a|\psi\rangle$ for some $a \in \mathbb{C}$, call a the eigenvalue.

- In Dirac notation, often label states via eigenvalues $A|a\rangle = a|a\rangle$

Spose $A, B, C, \ldots$ commute, label eigenstates $|a, b, c, \ldots\rangle$

- If Q is Hermitian, $Q|q\rangle = q|q\rangle$, then
  - $q\langle q|q\rangle = \langle q|Q|q\rangle = \overline{\langle q|Q|q\rangle} = \bar{q}\langle q|q\rangle$, so $q \in \mathbb{R}$
  - $(q_1 - q_2)\langle q_2|q_1\rangle = \langle q_2|Q|q_1\rangle - \overline{\langle q_1|Q|q_2\rangle} = 0$

    so if $q_1 \neq q_2$ then $\langle q_2|q_1\rangle = 0$

Set $\{|n\rangle\}$ of eigenstates of a Hermitian op form an orthonormal basis

- $Q = \sum_n q_n |n\rangle\langle n|$ so that $Q|\psi\rangle = Q\left(\sum_n c_n |n\rangle\right) = \sum_n c_n q_n |n\rangle$
  - identity operator on $\mathcal{H}$ can be written $1_{\mathcal{H}} = \sum_n |n\rangle\langle n|$
  - $f(Q) = \sum_n f(q_n)|n\rangle\langle n|$ defines $f(Q)$ provided $f(q_n)$ exist
- Matrix elements of an operator are $A_{km} = \langle k|A|m\rangle$ in this basis
  - $(AB)_{km} = \sum_n \langle k|A|n\rangle\langle n|B|m\rangle = \sum_n A_{kn} B_{nm}$ so composition as usual

Operators on ∞-dim Hilbert spaces

Ops on ∞-dim Hilb spcs such as $L^2(\mathbb{R}, dx)$ are more subtle

- Act on $\psi(x)$ as linear diff operators
- Operator A is <u>bounded</u> if $\exists M \in \mathbb{R}$ with $\| A|\psi\rangle \| < M \| \psi \|$ for $|\psi\rangle \in \mathcal{H}$
  - > bounded operators are lin maps $A : \mathcal{H} \to \mathcal{H}$
  - > unbounded operators restricted to some subspace $\mathrm{Dom}(A) \subset \mathcal{H}$
- position, momentum operators X, P are unbounded
  - > $x\psi(x)$ or $-i\hbar \frac{\partial}{\partial x}\psi$ many be non-normalizable even when $\|\psi\| < \infty$
  - > unbounded operators do not have normalizable eigenstates

    $\psi(x) = e^{ikx}$ eigenstate of $-i\hbar \partial/\partial x$

Using continuum states avoids / hides this complication

$$\begin{aligned} \langle x|P|\psi\rangle &= \int \langle x|p\rangle\langle p|P|\psi\rangle \, dp \\ &= \int e^{ixp/\hbar}\, p\, \tilde{\psi}(p) \frac{dp}{\sqrt{2\pi\hbar}} \\ &= -i\hbar \frac{\partial}{\partial x} \int e^{ixp/\hbar} \tilde{\psi}(p) \frac{dp}{\sqrt{2\pi\hbar}} \\ &= -i\hbar \frac{\partial}{\partial x} \langle x|\psi\rangle \end{aligned}$$

Operators on composite systems

Let $\{|e_a\rangle\}$ be a basis of $\mathcal{H}_1$, and $A : \mathcal{H}_1 \to \mathcal{H}_1$ lin op

Likewise $\{|f_\alpha\rangle\}$ for $\mathcal{H}_2$, $B : \mathcal{H}_2 \to \mathcal{H}_2$.

Define $A \otimes B$ by $(A \otimes B)(|e_a\rangle \otimes |f_\alpha\rangle) = (A|e_a\rangle) \otimes (B|f_\alpha\rangle)$

on basis elements and extend to all of $\mathcal{H}_1 \otimes \mathcal{H}_2$ by linearity

- $[A \otimes 1_{\mathcal{H}_2}, 1_{\mathcal{H}_1} \otimes B] = 0$ for all A, B
- Hydrogen atom described (roughly) by Hamiltonian

$$H = \frac{\underline{P}_p^2}{2m_p} \otimes 1_e + 1_p \otimes \frac{\underline{P}_e^2}{2m_e} - \frac{q^2}{4\pi\varepsilon_0} \frac{1}{|\underline{X}_e - \underline{X}_p|}$$

$(\underline{P}^2 = P_x^2 + P_y^2 + P_z^2)$

Using the isomorphism $L^2(\mathbb{R}^3_p \times \mathbb{R}^3_e) \cong L^2(\mathbb{R}^3_{cm} \times \mathbb{R}^3_{rel})$,

$$H = \frac{\underline{P}_{cm}^2}{2M} \otimes 1_{rel} + 1_{cm} \otimes \left[\frac{\underline{P}_{rel}^2}{2\mu} - \frac{q^2}{4\pi\varepsilon_0} \frac{1}{|\underline{X}_{rel}|} \right]$$

where $M = m_e + m_p$, $\mu = \frac{m_e m_p}{M}$, $\underline{P}_{cm} = \underline{P}_e + \underline{P}_p$, $\underline{P}_{rel} = \frac{m_p \underline{P}_e - m_e \underline{P}_p}{M}$

Postulates of Quantum Mechanics I

- The state of our system is specified by $|\psi\rangle \in \mathcal{H}$, $|\psi\rangle \neq |0\rangle$
- Any complete set of orthogonal states $\{|\phi_1\rangle, |\phi_2\rangle, \ldots\}$ is in 1-1 correspondence with the possible outcomes of a measurement
- The prob we observe that for $|\phi_n\rangle$ is $\dfrac{|\langle\phi_n|\psi\rangle|^2}{\langle\phi_n|\phi_n\rangle\langle\psi|\psi\rangle}$ ← can make 1

Born's rule is indep of scale of $|\psi\rangle, |\phi_n\rangle$

- Physical states really correspond to rays through the origin of $\mathcal{H}$ with $|\psi_1\rangle, |\psi_2\rangle$ in same ray if $|\psi_1\rangle = \lambda|\psi_2\rangle$ for $\lambda \in \mathbb{C}^\times$
  - > Geometrically, this is the projective Hilbert space $\mathbb{P}\mathcal{H}$
  - > Often simplest to pick representatives $\|\psi\| = \|\phi_n\| = 1$, phase though

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- Observable quantities are rep by Hermitian lin ops
- The expectation value $\langle Q\rangle_\psi$ of property corresponding to Q in state $|\psi\rangle$ is $\langle Q\rangle_\psi = \langle\psi|Q|\psi\rangle / \langle\psi|\psi\rangle$

We define rms deviation or uncertainty $\Delta_\psi Q$ of Q in state $|\psi\rangle$ as $\Delta_\psi Q = \sqrt{\langle Q^2\rangle_\psi - \langle Q\rangle_\psi^2}$

- Since Q is Hermitian, $\langle Q^2\rangle_\psi - \langle Q\rangle_\psi^2 = \langle\psi|(Q-\langle Q\rangle_\psi)^2|\psi\rangle$
  $= \|(Q-\langle Q\rangle_\psi)|\psi\rangle\|^2 \geq 0$,

so $\Delta_\psi Q$ is well defined, vanishes iff $Q|\psi\rangle = q|\psi\rangle$, some q

- Uncertainty principle for Hermitian A, B
  - > Let $|\psi_A\rangle = A|\psi\rangle - \langle A\rangle_\psi|\psi\rangle$, similarly for $|\psi_B\rangle$
  - > Then $\|\psi_A\| = \Delta_\psi A$, $\langle\psi_A|\psi_B\rangle = \langle\psi|AB|\psi\rangle - \langle A\rangle_\psi\langle B\rangle_\psi$
  - > $2i\,\mathrm{Im}\langle\psi_A|\psi_B\rangle = \langle\psi|AB|\psi\rangle - \overline{\langle\psi|AB|\psi\rangle}$
    $= \langle\psi|[A,B]|\psi\rangle$
  - > so by C-S, $(\Delta_\psi A)(\Delta_\psi B) = \|\psi_A\|\|\psi_B\| \geq |\langle\psi_A|\psi_B\rangle|$
    $\geq |\langle[A,B]\rangle_\psi|/2$

Remarks Nothing said about how we carry out a measurement

- In the Copenhagen interpretation, state collapses after we measure
- If we actually find a result q upon measuring Q, then immediately after the measurement $|\psi\rangle \rightsquigarrow |q\rangle$
- The Copenhagen interpretation doesn't say how/when collapse happens

At the least, carrying out a measurement involves coupling our system to some measuring apparatus – i.e. a change in the system's Hamiltonian

- Measuring property Q has nothing to do with applying Q to $|\psi\rangle$

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- The dynamical evolution of a system governed by

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \quad , \text{ TDSE}$$

for some operator H known as the Hamiltonian

- The form of H depends on the system
  - > often specify $H = H(\underline{X}, \underline{P}, \ldots)$
  - > suitably interpreted TDSE still applies relativistically
- Hilbert space does not involve time
  - > eg never integrate over t computing inner product on $L^2(\mathbb{R}, dx)$
  - > state $|\psi\rangle$ evolves but $\||\psi\|$ remains constant
- In Copenhagen interpretation, TDSE applies except during collapse

This is unsatisfactory :(

TLDW
- Operators are lin maps $A: \mathcal{H} \to \mathcal{H}$, form associative algebra
- Hermitian operators have real evals q and orthogonal estates

  They correspond to observables
- Certain to obtain result q when measuring Q iff $Q|\psi\rangle = q|\psi\rangle$

  Born rule gives probability of getting result for some estate
- Dynamics governed by TDSE, $i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$

Harmonic oscillators

- Any generic potential looks harmonic near a minimum → ubiquitous

Raising & lowering operators

The Hamiltonian of the d=1 harmonic oscillator is

$$H = \frac{1}{2m} P^2 + \frac{1}{2} m\omega^2 X^2$$

- Introduce dimensionless operators

$$A = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega X + iP) \quad , \quad A^\dagger = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega X - iP) \quad \text{s.t.}$$

$$A^\dagger A = \frac{1}{2m\hbar\omega} \left(P^2 + m^2\omega^2 X^2 + im\omega [X, P] \right) = \frac{H}{\hbar\omega} - \frac{1}{2}$$

- So can express

$$H = \hbar\omega (A^\dagger A + \tfrac{1}{2}) = \hbar\omega (N + \tfrac{1}{2})$$

↖ Hermitian number operator

Spectrum of N (and so H)

- From $[X, P] = i\hbar$; show that

$$[A, A^\dagger] = \frac{1}{2m\hbar\omega} ([m\omega X + iP, m\omega X - iP])$$
$$= \frac{-im\omega}{2m\hbar\omega} ([X, P] - [P, X]) = 1$$

and of course $[A, A] = [A^\dagger, A^\dagger] = 0$

▷ consequently $[N, A^\dagger] = A^\dagger [A, A^\dagger] = A^\dagger$,

$$[N, A] = -A$$

- This allows computation of spectrum of N

▷ Let $|n\rangle$ be normalized eigenstate $N|n\rangle = n|n\rangle$; $\langle n|n\rangle = 1$

▷ $NA^\dagger |n\rangle = ([N, A^\dagger] + A^\dagger N)|n\rangle$

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

▷ similarly $NA|n\rangle = (n-1) A|n\rangle$

Provided they don't vanish, $A^\dagger|n\rangle$, $A|n\rangle$ are also eigenstates of N, with eigenvalues $n+1$, $n-1$

The algebra $[A, A^\dagger]$ has shown a relation between eigenvalues, but so far we only know our initial $n \in \mathbb{R}$

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

have equality iff $A|n\rangle = 0$

$d=1$ harmonic oscillator has non-degenerate energy levels, so must have

$A^\dagger|n\rangle = c_n|n+1\rangle$ for some $c_n \in \mathbb{C}$

- $|c_n|^2 = \|A^\dagger|n\rangle\|^2 = \langle n|AA^\dagger|n\rangle$
  $= \langle n|N + [A, A^\dagger]|n\rangle$
  $= n+1$
- choose $c_n = \sqrt{n+1}$ (phase convention)

if $A|n\rangle = 0$ then $N|n\rangle = 0$ i.e. $|n\rangle = |0\rangle$

$A^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$
$A|n\rangle = \sqrt{n}\,|n-1\rangle$

Combining all this, harmonic oscillator has energy levels

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right) \quad \text{with} \quad n \in \mathbb{N}_0$$

The ground state $|0\rangle$ is defined by $A|0\rangle = 0$.

Higher normalized energy eigenstates are $|n\rangle = (A^\dagger)^n|0\rangle/\sqrt{n!}$

Position space wavefunctions

If needed, we can easily reproduce $\psi_0(x)$ via $\langle x|0\rangle$

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

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

normalized so that $\langle 0|0\rangle = 1$

recall $\langle x|P|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\psi(x)$

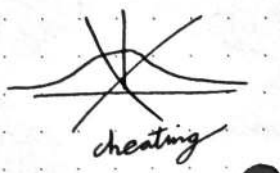
Higher energy states obtained by differentiating

- $\psi_1(x) = \langle x|A^\dagger|0\rangle = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega x\,\psi_0(x) - \hbar\psi_0'(x)\right) \propto 3xe^{-m\omega x^2/2\hbar}$
- repeated application generates the Hermite polynomials

Uncertainty in oscillator ground state

Recall $\Delta_\psi X\,\Delta_\psi P \geq |\langle [X,P]\rangle_\psi|/2 = \hbar/2$

- Recall $(\Delta_\psi X)^2 = \langle X^2\rangle_\psi - \langle X\rangle_\psi^2$
  - ▷ in terms of $A, A^\dagger$ have $X = \sqrt{\frac{\hbar}{2m\omega}}\,(A + A^\dagger)$
  - ▷ in any energy eigenstate $\langle n|X|n\rangle \propto \langle n|A + A^\dagger|n\rangle = 0$
    (A gives $\sim|n-1\rangle$; $A^\dagger$ gives $\sim|n+1\rangle$)



L3.3

▷ $(2m\omega/\hbar)\langle 0|X^2|0\rangle = \langle 0|(A+A^\dagger)^2|0\rangle = \langle 0|\, AA^\dagger + A^\dagger A\,|0\rangle = 1$

terms with A^2, $A^{\dagger 2}$ killed; $N+1$; killed

Similarly find

- $\langle 0|P|0\rangle = 0$, $\langle 0|P^2|0\rangle = \frac{m\hbar\omega}{2}$

$\therefore \Delta_0 X \,\Delta_0 P = \sqrt{\frac{\hbar}{2m\omega}} \cdot \sqrt{\frac{m\hbar\omega}{2}} = \frac{\hbar}{2}$ i.e. minimal uncertainty

▷ other states also have minimum uncertainty

A glimpse of QFT

The fact that energy levels are equally spaced means that an alternative interpretation of the $|n\rangle$ is both natural & intriguing

- a single particle living in the n^{th} excited state of the harmonic potential
- n (identical) particles excited out of the vacuum

- The identical particles do not interact; creating 2 particles cost exactly twice as much as just 1
- this observation is the starting point for quantization of a field theory

TLDW
- Used algebra to obtain spectrum, eigenstates
  - ▷ raising & lowering operators $[A, A^\dagger] = 1$
- Algebra fixed separation between eigenvalues,

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

  but also needed normalisation to fix starting point
- Energy level $E_n = (n+\frac{1}{2})\hbar\omega$ has corresponding normalized eigenstate $|n\rangle = (A^\dagger)^n|0\rangle/\sqrt{n!}$
  - ▷ can easily obtain position / space wavefunctions

Up next
- Transformations of quantum systems
  - ▷ study dynamics of oscillators

4 Translations

$p \to -i\hbar \frac{\partial}{\partial x}$ $\quad [\hat{x}, \hat{p}] = i\hbar$ WHAT

If we perform a transformation of our quantum system (e.g. translate / rotate)

- it will generically be in a different state after the transformation.
- Transformation will be rep by a lin op $U: \mathcal{H} \to \mathcal{H}$, $|\psi\rangle \mapsto |\psi'\rangle$

Transf^{n}s such as translations form a group, say G.

- U is a hom from G to the group $GL(\mathcal{H})$
  - ▷ $U(g_2 \circ g_1) = U(g_2) \circ U(g_1)$
  - ▷ $U(e) = 1_{\mathcal{H}}$ (see later)
- U must also be unitary; $U^{-1} = U^\dagger$
  - ▷ after transf^{n}, system will still be found somewhere, so we expect

$$\langle \psi | \psi \rangle = 1 \Rightarrow \langle \psi' | \psi' \rangle = \langle \psi | U^\dagger U | \psi \rangle = 1$$

  - ▷ holds for all $|\psi\rangle$ implies U is unitary

Thus we'll be concerned with unitary representations of our transf^{n} group on $\mathcal{H}$

$\langle \psi | \psi \rangle = \langle \psi | U^\dagger U | \psi \rangle$
Let $|\psi\rangle = |\phi\rangle + \lambda |\chi\rangle$,
$\langle \phi | \phi \rangle + |\lambda|^2 \langle \chi | \chi \rangle + \lambda \langle \phi | \chi \rangle + \bar{\lambda} \langle \chi | \phi \rangle$ LHS
$= \langle \phi | U^\dagger U | \phi \rangle + |\lambda|^2 \langle \chi | U^\dagger U | \chi \rangle + \lambda \langle \phi | U^\dagger U | \chi \rangle + \bar{\lambda} \langle \chi | U^\dagger U | \phi \rangle$
so $\langle \phi | U^\dagger U | \chi \rangle = \langle \phi | \chi \rangle$
varying $\lambda \in \mathbb{C}$

Transforming operators

Suppose $A: \mathcal{H} \to \mathcal{H}$ is some operator.
Expectation $\langle \psi | A | \psi \rangle$ originally;

$\langle \psi | U^\dagger A U | \psi \rangle$ after transform^{n}.

- Can alternatively view the transf^{n} acting on operators

$$A \mapsto A^\dagger = U^\dagger A U = U^{-1} A U$$

while leave states unchanged

- ▷ known as conjugation or similarity transform
- ▷ $A'B' = U^\dagger A U U^\dagger B U = U^\dagger A B U$ and $[A', B'] = U^\dagger [A, B] U$
- Similarity transforms preserve the spectrum
  - ▷ if $A|a\rangle = a|a\rangle$ then $A' U^\dagger |a\rangle = U^\dagger A |a\rangle = a U^\dagger |a\rangle$

Continuous transformations

Suppose our transf^n depends smoothly on some real parameter θ, with $\theta = 0$ identity

- For $\delta\theta \ll 1$, expand $U(\delta\theta) = 1_{\mathcal{H}} - i\,\delta\theta\, T + O(\delta\theta^2)$
  - T is called the generator of the transf^n ($-i$ convention)
  - unitary rel $U^\dagger U$ becomes
    $$1 = (1 + i\delta\theta\, T^\dagger)(1 - i\delta\theta\, T) + O(\delta\theta^2) = 1 + i\delta\theta(T^\dagger - T) + O(\delta\theta^2)$$
    which implies $T^\dagger = T$
  - generators are naturally Hermitian, good candidates for observables
- For states $|\psi'\rangle = (1 - i\delta\theta T + \cdots)|\psi\rangle$, $\delta|\psi\rangle = -i\delta\theta\, T|\psi\rangle$

For ops $A' = (1 + i\delta\theta T + \cdots) A (1 - i\delta\theta T + \cdots)$, $\delta A = i\delta\theta\,[T, A]$

- We can obtain a finite transf^n by exponentiation
  $$U(\theta) = \lim_{N\to\infty} \left(1 - i\frac{\theta}{N} T\right)^N = e^{-i\theta T}$$

Spatial Translations

Let's look at translations in $\mathbb{R}^3$

- Translating through $\underline{a} \in \mathbb{R}^3$ rep by unitary op $U(\underline{a})$
- Since $\mathbb{R}^3$ abelian, $U(\underline{a})\,U(\underline{b}) = U(\underline{a}+\underline{b}) = U(\underline{b}+\underline{a}) = U(\underline{b})\,U(\underline{a})$
  and also $U^\dagger(\underline{a}) = U^{-1}(\underline{a}) = U(-\underline{a})$

For infinitesimal $\delta\underline{a}$, write

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

($\underline{P}$: $\delta a_x \cdot P_x + \delta a_y \cdot P_y + \delta a_z \cdot P_z$)

Therefore $U(\underline{a}) = e^{-i\underline{a}\cdot\underline{P}/\hbar}$ by exponentiation

- By def^n $\underline{P}/\hbar$ are generators of translations in $\mathbb{R}^3$ — nothing about momenta yet
- $U(\delta\underline{a})\,U(\delta\underline{b}) = U(\delta\underline{b})\,U(\delta\underline{a})$ implies $[P_i, P_j] = 0$ so components commute

The canonical commutation relations

For $U(\underline{a})$ to indeed rep translation by $\underline{a}$, if $|\psi'\rangle = U(\underline{a})|\psi\rangle$,

- we must have $\langle \underline{X}^{\prime} \rangle_{\psi'} = \langle \psi | U^\dagger(\underline{a}) \underline{X} U^{\phantom\dagger}(\underline{a}) | \psi \rangle = \langle \underline{X} \rangle_\psi + \underline{a}$
- Since true for all $|\psi\rangle$, have $U^\dagger(\underline{a}) \underline{X} U^{\phantom\dagger}(\underline{a}) = \underline{X} + \underline{a}$ when acting on $\underline{X}$
- Infinitesimally, $(1 + i\delta\underline{a}\cdot\underline{P}/\hbar)\,\underline{X}\,(1 - i\delta\underline{a}\cdot\underline{P}/\hbar) + O(|\delta\underline{a}|^2) = \underline{X} + \delta\underline{a}$

and comparing coeffs we obtain $[X_i, P_j] = i\hbar\,\delta_{ij}\,1_{\mathcal{H}}$

$\left[\ \frac{i}{\hbar}[\delta\underline{a}\cdot\underline{P}, \underline{X}] = \delta\underline{a}\ \right]$

- ▷ asking where you are then translating not same as translating then asking
- ▷ nothing (yet!) about uncertainty

- Can't represent these commutation relations in non-trivial fd Hilbert space
- ▷ taking trace, $\dim(\mathcal{H}) = \mathrm{tr}(1_{\mathcal{H}}) = -i/\hbar\ \mathrm{tr}([X,P]) = 0$ so $\mathcal{H} = \{0\}$

This is why QM needs function spaces such as $L^2(\mathbb{R}, dx)$

Translating wavefunctions

- On the pos^{n} eigenstate $|\underline{x}\rangle$, $|\underline{x}'\rangle = U(\underline{a})|\underline{x}\rangle$
- $\underline{X}\,U(\underline{a})|\underline{x}\rangle = \left([\underline{X}, U(\underline{a})] + U(\underline{a})\,\underline{X}\right)|\underline{x}\rangle = (\underline{a} + \underline{x})\,U(\underline{a})\,|\underline{x}\rangle$

$\left[\ U^\dagger(\underline{a})\,\underline{X}\,U(\underline{a}) = \underline{X} + \underline{a}\ \text{ implies }\ \underline{X}\,U(\underline{a}) = U(\underline{a})\,\underline{X} + U(\underline{a})\,\underline{a}\ \right]$

- Consequently $U(\underline{a})|\underline{x}\rangle = c\,|\underline{x} + \underline{a}\rangle$ and we can fix $c = 1$ (exe)

Suppose $\psi(\underline{x}) = \langle \underline{x} | \psi \rangle$, and translate

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

$\left[\ \langle \underline{x} | U(\underline{a}) = \left(U(\underline{a})^\dagger |\underline{x}\rangle\right)^\dagger = \left(U(-\underline{a})|\underline{x}\rangle\right)^\dagger = \left(|\underline{x} - \underline{a}\rangle\right)^\dagger = \langle \underline{x} - \underline{a}|\ \right]$

- For an infinitesimal translation $\psi(\underline{x} - \delta\underline{a}) - \psi(\underline{x}) = -\delta\underline{a}\cdot\underline{\nabla}\psi$, but

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

and comparing for arb $\delta\underline{a}$ gives $\langle \underline{x} | \underline{P} | \psi \rangle = -i\hbar\,\underline{\nabla}\psi(\underline{x})$

- ▷ natural that $\underline{\nabla}$ describes an infinitesimal translation ☺

Ex Spose have eigenstate $|\underline{p}\rangle$, $\underline{P}|\underline{p}\rangle = \underline{p}|\underline{p}\rangle$

- After trans^n, get wavefunction

$$\langle \underline{x}|U(\underline{a})|\underline{p}\rangle = \langle \underline{x}|e^{-i\underline{a}\cdot\underline{P}/\hbar}|\underline{p}\rangle = e^{-i\underline{a}\cdot\underline{p}/\hbar}\langle \underline{x}|\underline{p}\rangle$$

- Hence $\psi_{\underline{p}}(\underline{x}-\underline{a}) = e^{-i\underline{a}\cdot\underline{p}/\hbar}\psi_{\underline{p}}(\underline{x})$ which is solved by

$$\psi_{\underline{p}}(\underline{x}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\underline{p}\cdot\underline{x}/\hbar}$$ where constant ensures "normalization"

$$\langle \underline{p}'|\underline{p}\rangle = \delta^{(3)}(\underline{p}'-\underline{p})$$

Next, let's translate the ground state $|0\rangle$ of 1d harmonic oscillator

- $\langle x|0\rangle = Ce^{-\alpha^2x^2/2}$ for some C, α
- Translated state $U(a)|0\rangle$ is known as a coherent state,

$$\langle x|U(a)|0\rangle = Ce^{-\alpha^2(x-a)^2/2}$$

▷ Gaussian of same variance, but now centred on $x=a$

▷ no longer an energy eigenstate, will oscillate

TL;DW • $U(g)$ gives hom from transf group G to the unitary group $U(\mathcal{H})$

- If transf depends on real param θ, expand $U(\delta\theta) = 1 - i\delta\theta\, T$

where T is Hermitian; ▷ $\underline{P}/\hbar$ generator of translations

- Algebra (comm rel^n) of generators just reflects properties of G.

▷ in particular $[P_i, P_j] = 0$ since trans^n commute, $[X_i, P_j] = i\hbar\delta_{ij}$

- For states $|\psi'\rangle = U|\psi\rangle$ or $\partial_\theta|\psi\rangle = -iT|\psi\rangle$ infinitesimally,

whereas for operators $A' = U^\dagger A U$ or $\partial_\theta A = i[T, A]$

▷ $\langle \underline{x}|\underline{P}|\psi\rangle = -i\hbar\underline{\nabla}\psi(\underline{x})$ now makes sense

Up Next • rotations, parity transforms

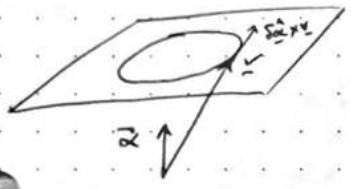
▷ subtle properties, dep on choice of Hilbert space

Rotations & Parity

Rotations on $\mathbb{R}^3$

Recall how rotations act on vectors $\underline{v} \in \mathbb{R}^3$

- An anticlockwise rotation through $|\underline{\alpha}|$ around the $\hat{\underline{\alpha}}$-axis can be represented by a rotation matrix $R(\underline{\alpha}) : \underline{v} \mapsto \underline{v}' = R(\underline{\alpha})\,\underline{v}$
  - ▷ since $\underline{v}'\cdot\underline{v}' = \underline{v}\cdot\underline{v}$ and $\det R(\underline{\alpha}) = +1$, rot group is $SO(3)$
  - ▷ $SO(3)$ is non-Abelian, $R(\underline{\beta})R(\underline{\alpha}) \neq R(\underline{\alpha})R(\underline{\beta})$ in general
- For an infinitesimal rotation $R(\delta\underline{\alpha})\,\underline{v} = \underline{v} + \delta\underline{\alpha} \times \underline{v} + O(|\delta\underline{\alpha}|^2)$



- Successive small rotations give

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

- The difference between rotations in opposite orders is

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

This is $R(\delta\underline{\alpha}\times\delta\underline{\beta}) - 1_{\mathbb{R}^3}$ to lowest order

← note this thingy? not sure about but who cares, cubic!

The rotation operator

We now apply our hom U to obtain a rotation operator $U(\underline{\alpha})$ on $\mathcal{H}$

hom slightly more than group hom?

- Let $U(\delta\underline{\alpha}) = 1 - i\,\delta\underline{\alpha}\cdot\underline{J}/\hbar + O(|\delta\underline{\alpha}|^2)$ where $\underline{J}/\hbar$ is generator
  - ▷ $\underline{J}$ has nothing to do with ang momentum (yet!)
  - ▷ for a finite rotation around fixed axis, $U(\underline{\alpha}) = e^{-i\underline{\alpha}\cdot\underline{J}/\hbar}$
- The relations $[R(\delta\underline{\alpha}), R(\delta\underline{\beta})]\,\underline{v} = R(\delta\underline{\alpha}\times\delta\underline{\beta})\,\underline{v} - \underline{v}$ imply

$$[U(\delta\underline{\alpha}), U(\delta\underline{\beta})] = U(\delta\underline{\alpha}\times\delta\underline{\beta}) - 1_{\mathcal{H}}$$

$$\Big[\,[1 - i/\hbar\,\delta\underline{\alpha}\cdot\underline{J},\ 1 - i/\hbar\,\delta\underline{\beta}\cdot\underline{J}] = -i/\hbar\,(\delta\underline{\alpha}\times\delta\underline{\beta})\cdot\underline{J}$$
$$-1/\hbar^2\,\delta\alpha_i\delta\beta_j[J_i, J_j] = -i/\hbar\,\varepsilon_{ijk}\,\delta\alpha_i\,\delta\beta_j\,J_k\,\Big]$$

- In terms of Cartesian components of the generators $\underline{J}/\hbar$ this is

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

which define the algebra $so(3)$ of inf rotations

- Considering rotations and translations we similarly obtain

$$[J_i, P_j] = i\hbar\,\varepsilon_{ijk}\,P_k$$

Rotating an operator

- The rotation operator $U(\underline{\alpha})$ should certainly rotate $\underline{X}$, so

$$U^\dagger(\underline{\alpha})\,\underline{X}\,U(\underline{\alpha}) = R(\underline{\alpha})\,\underline{X}$$

  - ▷ LHS involve similarity transform of each component of $\underline{X}$ whilst RHS just mixes up components
  - ▷ for an infinitesimal rotation this is

$$\left(1+\tfrac{i}{\hbar}\,\delta\underline{\alpha}\cdot\underline{J}\right)\underline{X}\left(1-\tfrac{i}{\hbar}\,\delta\underline{\alpha}\cdot\underline{J}\right) = \underline{X} + \delta\underline{\alpha}\times\underline{X}$$

  or equivalently $[J_i, X_j] = i\hbar\,\varepsilon_{ijk}\,X_k$ (exc)

- An operator $\underline{V}$ transforms under rotations as a vector whenever $U^\dagger(\underline{\alpha})\,\underline{V}\,U(\underline{\alpha}) = R(\underline{\alpha})\,\underline{V}$ so that infinitesimally $[J_i, V_j] = i\hbar\,\varepsilon_{ijk}\,V_k$
- An operator S transforms under rotations as a scalar wherever $U^\dagger(\underline{\alpha})\,S\,U^\dagger(\underline{\alpha}) = S$ so that infinitesimally $[J_i, S] = 0$
- If $\underline{V}$, $\underline{W}$ are vector operators, then $\underline{V}\cdot\underline{W}$ is a scalar

$$U^\dagger(\underline{\alpha})\,\underline{V}\cdot\underline{W}\,U(\underline{\alpha}) = \left(U^\dagger(\underline{\alpha})\,\underline{V}\,U(\underline{\alpha})\right)\cdot\left(U^\dagger(\underline{\alpha})\,\underline{W}\,U(\underline{\alpha})\right)$$
$$= R(\underline{\alpha})\,\underline{V}\cdot R(\underline{\alpha})\,\underline{W} = \underline{V}\cdot\underline{W}$$

Translations around a circle

For a point particle, we can build up a rotation by considering several successive small translations, each in slightly different directions.

- Suppose initially at vertex $\underline{x}$ of a regular N-gon, in plane with normal $\underline{n}$
- Translate through $\delta\underline{x} = (2\pi/N)\,\underline{n}\times\underline{x}$ to move along edge

Thus $U^\dagger(\delta\underline{x})\,\underline{X}\,U(\delta\underline{x}) = \underline{X} + (2\pi/N)\,\underline{n}\times\underline{X}$, so for these position-dependent translations

$$U(\delta\underline{x}) = 1 - \frac{i}{\hbar}\,\frac{2\pi}{N}\,(\underline{n}\times\underline{X})\cdot\underline{P} = 1 - \frac{i}{\hbar}\,\delta\underline{\alpha}\cdot\underline{L}$$

where $\underline{L} = \underline{X}\times\underline{P}$ and $\delta\underline{\alpha} = (2\pi/N)\,\underline{n}$

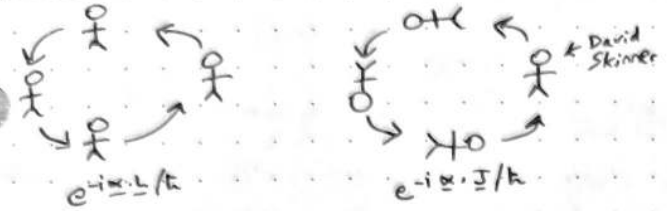
- As $N\to\infty$ describe translations around circular path
- From $[X_i, P_j] = i\hbar\,\delta_{ij}$ follows that

$$[L_i, L_j] = i\hbar\,\varepsilon_{ijk}\,L_k\,,\quad [L_i, X_j] = i\hbar\,\varepsilon_{ijk}\,X_k\,,\quad [L_i, P_j] = i\hbar\,\varepsilon_{ijk}\,P_k$$

so $\underline{L}$ and $\underline{J}$ act on $L^2(\mathbb{R}^3, d^3x)$ in exactly the same way

L5.3

Rotating a composite system



In QM, difference arises because $\mathcal{H}$ is now a tensor product, with $L^2(\mathbb{R}^3, dx)$ just describing CoM

- We define $\underline{S} = \underline{J} - \underline{L}$ or equiv $\underline{J} = \underline{L} + \underline{S}$

  ▷ $\underline{L}/\hbar$ generates translations of centre of mass around circular path whilst $\underline{S}/\hbar$ generates rotations around the centre of mass.

  $\underline{S}$ is known as the spin operator

- Perhaps $\underline{J} \stackrel{?}{=} \sum_a \underline{X}_a \times \underline{P}_a$ by summing over all particles ?

  ▷ Very unwieldy ▷ Dangerous to assume what the correct Hilbert for a sub-atomic sys is

Commutation relations for spin operator

Compute • First since $[J_i, X_j] = i\hbar \varepsilon_{ijk} X_k$, $[J_i, P_j] = i\hbar \varepsilon_{ijk} P_k$

and likewise with the L_i

• Hence $[S_i, X_j] = [S_i, P_j] = 0$, confirming that $\underline{S}$ doesn't affect the centre of mass wavefunction

• We can also compute among components

$$\begin{aligned}[S_i, S_j] &= [J_i, J_k] - [J_i, L_j] - [L_i, J_j] + [L_i, L_j] \\ &= i\hbar(\varepsilon_{ijk} J_k - \varepsilon_{ijk} L_k + \varepsilon_{ijk} L_k + \varepsilon_{ijk} L_k) \\ &= i\hbar \varepsilon_{ijk}(J_k - L_k) = i\hbar \varepsilon_{ijk} S_k\end{aligned}$$

confirming $\underline{S}/\hbar$ indeed generate rotations (around CoM)

Parity

Not all transf^{n}s depend on a cts parameter. Most obvious example is the parity group $\mathbb{Z}_2$ acting on space as $P : \underline{x} \mapsto -\underline{x}$

• Parity transformations act on all Cartesian components. We can reflect in a plane by combining P and a rotation

• Represented by unitary operator Π obeying $\Pi^2 = 1$, so evals ± 1

• Since $\mathbb{Z}_2$ is discrete, there is no generator

- We have $\Pi^{-1} \underline{X} \Pi = -\underline{X}$ or equiv $\{\Pi, X\} = \Pi \underline{X} + \underline{X} \Pi = 0$

On the other hand $\Pi^{-1} \underline{L} \Pi = \underline{L}$ and one can also show $\Pi^{-1} \underline{J} \Pi = \underline{J}$

▷ $\underline{X}$ is a vector operator, whilst $\underline{J}, \underline{L}$ are pseudovector operators

Π may act subtly on composite systems (like rotations)

- If $|\underline{x}\rangle$ is position eigenstate for com, then $\Pi |\underline{x}\rangle = |-\underline{x}\rangle$
- Physical particles can have intrinsic parity: if $|\psi\rangle$ is a Π-eigenstate,

$\langle \underline{x} | \Pi | \psi \rangle = \eta \psi(-\underline{x})$ with $\eta = \pm 1$ coming from 'internal' Hilbert space & actual wavefn

TL;DW • Algebra $[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k$ just reflects non-Abelian nature of rotⁿ

- Spin operator $\underline{S} = \underline{J} - \underline{L}$ generates rotation of composite system about com
  - ▷ which $\mathcal{H}$ we should use ultimately determined by experiment
  - ▷ $[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k$ and $[S_i, S_j] = i\hbar \varepsilon_{ijk} S_k$ but $[L_i, S_j] = 0$
- Since $\mathbb{Z}_2$ is discrete, parity operator Π has no generator
  - ▷ can again be 'intrinsic' spin from internal Hilbert space

Up next • Time translations, the Schrödinger and Heisenberg pictures

- Symmetries and conservation laws

Symmetries & conservation laws

Schrödinger's equation tells us that states evolve in time via

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

where H is the system's Hamiltonian.

- H is certainly Hermitian, so this looks like the infinitesimal version of a unitary transformation with $H/\hbar$ generator of time translations
- Provided H itself is time independent, integrate TDSE to find

  $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ where $U(t) = e^{-iHt/\hbar}$

  $U(t)$ is known as the time evolution operator
- Form of H can be constrained by group properties (e.g. Galilean group for NRQM, or $SO(3,1)$ for relativity) but not completely fixed
  - ▷ different from previous cases because basic Hilbert space $L^2(\mathbb{R}^3, d^3x)$ does not depend on time
- This formulation of QM is sometimes called the Schrödinger picture
  - ▷ states evolve in time, whilst operators such as $\underline{X}, \underline{P}, \underline{J}$ that contain no explicit time dependence are indeed constant in time

Time evolution in the Heisenberg picture

As with other transformations, there's an alternative point-of-view in which time dependance is carried instead by the operators

- Expected value of quantity Q at time t is $\langle\psi(0)|U^\dagger(t) Q U(t)|\psi(0)\rangle$ if system prepared to be in state $|\psi(0)\rangle$ when $t=0$
- In the Schrödinger picture, provided $\partial_t Q = 0$ time dependence of $\langle Q\rangle$ arises only because state changes
- In the Heisenberg picture, state is always $|\psi(0)\rangle$ whilst the operator itself evolves in time according to

$$Q_H(t) = U^\dagger(t) Q_S U(t) \quad \text{with} \quad U(t) = e^{-iHt/\hbar}, \quad Q_S = Q = Q_H(0)$$

- Differentiating, we obtain

$$\frac{d}{dt} Q_H(t) = \frac{i}{\hbar} U^\dagger \underbrace{[H, Q_S]}^{=0} U(t) = \frac{i}{\hbar}[H, Q_H(t)]$$

$$+ U^\dagger(t) \frac{\partial Q_S}{\partial t} U(t) \qquad + \frac{\partial Q}{\partial t}(t)\Big|_H \quad \leftarrow \text{explicit time dep}$$

Dynamics

To give life to the equations of motion, need to specify the form of H.

For motion in $\mathbb{R}^3$ we should choose $H = H(\underline{X}, \underline{P}, \dots)$ since $\underline{X}, \underline{P}$ are the fundamental operators on $L^2(\mathbb{R}^3, d^3x)$

- Any choice of $H(\underline{X}, \underline{P}, \dots)$ is known as a dynamical relation
- Simplest rotationally invariant choice is $H = \underline{P}^2/2m$
  - ▷ relates evolution through time (H) to translation through space (P)
- If our quantum system, may encounter obstacles, include

$$H = \frac{\underline{P}^2}{2m} + V(\underline{X}) = \frac{P_r^2}{2m} + \frac{\underline{L}^2}{2mR^2} + V(\underline{X})$$

so in Heisenberg picture

$$\frac{d\underline{X}(t)}{dt} = \frac{\underline{P}(t)}{m}, \qquad \frac{d\underline{P}(t)}{dt} = -\underline{\nabla} V(t) \qquad -\frac{dO_H}{dt} = i\hbar [O, H]\frac{i}{\hbar}$$

where $\underline{\nabla} V(t) = U^\dagger(t)\, \underline{\nabla} V(\underline{X})\, U(t)$

- Our intuition of momentum $\underline{P}$ comes from these equations
  - ▷ the dynamical relation says 'translation generator $\underline{P}$ = momentum'

Dynamics of oscillators

For an example, let's look again at $|0; x_0\rangle = e^{-ix_0 P/\hbar}|0\rangle$ (ground state of the harmonic oscillator displaced through x_0 in position space)

- In Heisenberg picture, show in probs 1 that

$$P(t) = U^\dagger(t)\, P\, U(t) = P\cos\omega t - Xm\omega \sin\omega t$$

- Evolving $|0, x_0\rangle$ for time t gives new state

$$U(t)|0; x_0\rangle = U(t)\, e^{-ix_0 P/\hbar}\, U^\dagger(t)\, \underline{U(t)}|0\rangle$$

$$= e^{-ix_0 P(-t)/\hbar}\, e^{-i\omega t/2}|0\rangle \qquad \underline{U(t)}|0\rangle \to e^{-i(E_0/\hbar)t}$$

since $P(-t)$ obtained from reversed conjugation

$$= e^{-i(m\omega x_0 X \sin\omega t + x_0 P\cos\omega t)/\hbar}\, e^{-i\omega t/2}|0\rangle$$

- If $[A,B]$ commutes with A & B then $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$, so

$$= e^{-i(m\omega x_0/\hbar)X\sin\omega t}\, e^{-i(x_0/\hbar)P\cos\omega t}\, e^{i\phi(t)}|0\rangle$$

This is a Gaussian centred at $x_0\cos\omega t$ and with momentum $m\dot{x}(t) = -m\omega x_0 \sin\omega t$ (phase $\phi(t)$ does not affect shape or location)

- Recovered oscillatory behaviour for a Gaussian lump of mass ☺

Conserved quantities

- If an operator Q is time independent even in Heisenberg picture, we say it is conserved

- Suppose $\partial_t Q = 0$ in Schrödinger picture. Then

$$\frac{dQ_H}{dt} = \frac{i}{\hbar}[H, Q(t)] = U^\dagger [H, Q] U$$

- Since $U(t)$ unitary, $Q_H(t)$ time independent iff $[H, Q] = 0$. Hence conserved operators commute with the Hamiltonian

Suppose we prepare our system to be in some Q eigenstate $|q\rangle$ at $t=0$

- At time t, $Q U(t)|q\rangle = U(t) Q |q\rangle = q U(t)|q\rangle$ so remains a Q eigenstate with same eigenvalue

  - ▷ state may change if $\dim(\mathcal{H}|_{Q=q}) > 1$
  - ▷ often useful to expand our states in basis of eigenstates of (possibly several) conserved quantities, because these basis states do not themselves change

Symmetries and Conserved Quantities

Important source of conserved quantities comes from symmetries

- Under any transformation, operators change by conjugation with some $U(\theta) = e^{-i\theta T}$, in particular $H \mapsto U^\dagger(\theta) H U(\theta)$

- A transformation is a symmetry if it leaves H unchanged, so $U^\dagger(\theta) H U(\theta) = H$ or $[T, H] = 0$ infinitesimally

- $[T, H] = 0$ also says generator is conserved, so symmetries of H correspond to conserved quantities

For example

- If $H(\underline{X}, \underline{P}, \ldots)$ is translationally invariant then momentum $\underline{P}$ is conserved
- If $H(\underline{X}, \underline{P}, \ldots)$ is rotationally invariant then angular momentum $\underline{J}$ is conserved

- Also true for discrete symmetries: if $[H, \Pi] = 0$ then parity is conserved
  - ▷ says two systems that are initially mirror images evolve so as to stay mirror images
  - ▷ remarkably, this is violated by radioactive β-decay

TL;DW • In Schrödinger pic, ops constant (if no explicit t)
while states evolve as $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$

- In Heisenberg pic, states remain $|\psi(0)\rangle$ for all t, but operators evolve as $Q_H = U^\dagger(t)\, Q\, U(t)$
- If H itself is time-independent then $U(t) = e^{-iHt/\hbar}$
- Symmetries of H correspond to conserved quantities
  - ▷ $[H, H] = 0$ trivially so (if $\partial_t H = 0$) energy always conserved
- ExSheet 1 is now free real estate

Up Next • Study repns of rotation algebra $[J_i, J_j] = i\hbar\,\varepsilon_{ijk}\,J_k$
▷ Application to observations of clouds of interstellar gas

Angular Momentum

The algebra $SO(3)$

- We found the generators $\underline{J}$ of infinitesimal rotations obey the $SO(3)$ algebra

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

- Unlike for $\underline{X}$ and $\underline{P}$, we can find finite dim unitary repns of $SO(3)$
  - ▷ if $\dim \mathcal{H} < \infty$ then $0 = \mathrm{tr}\,[J_i, J_j] = i\hbar\, \varepsilon_{ijk}\, \mathrm{tr}\, J_k$
  - ▷ each component of $\underline{J}$ will be rep by a traceless matrix
- No two components of $\underline{J}$ commute, but

$$[J_i, \underline{J}^2] = [J_i, J_j] J_j + J_j [J_i, J_j]$$
$$= i\hbar (\varepsilon_{ijk} J_k J_j + J_j \varepsilon_{ijk} J_k) = 0 \quad \text{(index } j \text{ summed)}$$

so cannot find a basis of simult eigenstates of diff components, but can diagonalize (say) J_z and $\underline{J}^2$.

- Let $|\beta, m\rangle$ obey $\underline{J}^2 |\beta, m\rangle = \beta\hbar^2 |\beta, m\rangle$

$$J_z |\beta, m\rangle = m\hbar |\beta, m\rangle$$

  - ▷ since eigenstates of Hermitian operators, must be orthogonal, and choose orthonormal $\langle \beta', m' | \beta, m \rangle = \delta_{\beta\beta'} \delta_{mm'}$

Raising and lowering operators

Possible values of β, m found as with harmonic oscillator

- Define $J_\pm = J_x \pm i J_y$
- Compute $[J_z, J_\pm] = [J_z, J_x] \pm i [J_z, J_y] = i\hbar (J_y \mp i J_x) = \pm \hbar J_\pm$
  - ▷ this is just a repackaging of the $SO(3)$ algebra
- We learn that

$$\underline{J}^2 (J_\pm |\beta, m\rangle) = ([\underline{J}^2, J_\pm] + J_\pm \underline{J}^2) |\beta, m\rangle = \beta\hbar^2 J_\pm |\beta, m\rangle$$
($[\underline{J}^2, J_\pm]$: zero)

$$J_z (J_\pm |\beta, m\rangle) = ([J_z, J_\pm] + J_\pm J_z) |\beta, m\rangle = (m \pm 1)\hbar (J_\pm |\beta, m\rangle)$$
($[J_z, J_\pm]$: $\pm\hbar J_\pm$)

Consequently, if non-vanishing, $J_\pm |\beta, m\rangle$ are again eigenstates of both $\underline{J}^2$ and J_z with eigenvalues $\beta\hbar^2$ and $(m \pm 1)\hbar$, resp

- ▷ $J_\pm$ reorient a system, adjusting how much ang momentum in z-axis, leave total ang momentum unaltered

Angular momentum spectrum

Just as with harmonic oscillator, must examine norm to fix initial β, m

- $\| J_+ |\beta, m\rangle \|^2 = \langle \beta, m | J_- J_+ | \beta, m \rangle$
  $= \langle \beta, m | \underline{J}^2 + J_y^2 + i[J_x, J_y] | \beta, m \rangle$
  $= \langle \beta, m | \underline{J}^2 - J_z^2 - \hbar J_z | \beta, m \rangle$
  $= \hbar^2 (\beta - m^2 - m) = \hbar^2 (\beta - m(m+1)) \geq 0$
- J_+ increases m whilst preserving β, so to stay in $\mathcal{H}$ we must have $\beta = j(j+1)$ for some j, where j is the maximum allowed value of m
  - ▷ on this state $\| J_+ |\beta, j\rangle \|^2 = 0$ so $J_+ |\beta, j\rangle = 0$
  - ▷ these states are called highest weight states in rep theory
- Similarly find $\| J_- |\beta, m\rangle \|^2 = \hbar^2 (\beta - (m-1)m)$ so also need $\beta = j'(j'-1)$ where j' is the minimum value of m
- So $\beta = j(j+1) = j'(j'-1) \Rightarrow j' = j+1$ or $\boxed{j' = -j}$, $j \geq 0$
  - ▷ $j - j' = 2j \in \mathbb{Z}_{\geq 0}$ because we change m in unit steps

Angular momentum eigenstates I

The story so far

- $\beta = j(j+1)$ where $2j \in \mathbb{Z}_{\geq 0}$. Since β is determined by j, we now relabel our states $|\beta, m\rangle \mapsto |j, m\rangle$
- For a fixed value of j, m can run from $-j$ to j in integer steps. This takes $2j$ steps, so $\dim(\mathcal{H}_j) = 2j+1$ *brah
- The operators act as

$$J_z |j, m\rangle = \hbar m |j, m\rangle, \qquad \underline{J}^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle$$

and $$J_+ |j, m\rangle = [j(j+1) - m(m+1)]^{1/2} |j, m+1\rangle$$
$$J_- |j, m\rangle = [j(j+1) - m(m-1)]^{1/2} |j, m-1\rangle$$

Note that these imply $J_+ |j, j\rangle = 0$, $J_- |j, -j\rangle = 0$, keeping us safely in $\mathcal{H}_j$

Angular Momentum Eigenstates II

Since $J_x = (J_+ + J_-)/2$, $J_y = (J_+ - J_-)/2i$, rotations around arbitrary axes map $U(\underline{\alpha}) : \mathcal{H}_j \to \mathcal{H}_j$, preserving j (trivial)

- Could equally well choose to work in J_x or J_y basis, but so long as j remains fixed, these still span $\mathcal{H}_j$ so nothing new
- When $j > 0$, states of definite J_z are never eigenstates of J_x or J_y

Physically, the highest weight state $|j,j\rangle$ is state with angular momentum aligned as well as possible along $\hat{z}$

- As a crude measure of this, compute

$$\frac{\langle j,j|\, J_x^2 + J_y^2 \,|j,j\rangle}{\langle j,j|\, J_z^2 \,|j,j\rangle} = \frac{j(j+1) - j^2}{j^2} = \frac{1}{j}$$

Thus in $|j,j\rangle$, roughly $1/\sqrt{j}$ of the angular momentum lies somewhere in the xy-plane. Negligible for macroscopic bodies ($j \gg 1$)

- $\langle j,j|J_x|j,j\rangle = \langle j,j|J_y|j,j\rangle = 0$ so 'extra' angular momentum equally likely to point in any direction in xy-plane

The classical limit

Suppose our system is in state $|j,j\rangle$ with ang mom maximally aligned with z. Let's measure $\underline{J}$ along $\underline{n} = (\sin\theta, 0, \cos\theta)$

- Classically we'll find $\hbar j \cos\theta$
- In QM, $\langle j,j|\, \underline{n}\cdot\underline{J} \,|j,j\rangle = \langle j,j|\cos\theta J_z + \sin\theta J_x|j,j\rangle = \hbar j\cos\theta$, so on average we agree with classical result
- We also compute

$$\langle (\underline{n}\cdot\underline{J})^2 \rangle = \cos^2\theta \langle J_z^2\rangle + \sin^2\theta \langle J_x^2\rangle + \cos\theta\sin\theta \underbrace{\langle J_x J_z + J_z J_x\rangle}_{\text{zero}}$$

$$= \hbar^2 j^2 \cos^2\theta + \frac{1}{4}\sin^2\theta \langle j,j|J_+J_-|j,j\rangle$$

$$\left[J_x^2 = \frac{(J_+ + J_-)(J_+ + J_-)}{4} = \frac{1}{4}(\underbrace{J_+^2}_{\text{zero}} + \underbrace{J_-^2}_{\text{zero}} + J_+J_- + \underbrace{J_-J_+}_{\text{zero}}) \right]$$

$$\left[J_-|j,m\rangle = [j(j+1) - m(m-1)]^{1/2}|j,m-1\rangle \quad \text{so } J_-|j,j\rangle = \sqrt{2j}\,|j,j-1\rangle \right.$$

$$\left. J_+|j,j-1\rangle = [j(j+1) - j(j-1)]^{1/2}|j,j\rangle = \sqrt{2j}\,|j,j\rangle \right]$$

Altogether, $\langle (\underline{n}\cdot\underline{J})^2\rangle = \hbar^2(j^2\cos^2\theta + \frac{j}{2}\sin^2\theta)$

so uncertainty $\Delta_{j,j}(\underline{n}\cdot\underline{J}) = \hbar|\sin\theta|\sqrt{j/2}$

- Thus, in this maximally aligned state $\Delta(\underline{n}\cdot\underline{J})/\langle\underline{n}\cdot\underline{J}\rangle \sim 1/\sqrt{j}$
  - ▷ negligible when $j \gg 1$ so macroscopic objects have very well-aligned angular momentum, but significant uncertainty for small j

Rotation spectrum of diatomic molecules

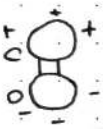
As a simple application of this formalism, consider an axisymmetric body with $I = I_x = I_y \neq I_z$. The Hamiltonian is

$$H = \frac{J_x^2}{2I_x} + \frac{J_y^2}{2I_y} + \frac{J_z^2}{2I_z} = \frac{J^2}{2I} + J_z^2\left(\frac{1}{2I_z} - \frac{1}{2I}\right)$$

so $|j,m\rangle$ is an energy eigenstate with

$$E_{j,m} = j(j+1)\hbar^2/2I + m^2\hbar^2\left(\frac{1}{2I_z} - \frac{1}{2I}\right)$$

- CO has $I_z \ll I$ so only states with $m=0$ accessible at low energies
- $|E_j - E_{j-1}| = j\hbar^2/I$ with corresponding frequency $\nu_j = \frac{2\pi\hbar j}{I}$



Large rotations

Our considerations so far have been local. Global / topological properties of the rotation group may impose further restrictions

- For example, consider Fourier series of a function on S^1
  - ▷ $\psi(\theta) = e^{ik\theta}$ is an L^2-eigenstate of $d^2/d\theta^2$ for any k
  - ▷ requirement $\psi(\theta+2\pi) = \psi(\theta)$ quantizes $k \in \mathbb{Z}$
- Suppose $|\psi\rangle \in \mathcal{H}_j$ and expand $|\psi\rangle = \sum_{m=-j}^{j} a_m |j,m\rangle$, $a_m \in \mathbb{C}$
- $U(\alpha\hat{z})|\psi\rangle = \sum_{m=-j}^{j} a_m e^{-i\alpha J_z/\hbar}|j,m\rangle = \sum_{m=-j}^{j} a_m e^{i\alpha m}|j,m\rangle$
  - ▷ in particular, $\alpha = 2\pi$ gives $\sum_{m=-j}^{j} a_m e^{-2\pi i m}|j,m\rangle$

In SO(3) a 2π rotation is the same as no rotation

- When $j \in \mathbb{Z}_{\geq 0}$ (hence $m \in \mathbb{Z}$) have $U(2\pi\hat{n}) = 1_{\mathcal{H}_j}$
- When $j \in \frac{1}{2} + \mathbb{Z}_{\geq 0}$ have $U(2\pi\hat{n}) = -1_{\mathcal{H}_j}$

Half-integer values of j are allowed because $\lambda 1_{\mathcal{H}}$ acts trivially on $\mathbb{P}\mathcal{H}$

- Since $U(2\pi\hat{n}) \neq 1_{\mathcal{H}}$, not a bona-fide repn of SO(3)

- Projective repn of $SO(3)$ (or true repn of $SU(2)$)

In physics, half-integer j-reps are called <u>spinors</u>

The Stern-Gerlach experiment

Not only are spinors permitted by the formalism, they occur in nature

- Atoms of mass M and spin s travel through region of magnetic field

$$H = \frac{p^2}{2M} - \underline{\mu}\cdot\underline{B} = \frac{p^2}{2M} - \frac{\mu B}{\hbar s} S_z$$

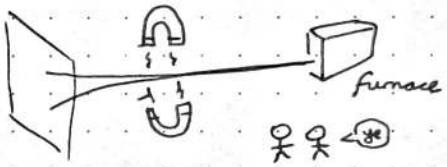
where $\underline{\mu} = \mu \underline{S}/\hbar s$ is the atom's magnetic dipole momentum

- Atoms feel a force

$$\frac{d}{dt}\langle \underline{p} \rangle = (\mu/\hbar s)\langle \underline{\nabla} B S_z \rangle$$

that depends on how well their spin is aligned with $\underline{B}$

- Beam separates into $2s+1$ rays
  - ▷ if $s \gg 1$ beam looks smeared
  - ▷ for silver atoms, split into two ($s = \frac{1}{2}$!)



- In fact, electrons, protons and neutrons each have spin-half

<u>TL;DW</u> • $\{|j,m\rangle\}$ basis of simultaneous J^2, J_z eigenstates

$$J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle \qquad J_z|j,m\rangle = \hbar m |j,m\rangle$$

- Angular momentum is quantized ∴

$$2j \in \mathbb{Z}_{\geq 0} \quad \text{and} \quad m \in \{-j, -j+1, \ldots, j-1, j\}$$

- Raising / lowering operators $J_\pm = J_x \pm i J_y$ act as

$$J_\pm |j,m\rangle = \left[j(j+1) - m(m\pm 1)\right]^{1/2} \hbar\, |j, m\pm 1\rangle$$

reorienting our system to place more / less ang momentum along z

- Projective reps with $j = \frac{1}{2}, \frac{3}{2}, \ldots$ are called spinors
  - ▷ eg electrons, protons, neutrons (and Ag atoms)

<u>Up Next</u> • Obtain explicit matrix representations for J_z, $J_\pm$ for low j

- Embed $j \in \mathbb{Z}_{\geq 0}$ reps inside $L^2(\mathbb{R}^3, d^3x)$ – orbital ang momentum

Spin and Orbital Angular Momentum

Spin rep"s

- The spin operators $\underline{S}$ and the orbital angular momentum operators $\underline{L} = \underline{X} \times \underline{P}$ obey the same $so(3)$ algebra

$$[S_i, S_j] = i\hbar \varepsilon_{ijk} S_k \qquad [L_i, L_j] = i\hbar \varepsilon_{ijk} L_k$$

as the rotation generators $\underline{J}$, so have the same reprs

- We let $|s, \sigma\rangle$ denote a spin eigenstate with

$$\underline{S}^2 |s,\sigma\rangle = s(s+1)\hbar^2 |s,\sigma\rangle \quad \text{and} \quad S_z |s,\sigma\rangle = \sigma\hbar |s,\sigma\rangle$$

where $2s \in \mathbb{Z}_{\geq 0}$ and $\sigma \in \{-s, -s+1, \ldots, s-1, s\}$

- Hilbert space of a spin-s particle is $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1} (\otimes \ldots)$

- The orbital angular momentum of a fundamental particle can be changed, but its spin (like its electric charge) is an inherent property

In this lecture, we'll construct explicit matrix reprs of the spin operators in this basis, for small values of s

Scalars

Particles with spin 0 are called scalars, e.g. Higgs boson

- When $s=0$, only one state $|0,0\rangle$ obeying $e^{-i\underline{\alpha}\cdot\underline{S}/\hbar}|0,0\rangle = |0,0\rangle \; \forall \underline{\alpha}$
- Scalars are perfectly spherical objects, uncharged by any rotation

Spin half

Electrons, protons, neutrons are all examples of spin-$\frac{1}{2}$ particles

- Just 2 lin indep states, $|\uparrow\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$ and $|\downarrow\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$.
  Generic spin state is $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$ with $|a|^2 + |b|^2 = 1$
- In this basis can represent

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

Using $S_x = (S_+ + S_-)/2$ and $S_y = (S_+ - S_-)/2i$ gives

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

[e.g. $S_x|\downarrow\rangle = \frac{1}{2}S_+|\downarrow\rangle = \frac{\hbar}{2}\sqrt{(\frac{1}{2})(\frac{1}{2}+1) - (-\frac{1}{2})(-\frac{1}{2}+1)}\,|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$]

- When $s = \frac{1}{2}$ we often write $\underline{S} = \frac{\hbar}{2}\underline{\sigma}$ where the $\underline{\sigma}$ are called Pauli matrices

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

Spin precession

Classically, when a magnetic dipole $\underline{\mu}$ is placed in a magnetic field $\underline{B}$ it experiences a torque $\dot{\underline{S}} = \underline{\mu} \times \underline{B}$

If also $\underline{\mu} = (\gamma) \underline{S}$ and $\underline{B}$ is constant, $\underline{S}$ precesses around $\underline{B}$ with angular velocity $\underline{\omega} = -\gamma \underline{B}$

(γ: gyromagnetic ratio)

- The proton dipole $\underline{\mu} = \gamma \underline{S}$ where $\gamma = g_p e / 2 m_p c$ with $g_p \approx 5.59$
- If the proton is not free to move through space (e.g. fixed in solid)

$$H = -\gamma \underline{S} \cdot \underline{B} = -\gamma B S_z \quad \text{where } \underline{B} = B \hat{\underline{z}}$$

$$\left[\frac{\partial S_i}{\partial t} = \frac{1}{i\hbar}[H, S_i] = -\frac{\gamma}{i\hbar} B_j [S_j, S_i] = -\gamma B_j \varepsilon_{jik} S_k = \gamma (\underline{B} \times \underline{S})_i \right]$$

- Suppose our proton is initially in state (ex Sh 2)

$$|\underline{n}\uparrow\rangle = e^{-i\phi/2} \cos\frac{\theta}{2} |\uparrow\rangle + e^{i\phi/2} \sin\frac{\theta}{2} |\downarrow\rangle$$

with spin maximally aligned along $\underline{n} = (\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta)$

- After time t, proton will be in state

$$|\underline{n}(t)\uparrow\rangle = U(t) |\underline{n}\uparrow\rangle = e^{i(\omega t/2 - \phi/2)} \cos\frac{\theta}{2} |\uparrow\rangle + e^{-i(\omega t/2 - \phi/2)} \sin\frac{\theta}{2} |\downarrow\rangle$$

  - ▷ θ independent of time, but $\phi(t) = \phi - 2\omega t$ $\quad !\underline{\omega} = -\gamma \underline{B}!$
  - ▷ $\underline{n}(t)$ precesses around $\underline{B}$ at ang freq $2\gamma B/2 = \frac{g_p e B}{m_p}$

Paramagnetic Resonance

Our spin precesses around the constant field $\underline{B}$ at frequency $\underline{\omega} = -\gamma \underline{B}$

- If we sit in a moving frame that rotates with angular frequency $\underline{\omega}_r$, then we see precession with $\underline{\omega} - \underline{\omega}_r$
  - ▷ see no net precession if our frame rotates at the same rate

We now add a further field $\underline{b}(t)$ with $\underline{b}(t) \cdot \underline{B} = 0$

- Choose to be resonant $\hat{\underline{b}}(t)$ rotates in lab frame at exactly the right frequency γB to stay constant in rotating frame
  - ▷ in rotating frame spin sees a constant field so precess around new axis
  - ▷ new precession freq $\gamma |\underline{b}|$ can be $\ll \gamma |\underline{B}|$

L 8.3

- This is the basis of MRI
  - ▷ protons held in place in molecules in body
  - ▷ heat bath (warm body!) actually means spins preferentially align with large static $\underline{B}$
  - ▷ small $\underline{b}(t)$ excites protons' spins : we observe their subseq decay
  - ▷ if $\nabla \underline{B} \neq 0$ only a thin slice will be resonant

Spin one

Spin-1 particles called W and Z bosons allow a pair of Hydrogen atoms to fuse into deuterium, powering nuclear fusion in the core of stars

- There are 3 lin indep states with $s=1$, $|+\rangle = |1,1\rangle$, $|0\rangle = |1,0\rangle$, $|-\rangle = |1,-1\rangle$
- In this basis the spin operators are

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} & 1 & \\ 1 & & 1 \\ & 1 & \end{pmatrix}, \quad S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} & -i & \\ i & & -i \\ & i & \end{pmatrix}, \quad S_z = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix}$$

use relations $S_+|0\rangle = \sqrt{2}\hbar|+\rangle$, $S_+|-\rangle = \sqrt{2}\hbar|0\rangle$

$S_-|0\rangle = \sqrt{2}\hbar|-\rangle$, $S_-|+\rangle = \sqrt{2}\hbar|0\rangle$ for S_x, S_y

Orbital angular momentum

We'll now examine orbital angular momentum $\underline{L} = \underline{X} \times \underline{P}$, starting from the repn theory point of view

- Consider a spinless particle described by $|\psi\rangle \in L^2(\mathbb{R}^3, dx)$
- For $U(\underline{\alpha}) = e^{-i\underline{\alpha}\cdot\underline{L}/\hbar}$ to describe a rotation, must have

$$U^\dagger(\underline{\alpha})\, \underline{X}\, U(\underline{\alpha}) = \underline{R}(\underline{\alpha})\, \underline{X}$$

so $U(\underline{\alpha})|\underline{x}\rangle = |\underline{R}(\underline{\alpha})\underline{x}\rangle$ on position eigenstates

- Under rotation, $|\psi\rangle \mapsto |\psi'\rangle = U(\underline{\alpha})|\psi\rangle$ with wavefunction

$$\langle \underline{x}|\psi'\rangle = \langle \underline{x}|U(\underline{\alpha})|\psi\rangle = (|\underline{R}^{-1}(\underline{\alpha})\underline{x}\rangle)^\dagger |\psi\rangle = \psi(\underline{R}^{-1}(\underline{\alpha})\underline{x})$$

  - ▷ inverse rotation ensures $\langle \underline{x}|U_2 U_1|\psi\rangle = \langle \underline{x}\underline{R}_2^{-1}\underline{R}_1^{-1}|\psi\rangle = \langle \underline{x}(R_2R_1)^{-1}|\psi\rangle$ ✓
- This representation is unitary, since

$$\langle \phi'|\psi'\rangle = \int \overline{\phi(\underline{R}^{-1}\underline{x})}\, \psi(\underline{R}^{-1}\underline{x})\, d^3x = \int \overline{\phi(\underline{x}')}\, \psi(\underline{x}')\, d^3x' = \langle \phi|\psi\rangle$$

where $\underline{x}' = \underline{R}^{-1}\underline{x}$ and $d^3x' = d^3x$, measure invariant

Reprns of orbital ang momentum

As usual, the algebra $[L_i, L_j] = i\hbar\,\varepsilon_{ijk} L_k$ means we can find a basis of simultaneous eigenstates of $\underline{L}^2$ and L_z

- We let $|\ell, m\rangle$ denote an eigenstate of $\underline{L}^2$ and L_z, with

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

- In $\mathbb{R}^3$ we can continuously shrink a circular path to zero size
  - ▷ must have $e^{-2\pi i \hat{\underline{\alpha}}\cdot \underline{L}/\hbar} = 1_{L^2(\mathbb{R}^3)}$ for all $\hat{\underline{\alpha}}$
  - ▷ unlike spin, only $\ell \in \mathbb{N}_{\geq 0}$ representations allowed (not $2\ell \in \mathbb{N}_0$)

We want to embed the $(2\ell+1)$-dim repn $\mathcal{H}_\ell$ inside the ∞-dim $L^2(\mathbb{R}^3)$

- Rotations act trivially on $r = |\underline{x}|$ so polar coords helpful
- $L^2(\mathbb{R}^3 \setminus \{0\}) \cong L^2(\mathbb{R}_{>0}) \hat{\otimes} L^2(S^2) \cong L^2(\mathbb{R}_{>0}) \hat{\otimes}_\ell \mathbb{C}^{2\ell+1}$
  - ▷ in IB language this is just separation of variables in spherical polars

Angular momentum eigenstates

- In position space we have

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

so if $L_z |\ell, m\rangle = m\hbar |\ell, m\rangle$ then position space wavefunction takes the form $\langle \underline{x} | \ell, m\rangle = e^{im\phi} K_{\ell,m}(r,\theta)$ for some function $K_{\ell,m}$

- Angular momentum raising & lowering operators act on position space wavefunctions as

$$\begin{aligned}\langle \underline{x} | L_\pm | \psi \rangle &= -i\hbar \left((y \mp ix)\frac{\partial}{\partial z} - z\left(\frac{\partial}{\partial y} \mp i\frac{\partial}{\partial x} \right) \right) \psi(\underline{x}) \\ &= \pm\hbar e^{i\pm\phi} \left(\frac{\partial}{\partial\theta} \pm i\cot\theta \frac{\partial}{\partial\phi} \right) \psi(\underline{x})\end{aligned}$$

- Highest weight state defined by $L_+ |\ell,\ell\rangle = 0$, which in pos^n space implies $\langle \underline{x} | \ell, \ell\rangle = R_\ell(r) e^{i\ell\phi} \sin^\ell\theta$ for some $R_\ell(r)$
- States with $m < \ell$ obtained by acting on this with L_-

Spherical harmonics

The eigenstates we've constructed are called spherical harmonics

- Often denoted $Y_\ell^m(\theta,\phi) = \langle \theta,\phi \mid \ell, m\rangle$
- Eigenstate condition

$$L^2|\ell,m\rangle = \ell(\ell+1)\hbar^2|\ell,m\rangle$$

implies $-\nabla^2_{S^2} Y_\ell^m(\theta,\phi) = \ell(\ell+1) Y_\ell^m(\theta,\phi)$

in position space, where $\nabla^2_{S^2}$ is the Laplacian on the unit sphere

↳ $\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\phi} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$

- Y_ℓ^m's obey the orthonormality condition

$$\int_{S^2} \overline{Y_{\ell'}^{m'}(\theta,\phi)}\, Y_\ell^m(\theta,\phi)\, d\mu = \delta_{\ell'\ell}\delta_{m'm}$$

by construction, where $d\mu = \sin\theta\, d\theta\, d\phi$ is natural measure

↳ T & parity

It's sometimes useful to think of spherical harmonics as the restriction to the unit sphere of homogeneous degree-ℓ harmonic polys on $\mathbb{R}^3$

- Let P_ℓ be the space of $\mathbb{C}$-valued, degree-ℓ hom polynomials in (x,y,z) or equivalently in $(x+iy, x-iy, z)$

$$\sum_{\ell_1,\ell_2,\ell_3} a_{\ell_1\ell_2\ell_3}(x+iy)^{\ell_1}(x-iy)^{\ell_2} z^{\ell_3} \in P_\ell \quad \text{with } \ell_1+\ell_2+\ell_3 = \ell$$

so $\dim(P_\ell) = \frac{(\ell+2)(\ell+1)}{2}$

- Taking Laplacian gives a surjective map $\nabla^2 : P_\ell \to P_{\ell-2}$ and hence $\dim\ker\nabla^2 = \frac{(\ell+2)(\ell+1)}{2} - \frac{\ell(\ell-1)}{2} = 2\ell+1$

recovering the $2\ell+1$ possible values of m

Under parity $\mathcal{P}: (x,y,z) \mapsto (-x,-y,-z)$; this construction shows

$$Y_\ell^m(-\hat{x}) = (-1)^\ell Y_\ell^m(\hat{x}) \quad \text{or} \quad Y_\ell^m(\pi-\theta,\pi+\phi) = (-1)^\ell Y_\ell^m(\theta,\phi)$$

TL;DW • Spin, orb ang mom have same repns as $\underline{J}$, except only integer ℓ allowed for $\underline{L}$

▷ Label eigenstates $|j,m\rangle$, $|s,\sigma\rangle$, $|\ell,m\rangle$

▷ Hilbert space of spin-s particle is (at least) $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$

- For finite s, can find explicit matrix repns of spin
- Orbital angular momentum eigenstates are spherical harmonics
  - ◆ $-\nabla^2_{S^2} Y_\ell^m = \ell(\ell+1) Y_\ell^m$ and $-i\partial_\phi Y_\ell^m = m Y_\ell^m$
  - ▷ Y_ℓ^m odd/even under parity when ℓ odd/even
- We've not yet shown how to change total orb ang mom
  - ▷ $L_\pm$ realign more/less along z, but $[L^2, L_\pm] = 0$

Up next • Investigate dynamical symmetries

▷ symmetries of H not inherited from transformations of $\mathbb{R}^3$

▷ 3d harmonic oscillator, gross structure of Hydrogen atom

Dynamical Symmetries

Motion in a Central Potential

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

- Since $[H, \underline{L}^2] = [H, L_z] = [\underline{L}^2, L_z] = 0$ we can use basis $|n, \ell, m\rangle$
  - ▷ energy, total ang mom & ang mom around z-axis all conserved
- Since $[H, L_\pm] = 0$, energy levels must be indep of m
  - ▷ clear that energy levels must be indep of m: no preferred z-axis
  - ▷ expect $(2\ell+1)$-fold degeneracy from raising / lowering L_z
- Generically we do expect energies to depend on ℓ

We occasionally find Hamiltonians with further degeneracy. It's natural to suspect these have a hidden, larger symmetry

- If algebra closes (including H), we say we have <u>dynamical</u> symmetry
  - ▷ only examples in $\mathbb{R}^3$ are isotropic oscillator & Coulomb potential
  - ▷ often transformations of <u>phase space</u> $\mathbb{R}^6 \ni (\underline{x}, \underline{p})$ not $\mathbb{R}^3$ itself

The 3d Isotropic Harmonic Oscillator

Hamiltonian is just the sum of three 1d oscillators, each with frequency ω

$$H = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + \frac{1}{2}m\omega^2(X^2 + Y^2 + Z^2) = H_x + H_y + H_z$$

- We introduce three sets of raising & lowering operators

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

  - ▷ these obey $[A_i^\dagger, A_j] = \delta_{ij}$, $[A_i, A_j] = 0 = [A_i^\dagger, A_j^\dagger]$
  - ▷ the Hamiltonian can be written $H = \hbar\omega(\underline{A}^\dagger \cdot \underline{A} + \frac{3}{2})$
- The energy eigenstates are

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

and have energy $E_n = (N + \frac{3}{2})\hbar\omega$ where $N = n_x + n_y + n_z$

- Degeneracy is $\frac{(N+2)(N+1)}{2}$
  - ▷ <u>why</u> is this degeneracy so large? (grows quadratically with N)

"bars"

Dynamical symmetry of the isotropic oscillator

Our Hamiltonian $H = \hbar\omega\left(\underline{A}^\dagger \cdot \underline{A} + \frac{3}{2}\right)$ has further symmetry, beyond rotational invariance

- H is invariant under $A_i \mapsto u_{ij} A_j$ (so $A_i^\dagger \mapsto A_k^\dagger u_{ki}^\dagger$) provided $u_{ki}^\dagger u_{ij} = \delta_{kj}$
  - ▷ $\underline{u}$ is a 3×3 unitary matrix acting on Cartesian components of the raising/lowering operators ($\underline{u}$ is not an operator in $\mathcal{H}$!)
  - ▷ $u_{ij} \in \mathbb{C}$, so action on mixes $\underline{X} \sim \mathrm{Re}(\underline{A})$ with $\underline{P} \sim \mathrm{Im}(\underline{A})$
- A 3×3 unitary matrix has 9 independent real parameters, so there should be 9 generators, each of which is conserved
- Infinitesimally $u_{ij} = \delta_{ij} - i\varepsilon_{ik} t_{kj}$ where $|\varepsilon_{ik}| \ll 1$ and $\underline{t}^\dagger = \underline{t}$ (hmm...)
  - ▷ $\exists$ unitary operator $U(\underline{u}) : \mathcal{H} \to \mathcal{H}$ with $U = 1_{\mathcal{H}} - i\varepsilon \underline{T}$ infinitesimally
  - ▷ we find $\underline{T} = \underline{A}^\dagger \otimes \underline{A}$ (i.e. $T_{ij} = A_i^\dagger A_j$)
- $\underline{T}$ is Hermitian and all its components are conserved

$$\frac{1}{\hbar\omega}[T_{ij}, H] = [A_i^\dagger A_j, A_k^\dagger A_k]$$
$$= A_i^\dagger \underbrace{[A_j, A_k^\dagger]}_{-\delta_{jk}} A_k + A_k^\dagger \underbrace{[A_i^\dagger, A_k]}_{\delta_{ik}} A_j$$
$$= -A_i^\dagger A_j + A_i^\dagger A_j = 0$$

Conserved quantities in the isotropic oscillator

To understand these, it's helpful to decompose into its trace, anti-sym and traceless sym parts

$$T_{ij} = \frac{\delta_{ij}}{3} \underline{A}^\dagger \cdot \underline{A} + \frac{A_i^\dagger A_j - A_j^\dagger A_i}{2} + \left[\frac{A_i^\dagger A_j + A_j^\dagger A_i}{2} - \frac{1}{3}\delta_{ij}\underline{A}^\dagger \cdot \underline{A}\right]$$

- The trace is essentially just H (or the total number operator)
- The 8 remaining components generate $SU(3) \cong U(3)/U(1)$
- The antisym part generates $SO(3) \subset SU(3)$

$$\varepsilon_{ijk} A_j^\dagger A_k = \frac{1}{2m\hbar\omega}\varepsilon_{ijk}(m\omega X_j - iP_j)(m\omega X_k + iP_k)$$
$$= \frac{i}{2\hbar}\varepsilon_{ijk}(X_j P_k - P_j X_k) = \frac{i}{2\hbar}\varepsilon_{ijk}(X_j P_k - X_k P_j) \quad \text{(swap)}$$
$$= \frac{i}{\hbar} L_i,$$

the usual orbital ang mom generators $\underline{L} = -i\hbar(\underline{A}^\dagger \times \underline{A})$

- Traceless sym part mixes $\underline{X}$ with $\underline{P}$
  - ▷ less familiar as special to isotropic oscillator

Hydrogen: Gross structure

With a Coulomb potential, the Hamiltonian

$$H = \frac{p^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0|\underline{x}|}$$

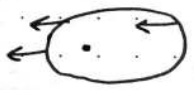
obeys $[H, \underline{L}] = 0$, so we can find a complete set $\{|n,\ell,m\rangle\}$ of eigenstates of $(H, \underline{L}^2, L_z)$

- Known (see probs 2) that energy levels are $E_{n,\ell,m} = -\frac{R}{n^2}$ where
  $R = \mu e^4/32\pi^2\epsilon_0^2\hbar^2 \approx 13.6\,eV$ is Rydberg's constant
  - ▷ agrees (somewhat coincidentally) with Bohr model
- At fixed energy, $\ell \in \{0,1,\dots,n-1\}$ so n^{th} energy level has degeneracy
  $$\sum_{\ell=0}^{n-1}(2\ell+1) = 2\cdot\frac{n(n-1)}{2} + n = n^2$$
- Why should the energies be independent of ℓ as well as m?
  - ▷ in fact degeneracy is lifted in real Hydrogen atom (see later)

The Runge-Lenz vector

In the classical Kepler problem orbits with $E<0$ are ellipses

- $\underline{\ell} = \underline{x}\times\underline{p}$ conserved $\Rightarrow$ orbits lie in plane
- Orbits closed because Runge-Lenz vector
  $$\underline{v} = \frac{1}{\mu}\underline{p}\times\underline{\ell} - \kappa\frac{\underline{x}}{|\underline{x}|} \quad (\text{where } V = -\tfrac{\kappa}{|\underline{x}|})$$



is also conserved,

$$\mu\dot{\underline{v}} = \dot{\underline{p}}\times\underline{\ell} - \kappa\frac{\mu\dot{\underline{x}}}{|\underline{x}|} + \kappa\mu\underline{x}\frac{\underline{x}\cdot\dot{\underline{x}}}{|\underline{x}|^3}$$

$$= -(\nabla V)\times(\underline{x}\times\underline{p}) - \kappa\frac{\underline{p}}{|\underline{x}|} + \kappa\underline{x}\frac{\underline{x}\cdot\underline{p}}{|\underline{x}|^3}$$

$$= -\frac{\kappa}{|\underline{x}|^3}\left(\underline{x}\times(\underline{x}\times\underline{p}) + \underline{p}(\underline{x}\cdot\underline{x}) - \underline{x}(\underline{x}\cdot\underline{p})\right) = 0$$

- Since $(\underline{x},\underline{p}) \in \mathbb{R}^6$ there must be relations between E, $\underline{\ell}$ & $\underline{v}$
  $$|\underline{v}|^2 = \kappa^2 + \frac{2E}{\mu}|\underline{\ell}|^2 \quad \text{with eccentricity } |\underline{v}|/\kappa$$

L9.4 $SU(2) \times SU(2)$ symmetry of the Coulomb potential (*)

- In the quantum theory we define the Runge-Lenz operator

$$\underline{R} = \frac{1}{2\mu}(\underline{P} \times \underline{L} - \underline{L} \times \underline{P}) - k\frac{\underline{X}}{|\underline{X}|}$$

▷ using $(\underline{P} \times \underline{L} - \underline{L} \times \underline{P})/2$ ensures $\underline{R}^\dagger = \underline{R}$

▷ $[H, \underline{R}] = 0$ and also $\underline{L} \cdot \underline{R} = \underline{R} \cdot \underline{L} = 0$ (Check!) UGH!

- We have $[L_i, R_j] = i\hbar\,\varepsilon_{ijk} R_k$ and $[R_i, R_j] = -\frac{2i\hbar}{\mu} H \varepsilon_{ijk} L_k$

▷ algebra of $H, \underline{L}, \underline{R}$ closes, so have dynamical symmetry

- The algebra is clearer if we introduce

$$\underline{A}_\pm = \frac{1}{2}\left(\underline{L} \pm \sqrt{\frac{\mu}{-2H}}\,\underline{R}\right)$$

▷ $\underline{A}_\pm$ are Hermitian provided we act on bound states (where $E<0$)

▷ no ordering ambiguity since $[H, \underline{R}] = 0$

▷ obey $so(3) \times so(3)$ algebra

$$[A_{+i}, A_{+j}] = i\hbar\,\varepsilon_{ijk} A_{+k} \qquad [A_{-i}, A_{-j}] = i\hbar\,\varepsilon_{ijk} A_{-k} \qquad [A_{+i}, A_{-j}] = 0$$

Energy levels & degeneracy of Coulomb potential

Since they each obey the same algebra as ang mom, evals of $\underline{A}_\pm^2$ take the familiar form $a_\pm(a_\pm+1)\hbar^2$ with $a_\pm \in \{0, \frac{1}{2}, 1, \ldots\}$

- Given $a_\pm$, there are $2a_\pm + 1$ possible evals $m_\pm$ for $A_{\pm z}$
- Since $\underline{L} \cdot \underline{R} = \underline{R} \cdot \underline{L} = 0$ we have

$$\underline{A}_+^2 = \underline{A}_-^2 = \frac{1}{4}\underline{L}^2 - \frac{\mu}{8H}\underline{R}^2 = -\frac{\mu k^2}{8H} - \frac{\hbar^2}{4}$$

▷ because $\underline{A}_+^2 = \underline{A}_-^2$ we must have $a_+ = a_- = a$ (but m_+, m_- still free)

- Energy levels determined by $2a \in \mathbb{Z}_{\geq 0}$ to be

$$E = -\frac{\mu k^2}{8} \cdot \frac{1}{a(a+1)\hbar^2 + \hbar^2/4} = -\frac{\mu k^2}{2} \cdot \frac{1}{(2a+1)^2} = -\frac{\mu k^2}{2} \cdot \frac{1}{n^2}$$

where $n = 2a+1 \in \{1, 2, 3, \ldots\}$

▷ degeneracy of the n^{th} level is $(2a+1)^2 = n^2$ (from possible $m_\pm$)

- This derivation was first given by (absolute chad) Wolfgang Pauli

▷ he did it in 1926; before Schrödinger's equation was published

TL;DW • Dynamical symmetries are symmetries of H that do not come from transformations of $\mathbb{R}^3$

▷ only examples in 3d are harmonic and Coulomb potentials

▷ closely related to integrable systems

- Presence of dynamical symmetry leads to enhanced degeneracy among energy levels
- For d-dim harmonic oscillator, dynamical symmetry is $SU(d)$
- For Coulomb potential, symmetry is $(SU(2) \times SU(2))/\mathbb{Z}_2 \cong SO(4)$

Up Next Revisit isotropic oscillator with spherical polars

The Isotropic Oscillator revisited

Look once more at $H = \frac{1}{2\mu}\underline{P}^2 + \frac{1}{2}\mu\omega^2\underline{X}^2$

- Simple to solve using Cartesian coordinates
  - ▷ Energy eigenstates take the form

$$|\underline{n}\rangle = |n_x\rangle \otimes |n_y\rangle \otimes |n_z\rangle \in L^2(\mathbb{R}^3) \cong L^2(\mathbb{R}) \hat{\otimes} L^2(\mathbb{R}) \hat{\otimes} L^2(\mathbb{R})$$

- This obscures the spherical symmetry of the problem
  - ▷ $[H, \underline{L}] = 0$ so label eigenstates as $|n,\ell,m\rangle \in L^2(\mathbb{R}_>) \hat{\otimes} L^2(S^2)$ where

$$L^2|n,\ell,m\rangle = \hbar^2\ell(\ell+1)|n,\ell,m\rangle$$

$$L_z|n,\ell,m\rangle = m\hbar|n,\ell,m\rangle$$

$$H|n,\ell,m\rangle = E_n|n,\ell,m\rangle$$

- ▷ pos^n space wavefunction $\langle \underline{x}|n,\ell,m\rangle = f_{n,\ell}(r)\, Y_\ell^m(\theta,\phi)$

The radial Hamiltonian

When acting on an L^2 eigenstate, we have

$$H|n,\ell,m\rangle = \left(\frac{1}{2\mu}P_r^2 + \frac{1}{2\mu}\frac{L^2}{|X|^2} + \frac{1}{2}\mu\omega^2|X|^2\right)|n,\ell,m\rangle$$

- $P_r = \langle \hat{\underline{X}}\cdot\underline{P} + \underline{P}\cdot\hat{\underline{X}}\rangle/2$ is the radial momentum operator and $R = |\underline{X}|$

$$= \left(\frac{1}{2\mu}P_r^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu R^2} + \frac{1}{2}\mu\omega^2R^2\right)|n,\ell,m\rangle = H_\ell|n,\ell,m\rangle$$

$$[R, P_r] = \frac{1}{2}\left[|\underline{X}|, \hat{\underline{X}}\cdot\underline{P}\right] + \frac{1}{2}\left[|\underline{X}|, \underline{P}\cdot\hat{\underline{X}}\right]$$

$$= \frac{1}{2}\frac{X_i}{|\underline{X}|}[|\underline{X}|, P_i] + \frac{1}{2}[|\underline{X}|, P_i]\frac{X_i}{|\underline{X}|} = 2\,\frac{i\hbar}{2}\,\frac{X_iX_i}{|\underline{X}|^2} = i\hbar \quad \checkmark \text{neat}$$

$$\downarrow$$

$$[\sqrt{X_jX_j}, P_i]$$

$$= i\hbar\frac{1}{\sqrt{X_iX_i}}X_j\delta_{ij}$$

- H_ℓ acts only in the radial direction
  - ▷ angular problem solved, just radial problem remains
  - ▷ H_ℓ related to full H only on L^2-eigenstates with eval $\ell(\ell+1)\hbar^2$

Raising & Lowering Operators

$$A_\ell = \frac{1}{\sqrt{2\mu\hbar\omega}}\left(\mu\omega R + iP_r \mp \frac{(\ell+1)\hbar}{R}\right)$$

- Related to radial Hamiltonian $H_\ell = \hbar\omega\left(A_\ell^\dagger A_\ell + \ell + \tfrac{3}{2}\right)$

$$\begin{aligned} A_\ell^\dagger A_\ell &= \frac{1}{2\mu\hbar\omega}\left(\mu\omega R - iP_r\right)\left(\mu\omega R + iP_r\right) \\ &\quad + \frac{1}{2\mu\hbar\omega}\left(\frac{(\ell+1)^2\hbar^2}{R^2} \mp \left(\mu\omega R - iP_r\right)\frac{(\ell+1)\hbar}{R} \mp \frac{(\ell+1)\hbar}{R}\left(\mu\omega R + iP_r\right)\right) \\ &= \ldots + \frac{1}{2\mu\hbar\omega}\left(\frac{(\ell+1)^2\hbar^2}{R^2} \mp 2\mu\omega(\ell+1)\hbar \mp i(\ell+1)\hbar\left[\frac{1}{R}, P_r\right]\right) \\ &\qquad\qquad \text{with } \left[\frac{1}{R}, P_r\right] \to -\frac{i\hbar}{R^2} \end{aligned}$$

- Commutation relations give

$$\begin{aligned} \left[A_\ell, A_\ell^\dagger\right] &= \frac{1}{2\mu\hbar\omega}\left[\mu\omega R + iP_r, \mu\omega R - iP_r\right] + \frac{2i(\ell+1)\hbar}{2\mu\hbar\omega}\left[\frac{1}{R}, P_r\right] \\ &= 1 + \frac{2(\ell+1)\hbar}{2\mu\omega R^2} = 1 + \frac{H_{\ell+1} - H_\ell}{\hbar\omega} \end{aligned}$$

- Correspondingly we find

$$\begin{aligned} \left[A_\ell, H_\ell\right] &= \hbar\omega\left[A_\ell, A_\ell^\dagger A_\ell\right] = \hbar\omega\left[A_\ell, A_\ell^\dagger\right]A_\ell \\ &= \left(\hbar\omega + H_{\ell+1} - H_\ell\right)A_\ell \end{aligned}$$

or equivalently $H_{\ell+1}A_\ell = A_\ell\left(H_\ell - \hbar\omega\right)$

- ▷ close to showing A_ℓ is a lowering operator for the energy
- ▷ presence of $H_{\ell+1}$ means we must consider all $\ell \in \mathbb{Z}_{\geq 0}$ simultaneously

Radial Spectrum

Suppose we have eigenstate $H_\ell|E_\ell\rangle = E_\ell|E_\ell\rangle$

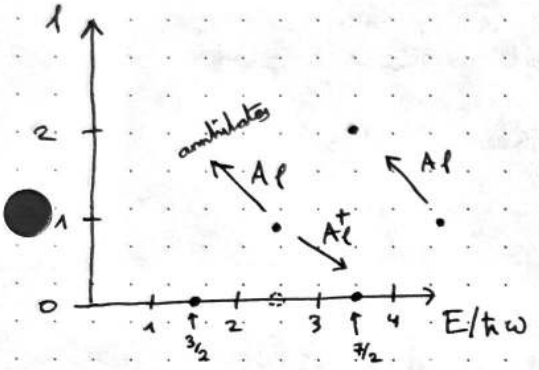
- $H_{\ell+1}\left(A_\ell|E_\ell\rangle\right) = A_\ell\left(H_\ell - \hbar\omega\right)|E_\ell\rangle = \left(E_\ell - \hbar\omega\right)\left(A_\ell|E_\ell\rangle\right)$
  - ▷ if non-vanishing, the radial state $\propto A_\ell|E_\ell\rangle$ is an eigenfunction of $H_{\ell+1}$ with decreased energy $E_\ell - \hbar\omega$
  - ▷ radial wavefunction $\langle r|A_\ell|E_\ell\rangle$ is appropriate for increased ang. mom
  - ▷ since $\left[L^2, A_\ell\right] = 0$, applying A_ℓ hasn't changed the total angular momentum – must do this 'by hand'

- Considering the norm

$$\frac{E}{\hbar\omega} - \ell - \frac{3}{2} = \langle E_\ell | A_\ell^\dagger A_\ell | E_\ell \rangle = \| A_\ell | E_\ell \rangle \|^2 \geq 0$$

- ▷ max possible angular mom at fixed energy E given by $\ell_{max} = \frac{E}{\hbar\omega} - \frac{3}{2} = n$
- Ground state occurs when $n = 0$ and has energy $E = \frac{3}{2}\hbar\omega$
  - ▷ since ground state has $n = \ell = 0$, it is spherically symmetric
  - ▷ agrees with conclusions from Cartesian perspective

Action of A_ℓ, $A_\ell^\dagger$



- For each given ℓ, there are $2\ell+1$ angular states
- For given energy, ℓ even or odd only
- A_ℓ, $A_\ell^\dagger$ act diagonally

Degeneracy of n^{th} energy level obtained

$$\sum_{\ell \text{ even/odd}}^{n} (2\ell+1) = \frac{(n+2)(n+1)}{2}$$

Radial wavefunctions

States of max possible ang mom ($\ell_{max} = n$) at given energy are defined by $A_{\ell_{max}} | E_{\ell_{max}} \rangle = 0$, so radial wavefunction obeys

$$0 = \sqrt{2\mu\omega}/\hbar \, \langle r | A_{\ell_{max}} | E_{\ell_{max}} \rangle = \left(\frac{d}{dr} + \frac{1}{r} - \frac{\ell_{max}+1}{r} + \frac{\mu\omega r}{\hbar} \right) \langle r | E_{\ell_{max}} \rangle$$

which is solved by

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

- Quantum equivalent of a circular orbit, but still has some non-zero radial kinetic energy
- Since $d^3x = r^2 dr \sin\theta \, d\theta \, d\phi$ the radial prob density

$$p(r) \sim r^{2(\ell_{max}+1)} e^{-r^2/2r_0^2}$$

- Radial states of more eccentric orbits obtained by acting with $A_\ell^\dagger$

TL;DW
- Natural to study isotropic harmonic oscillator using spherical polars
  - ▷ illuminates role of angular momentum more clearly
- Operator A_ℓ acts only on radial state $\in L^2(\mathbb{R}_>)$
  - ▷ lowers energy, but moves to radial state appropriate for $\ell \mapsto \ell+1$
  - ▷ does not affect angular part; must do this by hand with this method
- Recover same energy levels & degeneracy as before
- Prob Sheet 2 now free real estate ☺

UpNext
- Combine angular momentum of several constituent parts
  - ▷ decompose tensor product into irreps $R_1 \otimes R_2 = \oplus R_3$
  - ▷ go through simple examples and compare to classical intuition

Addition of Angular Momenta

Composite systems can store their angular momentum in several ways

- Angular momentum of bike comes from both revolving wheels
- Angular momentum of Hydrogen atom comes from spins of electron & proton, as well as relative orbital angular momentum

We want to understand how the angular momenta of the subsystems can combine to form total angular momentum

$$\underline{j}_{tot} = \underline{j}_1 + \underline{j}_2 \quad \text{classically}$$

$$|j_1| + |j_2| \geq |\underline{j}_{tot}| \geq |j_1| - |j_2|$$

Equalities hold only when $\underline{j}_1, \underline{j}_2$ are parallel or antiparallel

Combining quantum angular momenta

Suppose system has two indep degrees of freedom, each with fixed total ang momentum labelled by j_1, j_2 resp

- Let $\{|j_1, m_1\rangle\}$ be basis of eigenstates of $(\underline{J}_1^2, J_{1z})$ and $\{|j_2, m_2\rangle\}$ same for $(\underline{J}_2^2, J_{2z})$
- Then $\{|j_1, m_1\rangle \otimes |j_2, m_2\rangle\}$ is a basis for combined system and

$$\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} \ni |\psi\rangle = \sum_{m_1, m_2} a_{m_1 m_2} |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

- How do these states fit into multiplets of definite total ang mom for the combined system?
  - ▷ Physically, since angular momentum is quantized, what possible values of the total ang mom can arise?
  - ▷ Mathematically, we wish to decompose the combined Hilbert space into irreducible reprns of $so(3)$ as $\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} \cong \bigoplus_j \mathcal{H}_j$

Raising & lowering operators for combined system

this def" ← makes sense Ö

We define the combined ang mom operator

$$\underline{J} = \underline{J}_1 \otimes 1_2 + 1_1 \otimes \underline{J}_2 \quad \text{with} \quad \underline{J}^2 = \underline{J}_1^2 \otimes 1_2 + 1_1 \otimes \underline{J}_2^2 + 2\,\underline{J}_1 \cdot \underline{J}_2$$

Henceforth drop tensor product sign, writing

$$\underline{J} = \underline{J}_1 + \underline{J}_2 \quad \text{and} \quad \underline{J}^2 = \underline{J}_1^2 + \underline{J}_2^2 + 2\,\underline{J}_1 \cdot \underline{J}_2$$

We need to understand how $\underline{J}_1 \cdot \underline{J}_2 = J_{1x}J_{2x} + J_{1y}J_{2y} + J_{1z}J_{2z}$ acts on our basis states. [$\underline{J}_1^2, \underline{J}_2^2$ are nice]

- Since $J_x = (J_+ + J_-)/2$, $J_y = (J_+ - J_-)/2i$ we have

$$2\,\underline{J}_1 \cdot \underline{J}_2 = 2\left(\frac{J_{1+}+J_{1-}}{2} \cdot \frac{J_{2+}+J_{2-}}{2} + \frac{J_{1+}-J_{1-}}{2i} \cdot \frac{J_{2+}-J_{2-}}{2i} + J_{1z}J_{2z} \right)$$
$$= J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}$$

and therefore

$$\underline{J}^2 = \underline{J}_1^2 + \underline{J}_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}$$

whose action on each basis elt $|j_1, m_1\rangle |j_2, m_2\rangle$ we understand

The maximally alligned multiplet

Let's start with $|j_1, j_1\rangle |j_2, j_2\rangle$ where all ang mom of both subsystems is maximally aligned along $\underline{z}$

- We have $J_z(|j_1, j_1\rangle |j_2, j_2\rangle) = (J_{1z} + J_{2z})(|j_1, j_1\rangle |j_2, j_2\rangle)$
$$= (j_1 + j_2)\hbar\, |j_1, j_1\rangle |j_2, j_2\rangle$$

$$\underline{J}^2(|j_1, j_1\rangle |j_2, j_2\rangle) = (\underline{J}_1^2 + \underline{J}_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z})\,|j_1, j_1\rangle |j_2, j_2\rangle$$
$$= (j_1(j_1+1)\hbar^2 + j_2(j_2+1)\hbar^2 + \text{zeros} + 2j_1 j_2 \hbar^2)\,|j_1, j_1\rangle |j_2, j_2\rangle$$

since both raising operators J_{1+}, J_{2+} annihilate state

- So $\underline{J}^2 |j_1, j_1\rangle |j_2, j_2\rangle = (j_1 + j_2)(j_1 + j_2 + 1)\hbar^2 |j_1, j_1\rangle |j_2, j_2\rangle$

so we identify $|j_1, j_1\rangle |j_2, j_2\rangle$ as the state $|j, j\rangle$ of the combined system, where $j = j_1 + j_2$

- This state has the maximum ang mom we can form: j_1 and j_2 are perfectly aligned with each other, and also with the z-axis.

The max aligned multiplet

The remaining states in the $j = j_1 + j_2$ multiplet are obtained by acting on $|j, j\rangle$ with combined lowering operator $J_- = J_{1-} + J_{2-}$

- Recall that the lowering operator acts on any state as

$$J_- |j, m\rangle = \sqrt{j(j+1) - m(m-1)}\,\hbar\, |j, m-1\rangle$$

Consequently, $J_- |j, j\rangle = \sqrt{2j}\,\hbar\, |j, j-1\rangle$, while

$J_{1-}|j_1, j_1\rangle = \sqrt{2j_1}\,\hbar\,|j_1, j_1-1\rangle$ and $J_{2-}|j_2, j_2\rangle = \sqrt{2j_2}\,\hbar\,|j_2, j_2-1\rangle$

- Comparing these expressions, acting on $|j, j\rangle$ with $J_- = J_{1-} + J_{2-}$ we obtain

$$|j, j-1\rangle = \sqrt{\tfrac{j_1}{j}}\,|j_1, j_1-1\rangle|j_2, j_2\rangle + \sqrt{\tfrac{j_2}{j}}\,|j_1, j_1\rangle|j_2, j_2-1\rangle$$

- Acting with J_- again constructs the remaining states in this multiplet

- ~~Actu~~ ▷ $[J^2, J_-] = 0$, so all states obtained this way have $j = j_1 + j_2$
  - ▷ because $j = j_1 + j_2$, the two subsystems' ang. mom are still maximally aligned with each other, just not with the z-axis

Imperfectly aligned multiplets

Just as classically, it's also possible that the two subsystems are not aligned

- State $|j-1, j-1\rangle$ describes arrangement where subsystems are imperfectly aligned, but where the net angular momentum maximal along z
  - ▷ Since $J_z|j-1, j-1\rangle = (j_1 + j_2 - 1)\,\hbar\,|j-1, j-1\rangle$ we must have

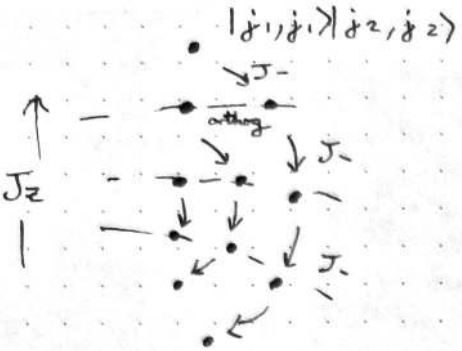
$$|j-1, j-1\rangle = a\,|j_1, j-1\rangle|j_2, j_2\rangle + b\,|j_1, j_1\rangle|j_2, j_2-1\rangle$$

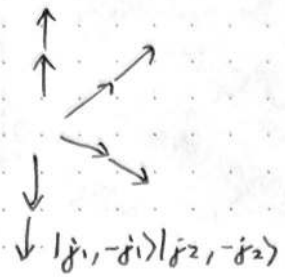
for some $a, b \in \mathbb{C}$

- ▷ Compute a, b using condition $\langle j, j-1 | j-1, j-1\rangle = 0$ together with normalization $|a|^2 + |b|^2 = 1$

Therefore we have

- $$|j-1, j-1\rangle = \sqrt{\tfrac{j_2}{j}}\,|j_1, j_1-1\rangle|j_2, j_2\rangle - \sqrt{\tfrac{j_1}{j}}\,|j_1, j_1\rangle|j_2, j_2-1\rangle$$
  - ▷ just swap coefficients from $|j, j-1\rangle$ and include relative $-$ sign
- Obtain the full $j = j_1 + j_2 - 1$ multiplet acting with J_- as before





- Moving along semicircles with $J_- = J_{1-} + J_{2-}$
  - ▷ preserves relative alignment between subsystems; but alters alignment $\hat{z}$
- Moving inwards between semi-circles uses orthogonality condition
  - ▷ preserves alignment with $\hat{z}$; but relative alignment between subsystems becomes worse

Clebsh-Gordan coefficients

Based on our classical picture; natural to conjecture lowest combined angular momentum is $|j_1 - j_2|$ with max anti-alignment

- Let's check this conjecture reproduces all the states
  - ▷ wlog assume $j_1 > j_2$, so combined $j \in \{j_1 + j_2, \ldots, j_1 - j_2\}$
  - ▷ total number of states obtained this way is

$$\sum_{j=j_1-j_2}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1)$$

in agreement with $\dim(\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}) = \dim(\mathcal{H}_{j_1}) \dim(\mathcal{H}_{j_2})$

- ▷ our conjectured range of j thus accounts for all the possible states

The numbers

$$C_{j,m}(j_1, m_1; j_2, m_2) = \langle j, m | (|j_1, m_1\rangle \otimes |j_2, m_2\rangle)$$

are known as Clebsch-Gordan coefficients

Trivial example

$j_1 \otimes 0 = j$

$\uparrow \quad \nwarrow |0,0\rangle$

$\{|j_1, m_1\rangle\}$

$\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$

The first non-trivial example is when $j_1 = j_2 = 1/2$, relevant to the ground state of hydrogen

- From above, we have $|1,1\rangle_H = |\uparrow\rangle_e |\uparrow\rangle_p$ $\qquad |\uparrow\rangle = |\tfrac{1}{2}, \tfrac{1}{2}\rangle$
- Applying $J_{-H} = J_{-e} + J_{-p}$ to this state gives

$$|1,0\rangle_H = \frac{1}{\sqrt{2}} \left(|\downarrow\rangle_e |\uparrow\rangle_p + |\uparrow\rangle_e |\downarrow\rangle_p \right)$$

$$|1,-1\rangle_H = |\downarrow\rangle_e |\downarrow\rangle_p$$

▷ further application of J_- kills

▷ note z-component of individual spins are anti-aligned, but net spin is 1

▷ components in xy-plane aligned, precise direction unknown

- Note that all three spin-1 states

$$|\uparrow\rangle_e |\uparrow\rangle_p, \quad \frac{1}{\sqrt{2}} \left(|\downarrow\rangle_e |\uparrow\rangle_p + |\uparrow e\rangle |\downarrow\rangle_p \right), \quad |\downarrow\rangle_e |\downarrow\rangle_p$$

are symmetric under exchange of the individual spins

- Remaining state $|0,0\rangle_H$ determined by ${}_H\langle 1,0|0,0\rangle_H = 0$, so

$$|0,0\rangle_H = \frac{1}{\sqrt{2}} \left(|\downarrow\rangle_e |\uparrow\rangle_p - |\uparrow\rangle_e |\downarrow\rangle_p \right)$$

and is antisymm under exchange of the individual spins

- This state clearly annihilated by $J_{zH} = J_{ze} + J_{zp}$ and also annihilated by J_{xH} and J_{yH}. For example

$$J_{xH} |0,0\rangle_H = \left(\frac{J_{+e} + J_{-e} + J_{+p} + J_{-p}}{2} \right) \left(\frac{|\uparrow\rangle_e |\downarrow\rangle_p - |\downarrow\rangle_e |\uparrow\rangle_p}{\sqrt{2}} \right)$$

$$= \frac{1}{2\sqrt{2}} \left(-|\uparrow\rangle_e |\uparrow\rangle_p + |\downarrow\rangle_e |\downarrow\rangle_p + |\uparrow\rangle_e |\uparrow\rangle_p - |\downarrow\rangle_e |\downarrow\rangle_p \right) = 0$$

- We've constructed $3 + 1 = 2 \times 2$ states altogether

▷ triplet of states with spin 1, each symm under exchange of individual spins

▷ singlet with spin 0, antisymm under exchange of individual spins

$1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$

- We obtain a $j = \frac{3}{2}$ multiplet

$$\left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle = |1,1\rangle|\uparrow\rangle$$

$$\left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle = \sqrt{\tfrac{2}{3}}\,|1,0\rangle|\uparrow\rangle + \sqrt{\tfrac{1}{3}}\,|1,1\rangle|\downarrow\rangle$$

$$\left|\tfrac{3}{2}, -\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{1}{3}}\,|1,-1\rangle|\uparrow\rangle + \sqrt{\tfrac{2}{3}}\,|1,0\rangle|\downarrow\rangle$$

$$\left|\tfrac{3}{2}, -\tfrac{3}{2}\right\rangle = |1,-1\rangle|\downarrow\rangle$$

- and also a $j = \frac{1}{2}$ multiplet

$$\left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle = \sqrt{\tfrac{1}{3}}\,|1,0\rangle|\uparrow\rangle - \sqrt{\tfrac{2}{3}}\,|1,1\rangle|\downarrow\rangle$$

$$\left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{2}{3}}\,|1,-1\rangle|\uparrow\rangle - \sqrt{\tfrac{1}{3}}\,|1,0\rangle|\downarrow\rangle$$

the classical limit

Classical ang mom has square magnitude $\underline{j}_1^2 + \underline{j}_2^2 + 2\underline{j}_1 \cdot \underline{j}_2$

- If we know nothing about the relative orientation, every point on sphere of radius $|\underline{j}_2|$ centred on $\underline{j}_1$ equally likely
- ▸ Let dP be the probability that angle between $\underline{j}_1, \underline{j}_2$ lies between $(\theta, \theta + d\theta)$
- ▸ $|\underline{j}_1|, |\underline{j}_2|$ fixed so

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

$$\left[\underline{j}^2 = \underline{j}_1^2 + \underline{j}_2^2 + 2\underline{j}_1 \cdot \underline{j}_2 = j_1^2 + j_2^2 + 2|\underline{j}_1||\underline{j}_2|\cos\theta\right]$$

- In the quantum case the proportion of states with net angular momentum j is $\dfrac{2j+1}{(2j_1+1)(2j_2+1)} \approx \dfrac{j}{2j_1 j_2}$ when $j_1, j_2 \gg 1$ in agreement with classical result

TL;DW · When we combine two states, the total ang mom can take values $j \in \{j_1 + j_2, \ldots, |j_1 - j_2|\}$

- ▸ if we combine an odd/even no. of half-integer spin particles, result will have half-int / int spin
- Construct combined $(\underline{J}^2, J_z)$ eigenstates from $|j_1, j_1\rangle|j_2, j_2\rangle$
- ▸ states obtained from $|j_1, j_1\rangle|j_2, j_2\rangle$ using lowering operators still have angular momentum aligned, but not along z-axis

- ▷ states with $\underline{J}_1, \underline{J}_2$ non-parallel obtained by orthogonalization
- ▷ the numbers $\langle j, m | \left(|j_1, m_1\rangle |j_2, m_2\rangle \right)$ are Clebsch-Gordan coeffs
- $\sum (2j+1) = (2j_1+1)(2j_2+1)$ states in all

Next lecture
- Operators can also carry angular momentum
- Wigner-Eckart theorem
  - ▷ selection rules with application to dipole radiative transitions

L13.1

Identical particles

Exchanging All electrons in Nature are indistinguishable (same for protons, photons, ...)

- Each e^- described by a copy of the same Hilbert space $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$
  - ▷ may differ in details of their motion & spin alignment, but labelled by same set of quantum numbers
  - ▷ no way to identify 'electron no. 1' or 'electron no. 2'
  - ▷ no explanation in QM but follows naturally from QFT

Whenever we have a 2 particle system, the state of the total system

$|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ with basis $\{|\alpha_1, \alpha_2\rangle = |\alpha_1\rangle|\alpha_2\rangle\}$

where α_a is a list of all quantum numbers of the a^{th} particle

- For indistinguishable particles, exchanging $1 \leftrightarrow 2$ maps

  $|\alpha_1, \alpha_2\rangle \mapsto |\alpha_2, \alpha_1\rangle = \lambda |\alpha_1, \alpha_2\rangle$ for some $\lambda \in \mathbb{C}^*$

- Exchanging twice $|\alpha_1, \alpha_2\rangle = \lambda^2 |\alpha_1, \alpha_2\rangle$, so $\lambda = \pm 1$ "statistics"
  - ▷ if $\lambda = +1$, particles called bosons (e.g. photons, H-atoms, Higgs bosons)
  - ▷ if $\lambda = -1$, particles called fermions (e.g. electrons, protons, neutrinos)

Pauli's exclusion principle

- For example, a pair of indistinguishable bosons are described by

$$|\Phi\rangle = \frac{|\alpha_1, \alpha_2\rangle + |\alpha_2, \alpha_1\rangle}{\sqrt{2}}$$

whereas state of indistinguishable fermions is antisymmetric

$$|\Psi\rangle = \frac{|\alpha_1, \alpha_2\rangle - |\alpha_2, \alpha_1\rangle}{\sqrt{2}}$$

- Pauli's exclusion principle: if $\alpha_1 = \alpha_2$ then $|\Psi\rangle = 0$, so no two fermions can be in the same state
- Important we exchange all the quantum numbers
  - ▷ e.g. for fermions, $\psi_{\sigma,\sigma'}(\underline{x}, \underline{x}') = -\psi_{\sigma',\sigma}(\underline{x}', \underline{x})$ but not necessarily any relation to $\psi_{\sigma,\sigma'}(\underline{x}', \underline{x})$
- Generalizes to states of N indistinguishable particles

$|\Phi_{\text{bos}}\rangle \in \text{Sym}^N \mathcal{H}$ $\quad |\Psi_{\text{ferm}}\rangle \in \bigwedge^N \mathcal{H}$

Spin and statistics

It turns out that particles with total spin $s \in \{0, 1, 2, \ldots\}$ are always bosons; whereas particles with spin $s \in \{\frac{1}{2}, \frac{3}{2}, \ldots\}$ are always fermions

- The reason spin & statistics are indeed related lies beyond QM, in realm QFT
  - ▷ if there is a relation, must be this one
  - ▷ adding an even no. of odd-half integer spins gives $s \in \mathbb{N}_0$, whereas adding an odd no. gives $s \in \frac{1}{2} + \mathbb{N}_0$
- Applies to composite particles (e.g. H-atom) as well as fundamental particles
  - ▷ exchanging two indistinguishable composites exchanges each of their constituents
  - ▷ if a composite consists of an even number of fermions (+ plus bosons), it is a boson; if an odd no. of fermions it is a fermion

Ideal quantum gases

Consider N indistinguishable fermions confined to a box of linear dimension L, but otherwise free $H = \sum_{a=1}^{N} \frac{\underline{p}_a^2}{2m}$

- Single particle energy eigenstates $|\underline{k}\rangle$ have energy $E = \hbar^2 \underline{k}^2 / 2m$ with $\underline{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$, $n_i \in \mathbb{Z}$ and wavefunction $\langle \underline{x} | \underline{k} \rangle = \frac{e^{-i\underline{k}\cdot\underline{x}}}{L^{3/2}}$
- Pauli exclusion principle prevents all N particles setting in ground state
- Energy levels are filled (accounting for spin) until all accommodated
- Highest filled energy defines Fermi energy $E_F = \hbar^2 \underline{k}_F^2 / 2m$
- Each electron[1] occupies $\underline{k}$-space volume $(2\pi/L)^3$ so for $N_e \gg 1$, we have $4\pi |\underline{k}_F|^3 / 3 = (2\pi/L)^3 N_e$ and total energy is

$$E_{tot} \overset{\uparrow}{=} \int_0^{|\underline{k}_F|} \frac{\hbar^2 k^2}{2m_e} \frac{4\pi k^2}{(2\pi/L)^3} dk = \frac{\hbar^2 |\underline{k}_F|^5 L^3}{20\pi^2 m_e} = \frac{\hbar^2}{20\pi^2 m_e} (6\pi^2 N_e)^{5/3} V^{-2/3}$$

(↑ used)

- Any reduction in size of the box is opposed by degeneracy pressure

$$P_{deg} = -\frac{\partial E_{tot}}{\partial V} = \frac{\hbar^2 (6\pi^2 N_e)^{5/3}}{30\pi^2 m_e} V^{-5/3}$$

- Assuming constant density, a star contains $4\pi\rho r^3/3$ within radius r. This attracts next shell containing mass $dm = 4\pi\rho r^2 dr$

L13.3

$$E_{grav} = -\int_0^R \frac{G_N}{r}\underbrace{\left(\frac{4\pi\rho r^3}{3}\right)}_{M}\underbrace{4\pi\rho r^2 dr}_{dm} = \frac{(4\pi\rho)^2 G_N}{15}R^5 = -\frac{3G_N M_{star}^2}{5R}$$

- Pressure at center due to gravitational attraction is

$$P_{grav} = -\frac{\partial E_{grav}}{\partial V} = -\frac{1}{5}G_N (m_n N_n)^2 \left(\frac{4\pi}{3}\right)^{1/3} V^{-4/3}$$

White dwarfs & Neutron stars

White dwarfs are cold stars whose nuclear fuel has been expended. They are supported by the electron degeneracy pressure

- $P_{deg} = -P_{grav}$ occurs roughly when

$$R \approx \frac{\hbar^2 N_e^{5/3}}{G_N m_e m_n^2 N_n^2} \approx \frac{\hbar^2}{G_N m_e m_N} N_n^{-1/3}$$

- which decreases as we add nucleons
- If white dwarf becomes too massive, pressure causes e^- to be absorbed into nucleus $(\cdot\cdot)^{n^0}$
- Star collapses to a neutron star causing a supernova

Exchange & parity

Exchanging indistinguishable particles is related to a parity transform

- Describe 2-particle spatial wavefunction using

$$\underline{X}_{com} = \frac{\underline{X}_1 + \underline{X}_2}{2} \qquad \underline{P}_{com} = \underline{P}_1 + \underline{P}_2$$

$$\underline{X}_{rel} = \underline{X}_1 - \underline{X}_2 \qquad \underline{P}_{rel} = \frac{\underline{P}_1 - \underline{P}_2}{2}$$

- Exchange sends $(\underline{X}_{com}, \underline{P}_{com}) \mapsto (\underline{X}_{com}, \underline{P}_{com})$ trivially, but $(\underline{X}_{rel}, \underline{P}_{rel}) \mapsto (-\underline{X}_{rel}, -\underline{P}_{rel})$ so acts like parity on rel coord
- Since $Y_\ell^m(-\hat{\underline{x}}) = (-1)^\ell Y_\ell^m(\hat{\underline{x}})$, if two indistinguishable particles have relative orbital ang mom ℓ, their spatial wavef^n is necessarily symmetric if ℓ even, antisymm if ℓ odd
- Behaviour of complete state under exchange also involves spin state
  - ▷ for bosons, spatial wavef^n same symmetry as spin state
  - ▷ for fermions, spin state must have opposite symm to spatial wavef^n

L13.4

Inelastic collisions

Particle stats have important consequences for collision processes

- Consider hydrogenic 'atom' formed from a pion (π^-) orbiting a deuterium nucleus (D^+)
  - ▷ energy levels have same Coulombic form as in H-atom, but with much smaller radius. Ground state is still $|n,\ell,m\rangle = |1,0,0\rangle$ with $\ell=0$
  - ▷ pion has $s=0$ whilst D^+ has $s=1$, so 'atom' has $j=1$
- Short-range strong nuclear force causes π^- to be absorbed and the atom disintegrates into a pair of neutrons

$$\pi^- + D^+ \longrightarrow N + N$$

- Neutrons are fermions with spin $\frac{1}{2}$, so final state must be antisymm under simultaneous exchange of spin & spatial wavefns
  - ▷ total ang mom conserved, so $j=1$ in final state
  - ▷ if net $s=0$ (antisymm), require ℓ even (symmetric), but then cannot obtain $j=1$ by combining ✗
  - ▷ if net $s=1$ (symm), require ℓ odd (antisym)
- The only possibility is $j=\ell=s=1$ in final state

TL;DW
- Multi-particle states are either symmetric or antisymm under exchange of indistinguishable particles
  - ▷ bosons symmetric under exchange
  - ▷ fermions antisymm
  - ▷ bosons have integer spin, while fermions have half-integer spin
- Pauli's exclusion principle: no two fermions in same quantum state
- Exchange acts as a parity transform on relative spatial wavefn
- Many corollaries / applications, from periodic table to supernovae

Up Next
- Perturbation theory
  - ▷ how to approach more realistic systems w/o exact solution

Time-Independent Perturbation Theory

Reality bites! Exploiting symmetry has allowed us to solve spectral problems exactly

- Unfortunately, most realistic systems are too complicated for this approach to work
  - more complicated objects typically have less symmetry
  - even the 3-body problem is (famously!) non-integrable
- To make headway with such realistic problems, we need to develop approximation methods

We hope to approximate our true system by a simpler one, ideally with the properties
- the simpler system is tractable
- but nonetheless provides a close approximation to the realistic one

An analytic expansion

Suppose H is the true Hamiltonian and H_0 is the simpler, model Hamiltonian whose eigenstates and eigenvalues we understand

- For $\lambda \in [0,1]$, define $H_\lambda = H_0 + \lambda \Delta H$ where $\Delta H = H - H_0$
  - H_λ interpolates between our model and true Hamiltonians
  - we hope the effects of turning on ΔH are 'small'
- We seek the eigenstates $|E_\lambda\rangle$ of H_λ
  - naively seems harder, as now need to solve 1-parameter family of Hamiltonians
- Key assumption: states $|E_\lambda\rangle$ and their associated energy levels $E(\lambda)$ vary analytically with λ so we have expansions

$$|E_\lambda\rangle = |\alpha\rangle + \lambda|\beta\rangle + \lambda^2|\gamma\rangle + \cdots$$

$$E(\lambda) = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots$$

- There are several ways this assumption can fail; will return to examine these later
- Plugging our expansions into $H_\lambda |E_\lambda\rangle = E(\lambda)|E_\lambda\rangle$ gives

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

- Since holds for $\lambda \in [0,1]$ must hold for each power individually, so

$$H_0|\alpha\rangle = E^{(0)}|\alpha\rangle$$

$$H_0|\beta\rangle + \Delta H|\alpha\rangle = E^{(0)}|\beta\rangle + E^{(1)}|\alpha\rangle$$

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

- Zeroth-order equation says $|\alpha\rangle$ is an eigenstate of H_0 with energy $E^{(0)}$
  - ▷ unsurprising as we're looking for energy eigenstates of H_λ and assumed analytic in λ
  - ▷ we choose $|\alpha\rangle = |n\rangle$ (so $E^{(0)} = E_n$) to study what happens to the n^{th} energy level of our model system as we make the system more realistic

First-order corrections

With $|\alpha\rangle = |n\rangle$ (assumed normalized), first order correction says

$$H_0|\beta_n\rangle + \Delta H|n\rangle = E_n|\beta_n\rangle + E_n^{(1)}|n\rangle$$

$|\beta_n\rangle$: 1st order correction to n^{th} energy e-state $|n\rangle$

E_n: $E^{(0)}$ n^{th} energy of unperturbed H_0

- Contract with $\langle n|$ to find $E_n^{(1)} = \langle n|\Delta H|n\rangle$
  - ▷ First order correction $E_n^{(1)}$ to the n^{th} energy level is just the expectation value of the perturbation ΔH in the original n^{th} eigenstate
- Contracting with $\langle m| \neq \langle n|$ gives $\langle m|\Delta H|n\rangle = (E_n - E_m)\langle m|\beta_n\rangle$
  - ▷ expand $|\beta_n\rangle = \sum b_k|k\rangle$ in basis of H_0 eigenstates with $b_m = \langle m|\beta_n\rangle$
- Provided $E_n \neq E_m$ (n^{th} level non-deg.) we have

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

  - ▷ can check (ex) $\langle E_\lambda|E_\lambda\rangle = 1$ at this order implies $b_n = \langle n|\beta_n\rangle = 0$
  - ▷ we'll consider degenerate perturbation theory later

Second-order corrections

At second order, the eigenstate condition $H_\lambda |E_\lambda\rangle = E(\lambda)|E_\lambda\rangle$ required

$$H_0|\gamma_n\rangle + \Delta H|\beta_n\rangle = E_n|\gamma_n\rangle + E_n^{(1)}|\beta_n\rangle + E_n^{(2)}|n\rangle$$

- Contracting with $\langle n|$ and using $\langle n|\beta_n\rangle = 0$ gives

$$E_n^{(2)} = \langle n|\Delta H|\beta_n\rangle = \sum_{m\neq n} \frac{|\langle n|\Delta H|m\rangle|^2}{E_n - E_m}$$

- If several states $|m\rangle$ have comparable mixing $|\langle n|\Delta H|m\rangle|$ with original state $|n\rangle$, nearby energy levels contribute most to perturbation of E_n
- Nearby energy levels are driven apart: degeneracy is generally lifted
  - ▷ degeneracy remains if perturbation preserves some symmetry of H_0
- 2nd-order correction to ground state energy is always negative
- Rarely required to go to higher order (not in Tripos lmao)

An illustrative example

Consider the 1d oscillator with Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2(X-\lambda x_0)^2 - \frac{1}{2}\lambda^2 m\omega^2 x_0^2$$
$$= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 X^2 - \lambda m\omega^2 x_0 X$$

- The exact energy levels are

$$E_n(\lambda) = \hbar\omega\left(n+\tfrac{1}{2}\right) - \frac{1}{2}\lambda^2 m\omega^2 x_0^2$$

and we'd never really use perturbation theory to study this

- Treating $\Delta H = -m\omega^2 x_0 X$ as a perturbation, our formalism gives

$$E_n(\lambda) = E_n + \lambda\langle n|\Delta H|n\rangle + \lambda^2 m^2\omega^4 x_0^2 \sum_{k\neq n} \frac{|\langle k|X|n\rangle|^2}{(n-k)\hbar\omega} + O(\lambda^3)$$

$$= \hbar\omega\left(n+\tfrac{1}{2}\right) - \frac{1}{2}\lambda^2 m\omega^2 x_0^2 + O(\lambda^3) \quad \text{☺}$$

$\lceil \langle n|X|n\rangle = 0$ since $X \sim \frac{A+A^\dagger}{2} \rfloor$

$\lceil \langle k|X|n\rangle \propto \langle k|A+A^\dagger|n\rangle = \sqrt{n+1}\,\langle k|n+1\rangle + \sqrt{n}\,\langle k|n-1\rangle$

- Perturbation hasn't really changed the character of our potential
  - ▷ for large enough x, perturbation negligible compared to original term
  - ▷ possible (but not trivial) to check $O(\lambda^3)$ terms indeed vanish
  - ▷ infinite radius of convergence

Consider the unperturbed oscillator, but with $\omega(\lambda) = \omega\sqrt{1+\lambda}$

- Exact energy levels are $E_n(\lambda) = \hbar\omega\sqrt{1+\lambda}\,(n+\frac{1}{2})$
- Treating $\lambda\Delta H = \frac{1}{2}m\omega^2\lambda X^2$ as a perturbation we find

$$E_n(\lambda) = E_n(0) + \frac{\lambda}{2}m\omega^2\langle n|X^2|n\rangle + \frac{\lambda^2}{4}m^2\omega^4\sum_{k\neq n}\frac{|\langle k|X^2|n\rangle|^2}{(n-k)\hbar\omega} + \dots$$

$$= (n+\tfrac{1}{2})\hbar\omega\left(1 + \frac{\lambda}{2} - \frac{\lambda^2}{8} + \dots\right)$$

in agreement with the expansion of $\sqrt{1+\lambda}$ to this order

- Going further, we'd find the perturbative series converges iff $|\lambda| < 1$
  - ▷ mathematically, this reflects the branch cut in $\sqrt{1+\lambda}$ at $\lambda = -1$
  - ▷ physically, finite radius of convergence because if $\lambda \leq -1$, potential becomes unbound for all energy states

An asymptotic series (*)

Finally, consider the Hamiltonian $H_\lambda = H_{SHO} + \lambda\varepsilon X^4$

- Not easy to solve exactly, but perturbatively we find

$$E_0(\lambda) = \tfrac{1}{2}\hbar\omega + \textstyle\sum_n (\lambda\varepsilon)^n a_n \quad \text{where}$$

$$a_n = \frac{(-1)^{n+1}3^n\sqrt{6}}{\pi^{3/2}}\Gamma(n+\tfrac{1}{2})\left(1 - \frac{95}{72}\frac{1}{n} + O(n^{-2})\right)$$

- ▷ $\Gamma(n+\frac{1}{2})$ grows faster than $n!$ as $n\to\infty$, so this series has zero radius of convergence
- ▷ turning on any λX^4 for $\lambda<0$; even with $|\lambda| \ll 1$, makes the potential unbounded and all oscillator states become unstable
- Perturbation theory gives us an asymptotic series

$$\lim_{\lambda\to 0^+}\frac{1}{\lambda^N}\left|E(\lambda) - \sum_n^N \lambda^n E^{(n)}\right| = 0 \quad \text{however} \quad \lim_{N\to\infty}\sum_{n=0}^N \lambda^n E^{(n)} = \infty$$

- ▷ most perturbation expansions in QM & QFT are asymptotic series
- ▷ often important physics in understanding which value of N is optimal

TL;DW • Time-indep perturb^n theory is appropriate for bound states of a complicated hamiltonian

- ▷ seek a model Hamiltonian H_0 tractable & 'close' to H
- ▷ write $H_\lambda = H_0 + \lambda\Delta H$ with $\Delta H = H - H_0$ and assume estates, energy analytic
- Provided H_0 is non-degenerate, perturbed n^{th} energy level is

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

whilst corresp estate is $|n(\lambda)\rangle = |n\rangle + \lambda\sum_{m\neq n}\frac{\langle m|\Delta H|n\rangle}{E_1 - E_m}|m\rangle + O(\lambda^2)$

UpNext • More realistic systems; relativistic corrections to H_2 atom

Hydrogen and Helium

Fine structure of hydrogen

- The spectrum of Hydrogen that follows from the Coulomb potential is often called its gross structure

- Binding energy of state $|n,l,m\rangle$ is $E_n = -\frac{1}{2}\mu c^2 \cdot \frac{\alpha^2}{n^2}$
  - ▷ $\mu = m_e m_p/(m_e+m_p) \approx m_e$ is the reduced mass
  - ▷ $\alpha = e^2/(4\pi\varepsilon_0 \hbar c) \simeq \frac{1}{137}$ is known as the fine structure constant
  - ▷ gross structure energy levels independent of l, m and e^-/p spin states

A more accurate description of Hydrogen comes from the Dirac equation.

- Since $|E_n| \propto \mu c^2$ we can treat relativistic corrections perturbatively

- At leading order, there are several competing relativistic effects:
  - ▷ correction to kinetic term from $E = \sqrt{\mu^2 c^4 + p^2 c^2}$
  - ▷ electron moves through Coulomb field so perceives a magnetic field
  - * Darwin term: 'smearing' the electrostatic potential at the nucleus

Kinetic correction

Expanding the relativistic dispersion relation we obtain

$$E = \sqrt{\mu^2 c^4 + p^2 c^2} \approx \mu c^2 + \frac{1}{2\mu} p^2 - \frac{1}{8\mu^3 c^2} p^4 + \cdots$$

- Since we expect $\langle \Delta H_{kin} \rangle / \langle H_0 \rangle \sim (v/c)^2 \sim \alpha^2$ we treat

$$\Delta H_{kin} = -\frac{(p^2)^2}{8\mu^3 c^2}$$

as a perturbation, so first order change in energy due to this term is

$$E^{(1,kin)}_{n,l,m} = \langle n;l;m| \Delta H_{kin} |n;l;m\rangle$$

- Non-degenerate perturbation theory justified since ΔH_{kin} does not mix degenerate states
  - ▷ ΔH_{kin} is rotationally invariant so $[L, \Delta H] = 0$
  - ▷ It follows that $\langle nl'm'| \Delta H_{kin} |nlm\rangle \propto \delta_{ll'}\delta_{mm'}$ since

$$0 = \langle nl'm'|[L^2, \Delta H_{kin}]|nlm\rangle = \hbar^2(l'(l'+1) - l(l+1))\langle nl'm'|\Delta H_{kin}|nlm\rangle$$

$$0 = \langle nl'm'|[L_z, \Delta H_{kin}]|nlm\rangle = \hbar(m'-m)\langle nl'm'|\Delta H_{kin}|nlm\rangle$$

Evaluating the kinetic correction

There's a trick to evaluate the first order correction

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

$$\left[(H_0 - V)^2 = \left(\frac{p^2}{2\mu}\right)^2 = \frac{(p^2)^2}{4\mu^2} \right]$$

- Virial theorem says $2\langle T \rangle = -\langle V \rangle$, so $E_n = \langle T \rangle + \langle V \rangle = \langle V \rangle / 2$ and

hence

$$\langle \Delta H_{kin} \rangle_{n,lm} = \frac{3E_n^2}{2\mu c^2} + \frac{\langle V^2 \rangle_{nlm}}{2\mu c^2} = \frac{1}{2}\mu c^2 \frac{3}{4}\frac{\alpha^4}{n^2} - \frac{\hbar^2}{2\mu}\left\langle \frac{\alpha^2}{r^2} \right\rangle_{nlm}$$

- Remaining term $\sim \langle 1/r^2 \rangle$ can be included in the effective potential (not)

$$V_{eff}(r) = \frac{\hbar^2}{2\mu}\left[\frac{l(l+1)}{r^2} + \frac{\alpha^2}{r^2}\right] - \frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{r}$$

$$= \frac{\hbar^2}{2\mu}\frac{l'(l'+1)}{r^2} - \frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{r}$$

where the fictitious ang mom $l' \notin \mathbb{N}_0$ is given by

$$l'(l'+1) = l(l+1) + \alpha^2$$

- If our original atom had orbital ang mom l', we'd find energy levels

$$E_n(l') = -\frac{1}{2}\mu\alpha^2 c^2 \frac{1}{(l'+1)^2}$$

- Perturbatively, only the first order correction is meaningful, so expanding the energy $E_n(l')$ to first order in $\delta l = l' - l$ gives

$$E_n(l+\delta l) = -\frac{1}{2}\mu\alpha^2 c^2 \left[\frac{1}{(l+1)^2} - \frac{2\delta l}{(l+1)^3} + \cdots\right]$$

$$= E_n + \frac{1}{2}\mu\alpha^2 c^2 \frac{\alpha^2}{n^3(l+\frac{1}{2})} + \cdots$$

$$\left[(l+\delta l)(l+\delta l+1) = l(l+1) + \alpha^2 \right]$$
$$\left[\Rightarrow \delta l = \frac{\alpha^2}{2l+1} \right]$$

- Combining all the terms we obtain

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

as the first-order correction coming from the modified kinetic term

Spin-orbit coupling

Classically, a charged particle moving through the Coulomb field with velocity $\underline{v}$ feels a magnetic field

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

- $\underline{B}$ couples to the electron's dipole moment $\underline{\mu}$ giving a spin-orbit coupling

$$\Delta H_{SO} = -\underline{\mu}\cdot\underline{B} = -\frac{e}{2\mu}\underline{B}\cdot\underline{S} = \frac{e^2}{8\pi\varepsilon_0\mu c^2}\frac{\underline{L}\cdot\underline{S}}{|\underline{x}|^3}$$

- Acts trivially on states with $\ell=0$ whilst action on other states also depends on electron's spin state $\{|\uparrow\rangle, |\downarrow\rangle\}$
- Writing $\underline{L}\cdot\underline{S} = (\underline{J}^2 - \underline{L}^2 - \underline{S}^2)/2$ we see that

$$\underline{L}\cdot\underline{S}\,|n,j,m_j;\ell\rangle = \frac{\hbar^2}{2}\left(j(j+1) - \ell(\ell+1) - \frac{3}{4}\right)|n,j,m_j;\ell\rangle$$

$$= \begin{cases} \frac{\hbar^2}{2}L\,|n,j,m_j;L\rangle & \text{when } j=\ell+\frac{1}{2} \\ -\frac{\hbar^2}{2}(L+1)\,|n,j,m_j;L\rangle & \text{when } j=\ell-\frac{1}{2}. \end{cases}$$

Evaluating the spin-orbit coupling

The spin-orbit coupling leads to a first order shift

$$E^{(1,SO)}_{n,j,\ell} = -\frac{1}{4\mu^2}\cdot\frac{e^2\hbar^2}{4\pi\varepsilon_0}\left\{\begin{array}{c}1\\ -(\ell+1)\end{array}\right\}\left\langle\frac{1}{|\underline{x}|^3}\right\rangle_{n,j,\ell}$$

- A further trick helps us compute $\langle 1/|\underline{x}|^3\rangle$. Recall

$$H_\ell = \frac{P_r^2}{2\mu} + \frac{L(L+1)\hbar^2}{2\mu R^2} - \frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{R}$$

- where $R=|\underline{x}|$ and the radial momentum P_r obeys $[R,P_r]=i\hbar$
- In any energy eigenstate $\langle[P_r,H_L]\rangle = 0$ and we compute

$$[P_r,H_L] = -i\hbar\left(-\frac{L(L+1)\hbar^2}{\mu R^3} + \frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{R^2}\right)$$

- Combining this with our previous result for $\langle 1/|\underline{x}|^2\rangle$ we obtain

$$\left\langle\frac{1}{|\underline{x}|^3}\right\rangle_{n,j,\ell} = \frac{\alpha\mu c}{\hbar}\cdot\frac{1}{L(L+1)}\left\langle\frac{1}{|\underline{x}|^2}\right\rangle_{n,j,\ell} = \frac{(\alpha\mu c)^3}{\hbar^3}\frac{1}{L(L+\frac{1}{2})(L+1)}\frac{1}{n^2}$$

Combining the fine structure corrections

Both the modified kinetic term and spin-orbit coupling lead to corrections at order α^4. Combining them we obtain the first-order corrections to the Hydrogen energy levels $E_{n,j,l} = -\frac{1}{2}\mu\alpha^2c^2\left[\frac{1}{n^2} - \frac{\alpha^2}{n^3}\left(\frac{3}{4n} - \frac{1}{j+\frac{1}{2}}\right) + \dots\right]$

- This accounts for the Darwin term means it also holds when $l=0$
- This holds for both $j = l \pm \frac{1}{2}$
- The degeneracy in l is lifted; Runge-Lenz vector no longer conserved

Proceeding down the periodic table, the innermost electron feels the attraction of Z protons in the nucleus. Since $\alpha \sim e^2$, replace $\alpha \to Z\alpha$.

- Relativistic corrections become more important for heavier atoms

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

▷ this is $\approx 4.53 \times 10^{-4}$ eV for the 2p states of Hydrogen

▷ by the middle of the periodic table, splitting is $\approx 10\%$ gross energy

Helium

The gross structure of the Helium atom is described by the Hamiltonian

$$H = \frac{\vec{p}_1^{\,2}}{2m_e} + \frac{\vec{p}_2^{\,2}}{2m_e} - \frac{2e^2}{4\pi\varepsilon_0}\left(\frac{1}{|\vec{x}_1|} + \frac{1}{|\vec{x}_2|}\right) + \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1 - \vec{x}_2|}$$

describing each electron's attraction to the nucleus and the e^-e^- repulsion

- We treat the e^-e^- repulsion as a perturbation, so model Hamiltonian is two copies of a Hydrogenic atom with $Z=2$
- Unperturbed single electron states are $|n,l,m\rangle \otimes |\psi_{spin}\rangle$ with energy

$$E_n = -\frac{1}{2}m_e Z^2\alpha^2c^2\frac{1}{n^2} = -2m_e\alpha^2c^2\frac{1}{n^2}$$

- Since electrons are fermions the total state must be antisymmetric

In particular, the unperturbed atomic 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

$$2E_{n=1} = 2\times(-54.4)\text{ eV} = -108.8\text{ eV}$$ from the two e^-s

Computing the repulsion

Let's compute $\langle \psi_0 | \Delta H | \psi_0 \rangle$

- ΔH is independent of spin, so

$$\frac{e^2}{4\pi\varepsilon_0}\left\langle \frac{1}{|\underline{x}_1 - \underline{x}_2|}\right\rangle_{\psi_0} = \int \overline{\psi_0(\underline{x}_1, \underline{x}_2)}\, \frac{\alpha\hbar c}{|\underline{x}_1 - \underline{x}_2|}\, \psi_0(\underline{x}_1, \underline{x}_2)\, d^3x_1\, d^3x_2$$

$$= \int \frac{\alpha\hbar c}{|\underline{x}_1 - \underline{x}_2|} |\psi_{100}(\underline{x}_1)|^2 |\psi_{100}(\underline{x}_2)|^2 d^3x_1\, d^3x_2$$

where ψ_{100} is the Hydrogenic ground state wavefunction

$$\psi_{100}(\underline{x}) = \frac{1}{\sqrt{\pi}}\left(\frac{2}{a_2}\right)^{3/2} e^{-r/a_2}, \quad a_2 = \frac{\hbar}{2\alpha m_e c} \quad \text{(half Bohr)}$$

- Performing the integral is tedious. With Z protons, we have

$$E_1(Z) = -4\alpha^2 m_e c^2\left(1 - \frac{5}{16}\frac{1}{Z} + \frac{25}{256}\frac{1}{Z^2} + \cdots\right)$$

  - ▷ for $Z = 2$ this gives $E_1 \approx -74.8\,\text{eV}$, whereas $E_1 \approx -79.0\,\text{eV}$ (expt)
  - ▷ including next order term gives $E_1 \approx -77.5\,\text{eV}$

Atomic first ionization energies

The first ionization energy E_1 is the energy required to liberate a single electron from the atom. It is usually of greater experimental interest (and accessibility!) than the full ground state binding energy

- For Hydrogen, $E_1 \approx 13.6\,\text{eV}$, just ground state energy
- For Helium, $E_1 \approx -79\,\text{eV} - (-54.4\,\text{eV}) = 24.6\,\text{eV}$
  - ▷ remaining electron feels full attraction of 2 protons so has energy $2^2(-13.6\,\text{eV}) = -54.4\,\text{eV}$

TL;DW
- Hydrogen atom has corrections to pure $1/n^2$ Coulomb energy levels coming from relativity
  - ▷ $p^4/8\mu^2c^4$ correction to electron's kinetic energy
  - ▷ spin-orbit coupling from electron moving thru Coulomb field
- Ground state of Helium can be approximated using pert^n theory in atomic number
  - ▷ also allows us to compute ionisation energies of Helium
  - ▷ 2nd order pertub^n in good agreement with expt
- Relativistic corrections to the ground state energy & first ionisation energies become more important further down the periodic table

Up Next
- How to do perturbation theory when the initial state is degenerate
  - ▷ application to atoms in external electric field (Stark effect)

Degenerate Perturbation Theory

Degenerate states

- If the model Hamiltonian contains degenerate states, even a tiny perturbation can have a dramatic effect

- A marble at rest in a bowl adjusts its position when the bowl is slightly tilted

- A marble resting on a flat table will run away if the table is tilted

We see this potential for large change in the coeffs

$$|n_\lambda\rangle = |n\rangle + \lambda \sum_{m\neq n} \frac{\langle m|\Delta H|n\rangle}{E_n - E_m}|m\rangle + O(\lambda^2)$$

of our perturbation expansion:

Perturbing with degeneracy

The original state mixes predominantly among those states with which it is degenerate. There are typically only finitely many of these.

- Let $V \subset \mathcal{H}$ be N-dim subspace for which $H_0|\psi\rangle = E_V|\psi\rangle \;\; \forall |\psi\rangle \in V$ and let $\{|r\rangle\}_{r=1}^{N}$ be an orthonormal basis of V

- We have a projection operator

$$P_V = \sum_{r=1}^{N} |r\rangle\langle r| : \mathcal{H} \longrightarrow V$$

and $P_\perp = 1 - P_V$ is the projector onto the orthogonal complement

$$V^\perp = \{|\chi\rangle \in \mathcal{H} : \langle\psi|\chi\rangle = 0 \text{ for all } |\psi\rangle \in V\}$$

- These projection operators obey the usual relations

$$P_V^2 = P_V, \quad P_\perp^2 = P_\perp, \quad P_V P_\perp = P_\perp P_V = 0$$

- Since V defined by H_0, they also obey $[P_V, H_0] = 0, \; [P_\perp, H_0] = 0$

Separating V and $V^\perp$

- Suppose $|\psi_\lambda\rangle$ is an eigenstate of the perturbed Hamiltonian, so

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

- Applying the projection operators P_V or $P_\perp$ on the left we learn

$$(E_V - E(\lambda) + \lambda P_V \Delta H)\,P_V|\psi_\lambda\rangle + \lambda P_V \Delta H P_\perp|\psi_\lambda\rangle = 0$$
$$(H_0 + \cancel{\lambda}\lambda P_\perp \Delta H - E(\lambda))P_\perp|\psi_\lambda\rangle + \lambda P_\perp \Delta H P_V|\psi_\lambda\rangle = 0$$

- As before, we expand

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

and choose $|\alpha\rangle \in V$

- At zeroth order we just learn $E^{(0)} = E_V$ as expected

Diagonalising and perturbation

- Using $P_V|\alpha\rangle = |\alpha\rangle$ and $P_\perp|\alpha\rangle = 0$, at first order we learn

$$(P_V \Delta H P_V)|\alpha\rangle = E^{(1)}|\alpha\rangle$$

This says we must choose $|\alpha\rangle$ to diagonalize the perturb^n within V

- ▷ to get an analytic expansion, we must start from a state that diagonalizes both $P_V \Delta H P_V$ and H_0
- ▷ diagonalising ΔH within the finite-dim subspace V is usually much simpler than doing so across full $\mathcal{H}$

- Choose our basis $\{|v\rangle\}_{r=1}^N$ of V so that it indeed diagonalizes the perturb^n, and set $|\alpha\rangle = |r\rangle$. Then we have

$$E_r^{(1)} = \langle r|P_V \Delta H P_V|r\rangle = \langle r|\Delta H|r\rangle$$

just as in the non-degenerate case

- Even tiny perturbations can easily break degeneracy, singling out states that are eigenstates of a (typically non-symmetric) perturbation
  - ▷ we'll see later that this is relevant to "collapse of the wavefunction"

The linear Stark effect

If a Hydrogen atom is placed in a constant electric field (external) $\underline{E}$ the

- Hamiltonian is modified by a new term $\Delta H = -e\Phi = e\underline{E}\cdot\underline{X} = e|\underline{E}|X_3$ ($\underline{X} = X_e - X_p$)
- By parity $\langle 1,0,0|X_3|1,0,0\rangle = 0$ so the ground state is unaffected to first order
- The first excited state ($n=2$) has degeneracy 4:

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

- Parity implies $\langle 2,\ell',m'|X_3|2,\ell,m\rangle$ vanishes unless $|\ell'-\ell|$ odd. Since $[L_z, X_3] = 0$ we also have $\langle 2,0,0|X_3|2,1,\pm 1\rangle = 0$
- Within our degenerate subspace V the perturbation acts as

$$\Delta H = e|\underline{E}| \begin{pmatrix} 0 & 0 & a & 0 \\ 0 & 0 & 0 & 0 \\ \bar{a} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{where } a = \langle 2,0,0|X_3|2,1,0\rangle = -3a_0$$

The electric dipole moment of the Hydrogen atom

The eigenvalues of this perturbation are $e|\underline{E}|a_0 \times \{3,0,0,-3\}$ with corresponding eigenstates

$$\frac{|2,0,0\rangle - |2,1,0\rangle}{\sqrt{2}}, \quad |2,1,1\rangle, \quad |2,1,-1\rangle, \quad \frac{|2,0,0\rangle + |2,1,0\rangle}{\sqrt{2}}$$

so the degeneracy between $|2,1,1\rangle$ and $|2,1,-1\rangle$ is not lifted

- Classically, the energy $-3ea_0|\underline{E}|$ suggests the $n=2$ states have an electric dipole moment of magnitude $3ea_0$
  - ▷ for a classical elliptical orbit, electron would spend more time near the apocentre than the pericentre

  - ▷ any small deviation from $1/r$ potential

causes the axis of the ellipse to precess, so time-averaged dipole moment will vanish

  - ▷ fine structure corrections are very small; so even a weak external field causes the $n=2$ states to align to $\frac{1}{\sqrt{2}}(|2,0,0\rangle + |2,1,0\rangle)$
- Quantum mechanically, the $|2,0,0\rangle$ state is usually metastable, decaying only via $\gamma\gamma$ emission (single photon decay forbidden)

▷ in the presence of $\underline{E}$ it decays rapidly through mixing with $|2,1,0\rangle$

The quadratic Stark effect

While $E_{n=1}^{(1)} = 0$, the spherically symm ground state is perturbed to

$$|\psi\rangle = |1,0,0\rangle + e|\underline{E}| \sum_{n=2}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} \frac{\langle n,l,m|X_3|1,0,0\rangle}{E_1 - E_n} |n,l,m\rangle$$

- Wigner-Eckart theorem shows that only states with $l=1$ and $m=0$ can contribute, so triple sum collapses
- The external $\underline{E}$ field polarizes the ground state, inducing an electric dipole moment $\underline{D} = e\langle \underline{X} \rangle_\psi = \alpha \underline{E}$ where the polarizability

$$\alpha = -2e^2 \sum_{n=2}^{\infty} \frac{|\langle n,1,0|X_3|1,0,0\rangle|^2}{E_1 - E_n} = \frac{9}{2} a_0^3 \quad \text{(*)}$$

- The induced polarization causes a 2nd order energy shift

$$E_{n=1}^{(2)} = -\frac{1}{2} \underline{E} \cdot \underline{D} = -\frac{9}{4} |\underline{E}|^2 a_0^3$$

TL;DW • When the state we wish to perturb lies in a degenerate subspace V, we must first diagonalize the perturbation within V

▷ with degeneracy; even small perturbation can have a dramatic effect

- If $|r\rangle$ diagonalizes both H_0 and ΔH then $E_r^{(1)} = \langle r|\Delta H|r\rangle$

▷ diagonalizing within subspace usually easier than solving full problem

- Problem Sheet 3 is now free real estate

Up Next • Time-dependent perturbation theory

▷ calculate transition rates between unperturbed energy levels

Time-dependent perturbation theory

An isolated system has a time-indep Hamiltonian, but these systems are often subject to transient perturbations from surrounding environment

- Key example: atoms being perturbed by passing radiation
  - ▷ absorption & stimulated emission of radiation by atom
- Can also view scattering theory this way
  - ▷ potential felt by particle changes as it approaches obstacle (see AQM)

Usually interested in the rate at which the perturbation causes transitions between the energy eigenstates of the original system

The interaction picture

Let $H(t) = H_0 + \Delta(t)$ where H_0 is a time-indep model Hamiltonian

- Let $\{|n\rangle\}$ be an o.n. basis of $\mathcal{H}$ with $H_0|n\rangle = E_n|n\rangle$ and expand a general state as $|\psi(t)\rangle = \sum_n e^{-iE_nt/\hbar} a_n(t)|n\rangle$
  - ▷ since $\{|n\rangle\}$ are a basis, any state can be expanded this way
  - ▷ $a_n(t)$ depend on time only because of presence of $\Delta(t)$
- Using this expansion in the TDSE $i\hbar\frac{\partial}{\partial t}|\psi\rangle = H(t)|\psi(t)\rangle$ gives
  $$\sum_n (a_n E_n + i\hbar\dot{a}_n) e^{-iE_nt/\hbar}|n\rangle = \sum_n a_n (E_n + \Delta(t)) e^{-iE_nt/\hbar}|n\rangle$$
- Contract with $\langle k|$ to obtain

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

or equivalently the integral equation

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

A perturbative expansion

Our treatment so far has been exact, but we must now approximate

- Since $\dot{a}_k \neq 0$ only because of the presence of perturbation $\Delta(t)$, as a first approximation we replace $a_n(t) \to a_n(t_0)$ inside the integral

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

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

where $\omega_{kn} = (E_k - E_n)/\hbar$

- Can go to higher order, plugging expression for $a_k(t)$ back in to get more accurate $a_k(t)$
- If we start in $|\psi(t_0)\rangle = |m\rangle$ at $t = t_0$, we have $a_n(t_0) = \delta_{mn}$ so to first order $a_k(t) = \delta_{km} + \frac{1}{i\hbar}\int_{t_0}^{t} e^{i\omega_{km}t'}\langle k|\Delta(t')|m\rangle\, dt'$
- To get further, need to specify the particular form of $\Delta(t)$

Prodding the harmonic oscillator

Consider a harmonic oscillator that receives a gentle 'push' near $t=0$, so

$$H(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 X^2 - F_0 X e^{-t^2/\tau^2}$$

where F_0, τ are constants. Treat $\Delta(t) = F_0 X e^{-t^2/\tau^2}$ term as perturbation

- Suppose oscillator was in state $|0\rangle$ for $t \to -\infty$. For $|k\rangle \neq |0\rangle$ we have

$$\begin{aligned}\lim_{t\to\infty} a_k(t) &\approx -\frac{F_0}{i\hbar}\int_{-\infty}^{\infty} e^{ik\omega t'} e^{-t'^2/\tau^2}\langle k|X|0\rangle\, dt' \\ &= i F_0 \sqrt{\frac{\pi\hbar}{2m\omega}}\,\tau\, e^{-k^2\omega^2\tau^2/4}\langle k|A^\dagger|0\rangle \\ &= i\delta_{k1} F_0 \sqrt{\frac{\pi\hbar}{2m\omega}}\,\tau\, e^{-\omega^2\tau^2/4}\end{aligned}$$

- Probability oscillator has transitioned to $|1\rangle$ after a long time is

$$\text{Prob}(|0\rangle \to |1\rangle) = \frac{\pi\hbar F_0^2}{2m\omega}\tau^2 e^{-\omega^2\tau^2/2}$$

▷ maximum probability occurs when $\tau \sim \omega^{-1}$; push 'resonantly'

▷ can reach higher states, but only at higher order in pert^n theory

Switching on a constant perturbation

Next consider the case our pert^n is switched on at $t=0$ and thereafter remains constant $\Delta(t) = \begin{cases} 0 & \text{for } t<0, \\ \Delta & \text{for } t \geq 0, \end{cases}$

with $\Delta(X, P, \ldots)$ a time-indep operator.

- If our system is in an eigenstates $|m\rangle$ for $t<0$ then find

$$\begin{aligned}a_k(t) &\approx \delta_{km} + \frac{1}{i\hbar}\int_0^t e^{i\omega_{km}t'}\langle k|\Delta|m\rangle\, dt' \\ &= \delta_{km} + \frac{\langle k|\Delta|m\rangle}{E_k - E_m}\left[1 - e^{i\omega_{km}t}\right]\end{aligned}$$

E E
if k=m.
then what

- Probability to find system in a different state $|k\rangle$ at $t>0$ is

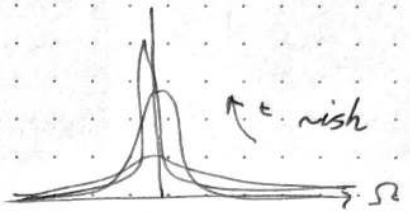
$$|a_k(t)|^2 = \frac{4}{\hbar^2}|\langle k|\Delta|m\rangle|^2 \frac{\sin^2(\omega_{km}t/2)}{\omega_{km}^2} \quad \text{to lowest order}$$

Transition rates

- For $\Omega \neq 0$ we have

$$\lim_{t\to 0}\left|\frac{\sin^2(\Omega t/2)}{\Omega^2 t}\right| \leq \lim_{t\to 0}\frac{1}{\Omega^2 t} = 0$$

and $\int_{-\infty}^{\infty}\frac{\sin^2(\Omega t/2)}{\Omega^2 t}\,d\Omega = \frac{\pi}{2}$



- Thus for $t\to\infty$ replace

$$\lim_{t\to\infty}\frac{\sin^2(\omega_{km}t/2)}{\omega_{km}^2 t} \longrightarrow \frac{\pi}{2}\delta(\omega_{km})$$

- We define the transition rate from $|m\rangle \to |k\rangle$ by

$$\Gamma(|m\rangle\to|k\rangle) = \lim_{t\to\infty}\frac{\partial}{\partial t}|a_k(t)|^2$$

- In the case of a constant perturbation switched on at $t=0$ we have

$$\Gamma(|m\rangle\to|k\rangle) = \frac{2\pi}{\hbar}|\langle k|\Delta|m\rangle|^2\,\delta(E_k - E_m)$$

▸ only (appreciable) transitions among states degenerate with $|m\rangle$

Monochromatic Perturbations

A very important case is that of monochromatic perturbations where

$$\Delta(t) = \begin{cases} 0 & \text{for } t<0, \\ \Delta e^{i\omega t} + \Delta^\dagger e^{i\omega t} & \text{for } t\geq 0, \end{cases}$$

where Δ is time-indep

- If our system is in state $|m\rangle$ at $t<0$ then for $t>0$ find

$$a_k(t) = \frac{\langle k|\Delta|m\rangle}{\hbar(\omega_{km}-\omega)}\left[e^{i(\omega_{km}-\omega)t}-1\right] + \frac{\langle k|\Delta^\dagger|m\rangle}{\hbar(\omega_{km}+\omega)}\left[e^{i(\omega_{km}+\omega)t}-1\right]$$

to first order, for $|k\rangle \neq |m\rangle$

- Comparing to previous case, as $t\to\infty$ we expect appreciable transitions only to states $|k\rangle$ with

either $E_k \approx E_m + \hbar\omega$ absorption

or $E_k \approx E_m - \hbar\omega$ stimulated emission

Fermi's Golden Rules

Only one term can be relevant for each process, so we find

$$|a_k(t)|^2 \approx \begin{cases} \frac{4}{\hbar^2} \frac{|\langle k|\Delta|m\rangle|^2}{(\omega_{km}-\omega)^2} \sin^2\left(\frac{(\omega_{km}-\omega)t}{2}\right) & \text{absorption} \\ \frac{4}{\hbar^2} \frac{|\langle k|\Delta^\dagger|m\rangle|^2}{(\omega_{km}+\omega)^2} \sin^2\left(\frac{(\omega_{km}+\omega)t}{2}\right) & \text{stimulated emission} \end{cases}$$

Consequently, at late time we find the lowest-order transition rates caused by a monochromatic perturbation to be

$$\Gamma(|m\rangle \to |k\rangle) = \begin{cases} \frac{2\pi}{\hbar} |\langle k|\Delta|m\rangle|^2 \delta(E_k - E_m - \hbar\omega) & \text{absorption} \\ \frac{2\pi}{\hbar} |\langle k|\Delta^\dagger|m\rangle|^2 \delta(E_k - E_m + \hbar\omega) & \text{stim emission} \end{cases}$$

- These results known as Fermi's golden rules
  - ▷ if (E_k, E_m) isolated and pert^n truly monochromatic, cannot tune frequency ω precisely enough to saturate δ-functions
  - ▷ consider ionization to continuum states, or range of frequencies ω

TL;DW Not doing this any longer, sorry TT

Up Next See ya in next lecture

Emission, Absorption and Ionization

Recall Fermi's golden rule(s) for the transition rate

$$\Gamma(|m\rangle \to |k\rangle) = \frac{2\pi}{\hbar} |\langle k|\Delta|m\rangle|^2 \, \delta(E_k - E_m \mp \hbar\omega)$$

caused by a harmonic pert^n $\Delta e^{-i\omega t} + \Delta^\dagger e^{i\omega t}$

- δ-f^n means purely monochromatic light does not cause appreciable transitions between discrete bound states
- Could have a range of frequencies, so some radiations guaranteed to have correct energy to cause transition
- ... or could ionize atom, exciting an electron from a bound state to the continuum of $E > 0$ states

Isotropic radiation bath

Suppose a Hydrogen atom is immersed in a bath of radiation

- For wavelengths $\gg$ Bohr radius, the dipole approximation gives

$$H = H_{atom} + e\underline{E}(t)\cdot\underline{X}$$

$\underline{D} = e(\underline{X}e - \underline{X}p)$

- Averaged over the radiation bath $\overline{\underline{E}(t)} = 0$ since the radiation could be pointing in any direction, whilst

$$\overline{E_i(t_1)E_j(t_2)} = \delta_{ij}\frac{1}{6\varepsilon_0}\int_{-\infty}^{\infty}\rho(\omega)e^{-i\omega(t_1-t_2)}d\omega$$

  - ▷ radiation isotropic; fluctuations in diff dir^{n}s uncorrelated
  - ▷ for $\underline{E}$ real, $\rho(\omega) = \rho(-\omega) = \rho^*(\omega)$ (so $\rho(\omega)$ is even & real)
  - ▷ energy density of E-M field is

$$\frac{\varepsilon_0}{2}\overline{(\underline{E}^2 + c^2\underline{B}^2)} = \varepsilon_0\overline{\underline{E}^2(t)} = \frac{1}{2}\int_{-\infty}^{\infty}\rho(\omega)\,d\omega,$$

  so $\rho(\omega)$ is the energy density in radiation at frequency ω

- For a transition $|m\rangle \to |k\rangle$ between two bound states of the atom, have

$$a_k(t) = -\frac{ie}{\hbar}\int_0^t e^{i\omega_{km}t'}\langle k|\,\underline{E}(t')\cdot\underline{X}\,|m\rangle\,dt'$$

- Taking mod-square and averaging over the radiation bath gives

$$\overline{|a_k(t)|^2} = \frac{e^2}{\hbar^2}\int_0^t\int_0^t \overline{E_i(t_1)E_j(t_2)}\, e^{i\omega_{km}(t_1-t_2)}\langle k|X_i|m\rangle\langle k|X_j|m\rangle\,dt_1\,dt_2$$

$$= \frac{e^2|\langle k|\underline{X}|m\rangle|^2}{6\varepsilon_0\hbar^2}\int_{-\infty}^{\infty}\int_0^t\int_0^t \rho(\omega)\,e^{i(\omega_{km}-\omega)(t_1-t_2)}\,dt_1\,dt_2\,d\omega$$

$$= \frac{e^2 |\langle k|\underline{X}|m\rangle|^2}{6\varepsilon_0 \hbar^2} \int_{-\infty}^{\infty} \rho(\omega) \left| \int_0^t e^{i(\omega_{km}-\omega)t'} dt' \right|^2 d\omega$$

$$= \frac{4e^2 |\langle k|\underline{X}|m\rangle|^2}{6\varepsilon_0 \hbar^2} \int_{-\infty}^{\infty} \rho(\omega) \frac{\sin^2((\omega_{km}-\omega)t/2)}{(\omega_{km}-\omega)^2} d\omega$$

$$\downarrow$$

$$\frac{\pi t}{2} \delta(\omega_{km}-\omega)$$

$$= \frac{4e^2 |\langle k|\underline{X}|m\rangle|^2}{6\varepsilon_0 \hbar^2} \frac{\pi t}{2} \rho(\omega_{km})$$

- Consequently, the transition rate

$$\Gamma(|m\rangle \to |k\rangle) = \frac{\pi e^2 \langle k|\underline{X}|m\rangle \cdot \langle m|\underline{X}|k\rangle}{3\varepsilon_0 \hbar^2} \rho(\omega_{km})$$

depends on energy density $\rho(\omega_{km})$ in field of just the right frequency to cause $|m\rangle \to |k\rangle$ transition:

Stimulated emission & absorption

Suppose our initial state $|m\rangle = |n, l, m\rangle$ and final state $|k\rangle = |n', l', m'\rangle$

- The matrix element $\langle n', l', m'|\underline{X}|n, l, m\rangle$ vanishes unless
  $|l'-l| = 1$ and $|m'-m| \leq 1$
  - ▷ consequence of parity and fact that operator $\underline{X}$ carries $l_{\underline{X}} = 1$
  - ▷ transitions violating these selection rules can occur, either at higher order in perturbation theory or beyond dipole approximation
- Reality conditions $\rho(\omega) = \rho(-\omega) = \rho^*(\omega)$ show transition rate $\Gamma \propto \rho(\omega_{n'n})$ is an even function of $\omega_{n'n} = (E_{n'} - E_n)/\hbar$
- Rate for absorption ($E_{n'} > E_n$) is the same as the rate for emission ($E_{n'} < E_n$) stimulated by background radiation field

Spontaneous decay

The above calculations allow us to understand the presence of a radiation bath can stimulate an atom to decay from $|k\rangle \to |m\rangle$

- If an isolated system is in an energy eigenstate, even a highly excited one, according to QM it will remain there forever.

Einstein produced an ingenious argument that helps us understand decays of an isolated atom (during his time off from revolutionizing gravity ...)

- Immerse atom in radiation bath of energy density $\rho(\omega)$ and write

$$\Gamma_{m\to k} = \rho(\omega_{km})\, B_{m\to k}(\omega_{km}) \quad \text{and} \quad \Gamma_{k\to m} = \rho(\omega_{km})\, B_{k\to m}(\omega_{km})$$

for the rates of absorption and stimulated emission

- ▷ $B_{m\to k} = B_{k\to m}$ calculated above, but used dipole approximation, first order pert^{n} theory, ...
- Let $A_{k\to m}(\omega_{km})$ denote rate of spontaneous emission
  - ▷ $A_{k\to m}$ exists because we also need to quantize the EM field (QFT)

Einstein's A & B coefficients

To make further progress we borrow some results from Statistical Physics:

- If system in (thermo^{c}) equilibrium with n_m atoms in state $|m\rangle$ and n_k in state $|k\rangle$ (with $E_k > E_m$), must have

$$n_k\left[A_{k\to m}(\omega_{km}) + \rho(\omega_{km})\, B_{k\to m}(\omega_{km})\right] = n_m\, \rho(\omega_{km})\, B_{m\to k}(\omega_{km})$$

- For atoms & radiation in thermal equilibrium at temperature T

$$\frac{n_m}{n_k} = \frac{e^{-E_m/k_BT}}{e^{-E_k/k_BT}} = e^{\hbar\omega_{km}/k_BT}, \qquad \rho(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3}\,\frac{1}{e^{\hbar\omega/k_BT}-1}$$

- Combining the above and setting $\omega = \omega_{km}$ gives

$$A_{k\to m}(\omega_{km}) = \frac{\hbar\omega_{km}^3}{\pi^2 c^3}\,\frac{1}{e^{\hbar\omega_{km}/k_BT}-1}\left[e^{\hbar\omega_{km}/k_BT}\, B_{m\to k} - B_{k\to m}\right]$$

- $A_{k\to m}$ must be independent of temperature, so $B_{m\to k} = B_{k\to m}$

and $A_{m\to k}(\omega_{km}) = \dfrac{\hbar\omega_{km}^3}{\pi^2 c^3}\, B_{m\to k}(\omega_{km}) = \dfrac{e^2\omega_{km}^3}{3\varepsilon_0\pi\hbar c^3}\,|\langle k|\underline{X}|m\rangle|^2$

- Dirac later calculated $A_{m\to k}(\omega_{km})$ from first principles in QFT

Ionization by monochromatic light

If the radiation is suff energetic, it can ionize the atom, liberating the electron into the continuum of states with $E > 0$

- Assume Hydrogen atom is initially in ground state $\langle \underline{x} | 1,0,0 \rangle = e^{-r/a}/\sqrt{\pi a^3}$ and look for probability for electron to be ionized into plane wave $\langle \underline{x} | \underline{k} \rangle = e^{i\underline{k}\cdot\underline{x}}/(2\pi\hbar)^{3/2}$
- In the dipole approximation, take perturbation to be

$$\Delta(t) = e\left(\underline{E}\cdot\underline{X}\, e^{-i\omega t} + \underline{E}^*\cdot\underline{X}\, e^{i\omega t}\right)$$

for radiation of freq ω and can choose $\underline{E}$ to define $\underline{z}$ axis

- The matrix element $\langle \underline{k} | X_3 | 1,0,0 \rangle$ evaluates to

$$\int \frac{e^{-i\underline{k}\cdot\underline{x}}\, z\, e^{-r/a}}{(2\pi\hbar)^{3/2}\sqrt{\pi a^3}}\, d^3x = \frac{4\pi k_z}{i(2\pi\hbar)^{3/2}\sqrt{\pi a^3}} \cdot \frac{8a^5}{(1+|\underline{k}|^2a^2)^3} \approx \frac{8\sqrt{2}\cos\theta}{i\pi\hbar^{3/2}|\underline{k}|^5 a^{3/2}}$$

since $|\underline{k}|a \gg 1$ in the dipole approximation, where $\cos\theta = \hat{\underline{E}}\cdot\hat{\underline{k}}$

Differential ionization rate

- Transition necessarily absorbs energy, so from Fermi's golden rule

$$\Gamma_{|100\rangle \to |\underline{k}\rangle} = \frac{2\pi}{\hbar} e^2 \underline{E}^2 |\langle \underline{k}|X_3|1,0,0\rangle|^2 \delta(E_k - E_{100} - \hbar\omega)$$

- We define the differential ionization rate

$$d\Gamma_{|100\rangle \to |\underline{k}\rangle} = \frac{2\pi}{\hbar} e^2 \underline{E}^2 |\langle \underline{k}|X_3|1,0,0\rangle|^2 \delta(E_k - E_{100} - \hbar\omega)\, \hbar^3 |\underline{k}|^2 d|\underline{k}|\, d\Omega$$

describing rate of ionization to momenta in the range $(\underline{k}, \underline{k}+d\underline{k})$

▷ δ-fn sets $\hbar|\underline{k}| = \sqrt{2m(\hbar\omega + E_{100})} \approx \sqrt{2m\hbar\omega}$

- Putting everything together & integrating over $|\underline{k}|$ gives

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

▷ valid for radiation wavelengths λ obeying $a \ll \lambda \ll 2\pi/\alpha a$ (large compared to the scale of atom, but still small enough that we can neglect binding energy E_{100}.

The density operator

Realistic systems are never completely isolated from their environment

- We can't possibly know the precise quantum state of $\sim 10^{23}$ particles!
- Need a way to discuss quantum systems even when we're not sure which state they're in

We define the density operator

$$\rho = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$$

where p_α is the classical probability our system is in state $|\psi_\alpha\rangle$

- No requirement for the $|\psi_\alpha\rangle$s to be orthogonal (normalised?) ✓
  - ▷ in particular, we're not saying the system is in state "$\sum_\alpha \sqrt{p_\alpha}|\psi_\alpha\rangle$"
- If $\exists |\chi\rangle \in \mathcal{H}$ such that $\rho = |\chi\rangle\langle\chi|$, the system is said to be pure
- ρs that cannot be written in this way are called impure or mixed

Properties of ρ

- The density operator $\rho : \mathcal{H} \to \mathcal{H}$ is defined by the properties

  $\rho = \rho^\dagger$ probs are real,

  $\rho \geq 0$ non-negative,

  $\mathrm{tr}_{\mathcal{H}}(\rho) = 1$ sum to 1

where positivity property is short for $\langle\phi|\rho|\phi\rangle \geq 0$ for all $|\phi\rangle \in \mathcal{H}$.

- Any operator ρ' with the above properties could be the density operator of some system
  - ▷ Let $\{|n\rangle\}$ be eigenstates of ρ' with $\rho'|n\rangle = p_n|n\rangle$
  - ▷ in this basis $\rho' = \sum_n p_n |n\rangle\langle n|$
  - ▷ $p_n \in \mathbb{R}$ since $\rho'^\dagger = \rho'$, $p_n = \langle n|\rho'|n\rangle \geq 0$ by positivity and $\sum p_n = 1$
- The system is pure iff $\rho^2 = \rho$
  - ▷ if $\rho = |\psi\rangle\langle\psi|$ then $\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho$
  - ▷ conversely if $(\rho - 1)\rho = 0$ then evals of ρ are either 0 or 1
  - ▷ $\mathrm{tr}\,\rho = 1$ so can't all vanish; exactly one is 1, so $\exists$ normalised state $|\chi\rangle \in \mathcal{H}$ for which $\rho = |\chi\rangle\langle\chi|$

QM in terms of ρ

- Since $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ where $U(t)$ is the time evolution operator,

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \quad \text{or} \quad \frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H, \rho(t)]$$

(analogous to Liouville's equation in Classical Dynamics)

- When a system is described by ρ; the average value of an observable Q is

$$\begin{aligned} \mathrm{tr}_{\mathcal{H}}(\rho Q) &= \sum_\alpha p_\alpha \, \mathrm{tr}_{\mathcal{H}}(|\psi_\alpha\rangle\langle\psi_\alpha| Q) \\ &= \sum_\alpha p_\alpha \langle \psi_\alpha | Q | \psi_\alpha \rangle \quad \text{lol!} \end{aligned}$$

▷ combines quantum expectation value of Q in state $|\psi_\alpha\rangle$ together with classical probability system is actually in state $|\psi_\alpha\rangle$

Density operators play an important role in Quantum Info & Quantum Computing; where maintaining purity is crucial

- We can formulate QM entirely in terms of operators on $\mathcal{H}$, together with a trace map $\mathrm{tr} : \mathrm{End}(\mathcal{H}) \longrightarrow \mathbb{C}$

An example

Consider a 2-state system (called a qubit) with basis $\{|\uparrow\rangle, |\downarrow\rangle\}$

- If we're sure the system is in state $|\uparrow\rangle$ then $\rho = (\langle\uparrow|)^\dagger\langle\uparrow|$
- If the system has probability $\frac{1}{2}$ to be in either $|\uparrow\rangle$ or $|\downarrow\rangle$ then

$$\rho = \tfrac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \tfrac{1}{2}1_{\mathcal{H}} = \tfrac{1}{2}(|\uparrow_x\rangle\langle\uparrow_x| + |\downarrow_x\rangle\langle\uparrow_x|)$$

▷ with this ρ we have no information about the system's state

- If there's probability $\frac{1}{2}$ the system is in either $|\uparrow\rangle$ or $|\uparrow_x\rangle$ then

$$\begin{aligned} \rho &= \tfrac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\uparrow_x\rangle\langle\uparrow_x|) \\ &= \tfrac{1}{2}|\uparrow\rangle\langle\uparrow| + \tfrac{1}{4}(|\uparrow\rangle + |\downarrow\rangle)(\langle\uparrow| + \langle\downarrow|) \\ &= \tfrac{1}{4}1_{\mathcal{H}} + \tfrac{1}{2}|\uparrow\rangle\langle\uparrow| + \tfrac{1}{4}|\uparrow\rangle\langle\downarrow| + \tfrac{1}{4}|\downarrow\rangle\langle\uparrow| \quad \text{⇝} \end{aligned}$$

The Bloch Ball

Any 2×2 Hermitian matrix can be written as a linear combination of the identity and Pauli matrices, so for any 2-state system with $\mathcal{H} = \mathbb{C}^2$

$$\rho = \tfrac{1}{2}(1_{\mathcal{H}} + \underline{b}\cdot\underline{\sigma})$$

$$= \frac{1}{2}\begin{pmatrix} 1+b_z & b_x - ib_y \\ b_x + ib_y & 1-b_z \end{pmatrix}$$

- Since $\mathrm{tr}\,\underline{\sigma} = 0$, coeff of $1_{\mathcal{H}}$ fixed by $\mathrm{tr}\,\rho = 1$
- To ensure both eigenvalues of ρ are non-negative, must also require

$$\det(\rho) = \tfrac{1}{4}(1 - \underline{b}\cdot\underline{b}) \geq 0 \quad \Rightarrow \quad |\underline{b}| \leq 1$$

which is known as the Bloch Ball (or the Bloch sphere ☺)

- ▷ if $|\underline{b}| = 1$ the system is pure, with spin aligned along $\underline{b}$
- ▷ if $|\underline{b}| < 1$, both evals > 0 so $\rho \neq |{\uparrow_n}\rangle\langle{\uparrow_n}|$ for any $\underline{n}$
- ▷ if $\underline{b} = 0$, $\rho = \frac{1}{2}1_{\mathcal{H}}$ and we are maximally ignorant about the state

⌈if $\underline{b} \neq 0$ the spin is preferentially aligned along $\underline{b}$⌋

The no cloning theorem

We could learn the precise state of our system if we were able to measure all aspects of it, but any measurement will disturb the system

- Perhaps try to duplicate the system many times and assemble complete information by repeated measurements?
- Suppose we try to copy a normalized state $|\psi\rangle \in \mathcal{H}_1$ to another system $\mathcal{H}_2 \cong \mathcal{H}_1$ initially in some (normalized) 'blank' state $|e\rangle$

$$C : |\psi\rangle \otimes |e\rangle \mapsto e^{-i\alpha(\psi,e)}\,|\psi\rangle \otimes |\psi\rangle$$

where $\alpha(\psi,e)$ is some unobservable phase

- In QM, C must be a unitary operator (time evol^n wrt some H), so

$$\langle\phi|\psi\rangle = (\langle\phi|\langle e|)(|\psi\rangle|e\rangle) = (\langle\phi|\langle e|)\,C^\dagger C\,(|\psi\rangle|e\rangle)$$

$$= e^{i(\alpha(\phi,e) - \alpha(\psi,e))}\langle\phi|\psi\rangle^2$$

so $|\langle\phi|\psi\rangle| = |\langle\phi|\psi\rangle|^2$ which implies $|\langle\phi|\psi\rangle| = 1$ or 0

- Cannot be true for all $|\phi\rangle, |\psi\rangle \in \mathcal{H}_1$, so ∄ such a unitary C

Entropy

The von Neumann entropy

$$S(\rho) = -\mathrm{tr}_{\mathcal{H}}(\rho \ln \rho)$$

quantifies how much information knowing ρ gives us about our system

- All eigenvalues of ρ lie in $[0,1]$, so $S(\rho) \geq 0$ with equality iff pure

  [If $\rho = \sum p_n |n\rangle\langle n|$ in o.n. basis then
  $\mathrm{tr}(\rho \ln \rho) = -\sum p_n \ln p_n$]

- $S(\rho)$ is concave: if ρ_i are a collection of density operators and $\kappa_i \geq 0$ obey $\sum \kappa_i = 1$ then $S(\sum_i \kappa_i \rho_i) \geq \sum_i \kappa_i S(\rho_i)$

- To find max entropy subject to $\mathrm{tr}\,\rho = 1$, use a Lagrange mult λ and extremise $S(\rho) - \lambda(1 - \mathrm{tr}_{\mathcal{H}}\rho)$:

$$\begin{cases} 0 = -\mathrm{tr}_{\mathcal{H}}(\delta\rho \ln\rho + \rho\rho^{-1}\delta\rho - \lambda\delta\rho) \\ 0 = \delta\lambda(\mathrm{tr}_{\mathcal{H}}\rho - 1) \end{cases} \quad \Big\downarrow$$

$$\ln\rho + 1 - \lambda = 0$$

$$\Rightarrow \rho = e^{\lambda - 1}\, id_{\mathcal{H}}$$

$$\Rightarrow \rho_{max} = \frac{1}{\dim(\mathcal{H})} 1_{\mathcal{H}}$$

- If $\dim(\mathcal{H}) < \infty$, maximal entropy is $S_{max} = S(\rho_{max}) = \ln \dim(\mathcal{H})$ and all states are equally likely

Entanglement & Decoherence

Entanglement Suppose our system has two (or more) parts, so

$$\mathcal{H} \cong \mathcal{H}_A \otimes \mathcal{H}_B$$

- We'll often think of A as the subsystem we're interested in, while B is the 'environment' (or the 'rest of the universe')
- A state $|\psi\rangle \in \mathcal{H}$ is called entangled if it cannot be written as $|\psi\rangle = |\phi\rangle \otimes |\chi\rangle$ for any $|\phi\rangle \in \mathcal{H}_A$, $|\chi\rangle \in \mathcal{H}_B$
- e.g. if A, B are each a single qubit, the states

$$|\phi\rangle = |\uparrow\rangle|\downarrow\rangle \quad \text{and} \quad |\psi\rangle = \left(\frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}\right)|\downarrow\rangle$$

are not entangled whereas the state

$$|EPR\rangle = \frac{|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle}{\sqrt{2}}$$

is entangled (we'll see more of this state later...)

- 'Entangled' just means the states of the subsystems are correlated

Reduced density operators

Define the reduced density operator for subsystem A as

$$\rho_A = \mathrm{tr}_{\mathcal{H}_B}(\rho_{AB})$$

ρ_A is useful if we only monitor behaviour of A

- For example, the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)_A \otimes |\downarrow\rangle_B$ has

$$\rho_A = \mathrm{tr}_{\mathcal{H}_B}\rho_{AB} = \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle)(\langle\uparrow| + \langle\downarrow|)$$

← $\rho_{AB} = |\psi\rangle\langle\psi|$ so $\rho_A = |\uparrow\rangle|\psi\rangle\langle\psi|\uparrow\rangle + \langle\downarrow|\psi\rangle\langle\psi|\downarrow\rangle$

whereas the EPR state $|EPR\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_A|\downarrow\rangle_B - |\downarrow\rangle_A|\uparrow\rangle_B)$ gives

$$\rho_A = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2}1_A$$

- If an observable Q depends only on properties of A then $Q = Q_A \otimes 1_B$ so its expectation value can be written

$$\mathrm{tr}_{\mathcal{H}_A \otimes \mathcal{H}_B}(\rho_{AB}(Q_A \otimes 1_B)) = \mathrm{tr}_{\mathcal{H}_A}(\rho_A Q_A)$$

expressed purely in terms of operators acting on $\mathcal{H}_A$

Entanglement entropy

Entanglement entropy quantifies how entangled two systems are

$$S_A = -\mathrm{tr}_{\mathcal{H}_A}(\rho_A \ln \rho_A)$$

It's just the von Neumann entropy of the reduced density operator

- If total system is both pure and unentangled then

$|\psi\rangle = |\phi\rangle \otimes |\chi\rangle \Rightarrow \rho_A = \mathrm{tr}_{\mathcal{H}_B}(|\phi\rangle\langle\phi| \otimes |\chi\rangle\langle\chi|) = |\phi\rangle\langle\phi| \Rightarrow S_A = 0$

- If ρ_{AB} is pure but ~~un~~entangled, $|\psi\rangle = \sum_{ab} c_{ab}|a\rangle|b\rangle$ with $c_{ab} \neq \alpha_a \beta_b$, then

$$\rho_A = \sum_{aba'b'} c_{ab}\overline{c_{ba'}}\,\mathrm{tr}_{\mathcal{H}_B}(|a^{\sharp}\rangle\langle a'| \otimes |b^{\sharp}\rangle\langle b'|)$$
$$= \sum_{aa'} C_{aa'}|a\rangle\langle a'|$$

where $C_{aa'} = \sum_b c_{ab}\overline{c_{ba'}}$ (assuming $\{|a\rangle\}$, $\{|b\rangle\}$ orthonormal)

and entanglement entropy $S_A > 0$ even though $S_{A\cup B} = 0$

If our monitored system A is entangled with the environment B, we lose information about A when tracing over the state of B.

Schmidt decomp^{n}

If the total system is in a pure ~~sty~~ state $|\psi\rangle$ then the entanglement entropy is symmetric, $S_A = S_B$. This implies S_A cannot be extensive.

↗ $-\mathrm{tr}_{\mathcal{H}_A} \rho_A \ln \rho_A$ where $\rho_A = \mathrm{tr}_{\mathcal{H}_B} \rho_{AB}$ & the other Lda

⌈* Let $\{|a\rangle\}$ be basis of $\mathcal{H}_A$ diagonalising ρ_A so that $\rho_A = \sum_a p_a |a\rangle\langle a|$

▸ any pure state of full system can be written

$|\psi\rangle = \sum_{aj} c_{aj}|a\rangle|j\rangle$ using arbitrary $\{|j\rangle\}$ for $\mathcal{H}_B$

Set $|\chi_a\rangle = \sum_j c_{aj}|j\rangle \in \mathcal{H}_B$ so that $|\psi\rangle = \sum_a |a\rangle|\chi_a\rangle$

$$\rho_A = \sum_{a'a} \mathrm{tr}_{\mathcal{H}_B}(|a\rangle\langle a'| \otimes |\chi_a\rangle\langle\chi_{a'}|) = \sum_{a'a} \langle\chi_{a'}|\chi_a\rangle\,|a\rangle\langle a'|$$

▸ $|\chi_a\rangle$ not constructed to be orthog, but comparison to above shows we must have $\langle\chi_{a'}|\chi_a\rangle = p_a \delta_{aa'}$ so $|\tilde{\chi}_a\rangle = \frac{1}{\sqrt{p_a}}|\chi_a\rangle$ are an.

▸ $\{|\chi_a\rangle\}$ are not a basis of $\mathcal{H}_B$ if $\dim(\mathcal{H}_B) > \dim(\mathcal{H}_A)$ ⌋

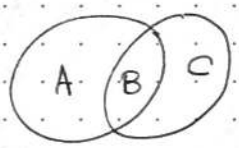
$$\rho_A = \sum_a p_a |a\rangle\langle a|, \quad \rho_B = \sum_a p_a |\tilde{\chi}_a\rangle\langle\tilde{\chi}_a| \Rightarrow S_A = S_B = -\sum_a p_a \ln p_a$$

Subadditivity The entropy of the total system is no greater than the sum of the entanglement entropies of its parts $S_{A\cup B} \leq S_A + S_B$

- * Proof uses Jensen's inequality $\langle f(X)\rangle \leq f(\langle X\rangle)$ for f convex in

$$\begin{aligned} S_{A\cup B} - S_A - S_B &= -\mathrm{tr}_{\mathcal{H}_A\otimes\mathcal{H}_B}(\rho_{AB}\ln\rho_{AB}) + \mathrm{tr}_{\mathcal{H}_A}(\rho_A\ln\rho_A) + \mathrm{tr}_{\mathcal{H}_B}(\rho_B\ln\rho_B) \\ &= -\mathrm{tr}_{\mathcal{H}_A\otimes\mathcal{H}_B}\left(\rho_{AB}\left(\ln\rho_{AB} - \ln[\rho_A\otimes 1_B] - \ln[1_A\otimes\rho_B]\right)\right) \\ &= \mathrm{tr}_{\mathcal{H}_A\otimes\mathcal{H}_B}\left(\rho_{AB}\underbrace{\ln\left[\rho_{AB}^{-1}\circ(\rho_A\otimes\rho_B)\right]}_{f(X)}\right) \\ &\leq \ln\left[\mathrm{tr}_{\mathcal{H}_A\otimes\mathcal{H}_B}\left(\rho_{AB}\circ\rho_{AB}^{-1}\circ(\rho_A\otimes\rho_B)\right)\right] \\ &= \ln(1) = 0. \ * \end{aligned}$$

- Strong subadditivity [Lieb & Ruskai 1973] says this is true even if the subsystems have parts in common



$$S_{A\cup B\cup C} \leq S_{A\cup B} + S_{B\cup C} - S_B$$

Decoherence Suppose the whole 'universe' starts from a pure & unentangled state $\rho(0) = |\psi_0\rangle\langle\psi_0|$ for some $|\psi_0\rangle = |\phi\rangle\otimes|\chi\rangle \in \mathcal{H}_A\otimes\mathcal{H}_B$

- Under unitary time evolution the density operator behaves as

$$\rho(t) = U_{AB}(t)\,\rho(0)\,U_{AB}^\dagger(t) = U_{AB}(t)|\psi_0\rangle\langle\psi_0|U_{AB}^\dagger(t)$$

- If $U_{AB}(t) = U_A(t)\otimes U_B(t)$ (no interaction between A, B) then ρ_A remains pure

- More generally we have

$$\rho_A(t) = \mathrm{tr}_{\mathcal{H}_B}\left(U_{AB}(t)|\psi_0\rangle\langle\psi_0|U_{AB}^\dagger(t)\right) = \sum_\beta M_\beta(t)\,\rho_A(0)\,M_\beta^\dagger(t)$$

where $M_\beta(t) = \langle\beta|U_{AB}(t)|\chi\rangle$ and $\{|\beta\rangle\}$ a basis of $\mathcal{H}_B$

▷ $M_\beta(t): \mathcal{H}_A \to \mathcal{H}_A$ since defined using full evolution $U_{AB}(t)$

▷ $\sum_\beta M_\beta^\dagger(t)M_\beta(t) = \sum_\beta \langle\chi|U_{AB}^\dagger|\beta\rangle\langle\beta|U_{AB}|\chi\rangle = 1_{\mathcal{H}_A}$ using $\langle\chi|\chi\rangle = 1$

- Interactions cause A and B to become entangled, leading to mixed ρ_A. This is decoherence

Decoherence & Measurement

Suppose system A is a single qubit with basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ while the measuring apparatus B has basis $\{|0\rangle, |1\rangle, |2\rangle\}$

- Ideal measurements of A change the state of B w/o affecting A

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

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

so evolution via U causes apparatus to register $|1\rangle$ if A in $|\uparrow\rangle$ and to register $|2\rangle$ if A in $|\downarrow\rangle$ each with probability p

- For this evolution we have

$$M_0 = \langle 0|U|0\rangle = \sqrt{1-p}\,1_A$$

$$M_1 = \langle 1|U|0\rangle = \sqrt{p}\,|\uparrow\rangle\langle\uparrow|$$

$$M_2 = \langle 2|U|0\rangle = \sqrt{p}\,|\downarrow\rangle\langle\downarrow|$$

- In the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis, the reduced density operator ρ_A evolves as

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

- Suppose U acts over time δt and assigns a rate $\Gamma = p/\delta t$. After time $t = N\delta t$ with $N \gg 1$, off-diagonal elements suppressed by

$$(1-p)^N = \left(1 - \frac{\Gamma t}{N}\right)^N \approx e^{-\Gamma t}$$

- Phase damping: spose initially A in state $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$.

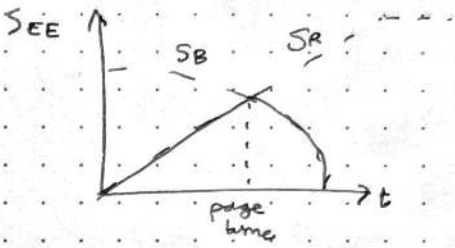
Then $$\lim_{t\to\infty} \rho_A(t) = \lim_{t\to\infty} \begin{pmatrix} |a|^2 & e^{-\Gamma t} b\bar{a} \\ e^{-\Gamma t}\bar{b}a & |b|^2 \end{pmatrix} = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}$$

- As A entangles itself with the measuring apparatus, we're unlikely to find A in a superposition in the basis preferred by the apparatus
  - ▷ related to what we saw in degenerate perturbation theory
  - ▷ locality determines preferred interactions in QFT

Hawking Radiation & the Black Hole Information Paradox

Hawking discovered that quantum fluctuations mean black holes radiate

- The radiation is entangled with the state of the black hole
- As the black hole evaporates, what happens to information trapped inside? Is quantum gravity non-unitary?



Bell Inequalities

The Einstein-Podolsky-Rosen Gedankenexperiment

Einstein believed that the probabilistic aspects of QM were attributable purely to our lack of understanding of hidden 'aspects of reality'

- EPR devised a thought experiment aiming to show that QM could not be a complete theory of nature
- Wavef^n $\psi(x_1, x_2) = \delta(x_1 - x_2 - x_0)$ has

$$(X_1 - X_2)\,\psi(x_1, x_2) = x_0\,\psi(x_1 - x_2)$$

$$(P_1 + P_2)\,\psi(x_1, x_2) = 0$$

noting that $[X_1 - X_2,\ P_1 + P_2] = 0$.

If we find x_1 when measuring X_1, we know particle 2 has position $x_1 + x_0$.

- Suppose we now measure P_1 and find some value p.

Doesn't this mean particle 2 has momentum $-p$?

- How can measuring particle 1 disturb the (perhaps distant) particle 2?

Bohm's refinement of the EPR experiment

In Bohm's 1951 version, an e^-e^+ pair are created in the spin-0 state

$$|EPR\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right) = \frac{1}{\sqrt{2}}\left(|\uparrow_a\rangle|\downarrow_a\rangle - |\downarrow_a\rangle|\uparrow_a\rangle\right)$$

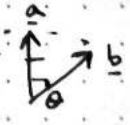
(perhaps by nuclear decay) and subsequently travel to Alice & Bob

- When e^- reaches Alice, she measures its spin along an axis $\underline{a}$ of her choice. If Alice measures $+\hbar/2$, Copenhagen interpretation says

$$|EPR\rangle \mapsto |\uparrow_a\rangle|\downarrow_a\rangle$$

- Bob now measures the spin of e^+ along an axis $\underline{b}$ of his choice
- We can expand Bob's state $|\uparrow_b\rangle$ in basis adapted to $\underline{a}$

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



so if Alice found the e^- to be in $|\uparrow_a\rangle$, probability Bob finds the e^+ to be in $|\uparrow_b\rangle$ is

$$|\langle\uparrow_b|\downarrow_a\rangle|^2 = \sin^2\left(\frac{\theta}{2}\right) \quad \text{where } \theta = \cos^{-1}(\hat{a}\cdot\hat{b})$$

No Violation of Causality

Since Bob and Alice are space-like separated (and perhaps very distant), who made their measurement 'first' depends on the frame of the observer

- Above result not in conflict with this, since depends on Alice & Bob's choices only through $\underline{a} \cdot \underline{b}$ so symmetric under exchange $A \leftrightarrow B$

However, there's a direction ($\underline{a}$) along which Bob never finds spin $+\hbar/2$ and this direction depends on what Alice chooses to measure

- Einstein deplored this 'spooky action at a distance'
  - ▷ perhaps e^- and e^+ each already have definite spin directions when created (unlike in $|EPR\rangle$) just that we don't know what they are

Hidden variables

Following Einstein, suppose that the result of measuring an electron's spin along unit vector $\underline{a}$ is completely determined by some 'hidden variables', say $\underline{v} \in \mathbb{R}^n$, whose value was fixed when the $e^- e^+$ pair was created

- In such theories, spin along a direction $\underline{a}$ is a function

$$S_e : S^2 \times \mathbb{R}^n \longrightarrow \left\{ +\frac{\hbar}{2}, -\frac{\hbar}{2} \right\}$$

whose value is completely determined by $(\underline{a}, \underline{v})$: Outcome of Alice's measurement uncertain only because she doesn't know value of $\underline{v}$

- Let $p(\underline{v})\, d^n v$ be prob the hidden variables lie in the range $(\underline{v}, \underline{v} + d\underline{v})$

We want to compute

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

and compare to quantum result

- Conservation of angular momentum says $S_e(\underline{a}, \underline{v}) + S_p(\underline{a}, \underline{v}) = 0$ for any unit vector $\underline{a} \in S^2$, so $\langle S_e(\underline{a})\, S_p(\underline{b}) \rangle = -\langle S_p(\underline{a})\, S_p(\underline{b}) \rangle$

Bell's Inequality

Bob could choose to measure the spin along $\underline{b}'$ instead of $\underline{b}$

- Since $s_p(\underline{b},\underline{v})^2 = \hbar^2/4$ always, we have

$$\langle s_e(\underline{a})\, s_p(\underline{b})\rangle - \langle s_e(\underline{a})\, s_p(\underline{b}')\rangle = \int_{\mathbb{R}^n} s_e(\underline{a},\underline{v})\left[s_p(\underline{b},\underline{v}) - s_p(\underline{b}',\underline{v})\right] p(\underline{v})\, d^n v$$

$$= \int_{\mathbb{R}^n} s_e(\underline{a},\underline{v})\, s_p(\underline{b},\underline{v})\left[1 - \frac{4}{\hbar^2} s_p(\underline{b},\underline{v}) s_p(\underline{b}',\underline{v})\right] p(\underline{v})\, d^n v$$

$$= -\int_{\mathbb{R}^n} s_p(\underline{a},\underline{v}) s_p(\underline{b},\underline{v})\left[1 - \frac{4}{\hbar^2} s_p(\underline{b},\underline{v}) s_p(\underline{b}',\underline{v})\right] p(\underline{v})\, d^n v$$

- The expression $\left[1 - \frac{4}{\hbar^2} s_p(\underline{b},\underline{v})\, s_p(\underline{b}',\underline{v})\right]$ is non-negative, whilst $s_p(\underline{a},\underline{v})\, s_p(\underline{b},\underline{v})$ fluctuates between $\pm\hbar^2/4$ according to $\underline{v}$

- Replace fluctuating term by $\hbar^2/4$ everywhere to find Bell's inequality

$$\left|\langle s_p(\underline{a})\, s_p(\underline{b})\rangle - \langle s_p(\underline{a})\, s_p(\underline{b}')\rangle\right| \leq \int_{\mathbb{R}^n}\left[\frac{\hbar^2}{4} - s_p(\underline{b},\underline{v})\, s_p(\underline{b}',\underline{v})\right] p(\underline{v})\, d^n v$$

$$= \frac{\hbar^2}{4} - \langle s_p(\underline{b})\, s_p(\underline{b}')\rangle$$

which must be obeyed in any theory of hidden variables.

Quantum Mechanics violates Bell's inequality

- Since $(\underline{s}_e \otimes 1_p + 1_e \otimes \underline{s}_p)\,|EPR\rangle = 0$, we have

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

$$= -1_e \otimes (\underline{a}\cdot\underline{s}_p \,\not\!\!\not\, \underline{b}\cdot\underline{s}_p)\,|EPR\rangle$$

- We now use

$$\underline{a}\cdot\underline{s}\;\underline{b}\cdot\underline{s} = \frac{\hbar^2}{4}\underline{a}\cdot\underline{b}\,1_{\mathcal{H}} + \frac{i\hbar}{2}(\underline{a}\times\underline{b})\cdot\underline{s} \quad \text{and} \quad \langle EPR|\,\underline{s}_p\,|EPR\rangle = 0$$

to learn $\langle \underline{a}\cdot\underline{s}_p\;\underline{b}\cdot\underline{s}_p\rangle_{EPR} = \hbar^2/4\;\underline{a}\cdot\underline{b}$ ⊁

- In quantum mechanics, the LHS of Bell's inequality is

$$\left|\langle \underline{a}\cdot\underline{s}_p\,\underline{b}\cdot\underline{s}_p\rangle_{EPR} - \langle \underline{a}\cdot\underline{s}_p\,\underline{b}'\cdot\underline{s}_p\rangle_{EPR}\right| = \frac{\hbar^2}{4}\left|\underline{a}\cdot(\underline{b}-\underline{b}')\right|$$

whilst the RHS becomes

$$\frac{\hbar^2}{4} - \langle \underline{b}\cdot\underline{s}_p\,\underline{b}'\cdot\underline{s}_p\rangle_{EPR} = \frac{\hbar^2}{4}(1 - \underline{b}'\cdot\underline{b})$$

- e.g. $\underline{a} = \underline{i}$, $\underline{b} = \underline{k}$, $\underline{b}' = \frac{1}{\sqrt{2}}(\underline{i}+\underline{k})$ shows QM violates Bell's inequality

The Clauser-Horne-Shimony-Holt inequality

The original form of Bell's inequality is difficult to test directly

- Consider a theory of hidden variables where Alice and Bob can each measure only one of two things, each of which takes values ± 1. Then

$$a_i : \mathbb{R}^n \to \{\pm 1\} \quad \text{and} \quad b_j : \mathbb{R}^n \to \{\pm 1\}$$

- Define $C = (a_1 + a_2)\, b_1 + (a_1 - a_2)\, b_2$ so that on average

$$\langle C \rangle = \int \left[(a_1(\underline{v}) + a_2(\underline{v}))\, b_1(\underline{v}) + (a_1(\underline{v}) - a_2(\underline{v}))\, b_2(\underline{v}) \right] p(\underline{v})\, d^n v$$

- Depending on the hidden variable $\underline{v}$,

either $a_1(\underline{v}) + a_2(\underline{v}) = \pm 2$ while $a_1(\underline{v}) - a_2(\underline{v}) = 0$

or $a_1(\underline{v}) + a_2(\underline{v}) = 0$ while $a_1(\underline{v}) - a_2(\underline{v}) = \pm 2$

and multiplying the non-zero term by $b_i(\underline{v})$ at most changes its sign

- Thus we find the CHSH inequality $-2 \leq \langle C \rangle \leq 2$

Quantum violations of the CHSH inequality

In the quantum context we assume we have operators A_i and B_j each with eigenvalues ± 1 and define $C = (A_1 + A_2) B_1 + (A_1 - A_2) B_2$

- Assume $[A_i, B_j] = 0$ so Alice & Bob's measurements don't interfere with one another, but don't assume $[A_i, A_j]$, $[B_i, B_j]$ vanish
- Since evals are ± 1, must have $A_i^2 = B_j^2 = 1$. Hence

$$C^2 = 4 - [A_1, A_2]\,[B_1, B_2] \quad \text{(direct calculation)}$$

- For any operators A_i with evals ± 1 we have

$$|\langle [A_1, A_2] \rangle| \leq |\langle A_1 A_2 \rangle| + |\langle A_2 A_1 \rangle| \leq 2$$

and also $\langle C^2 \rangle \geq \langle C \rangle^2$ for any Hermitian operator C

- In quantum mechanics, we have only the weaker Tsirelson bound

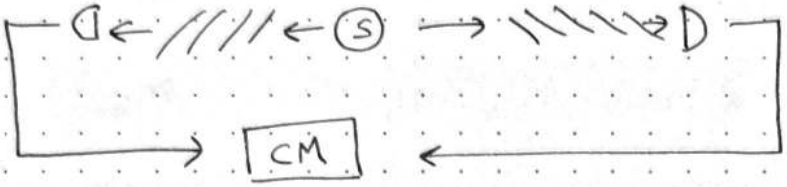
$$-2\sqrt{2} \leq \langle C \rangle \leq 2\sqrt{2}$$

- Saturated by $|EPR\rangle$ if we take $A_i = \underline{n}_i \cdot \underline{\sigma}$ and $B_j = \underline{m}_j \cdot \underline{\sigma}$ with

$$\underline{n}_1 = \underline{i}, \quad \underline{n}_2 = \underline{k}, \quad \underline{m}_1 = \frac{\underline{i} + \underline{k}}{\sqrt{2}}, \quad \underline{m}_2 = \frac{\underline{i} - \underline{k}}{\sqrt{2}}$$

Nature speaks...

The CHSH form of Bell's inequality was tested by Aspect & Roger in 1982



- Two photons emitted from successive decays of excited states of $_{55}Cs$
  - ▷ first from decay of $j=0^+$ state to short-lived $j=1^-$ state
  - ▷ second from decay of this $j=1^-$ state down to a lower $j=0^+$ state
- Photons enter photomultipliers (detectors) that read out ± 1 according to whether photons found to be linearly polarised along $\underline{a}/\underline{b}$
- Expt measured $\langle C\rangle_{expt} = 2.697 \pm 0.015 > 2$, ruling in favour of quantum mechanics
  - ▷ $\langle C\rangle_{expt} < 2\sqrt{2}$ only largely due to imperfect polarizers

The GHZ state

An even sharper conflict between QM and any hidden variables theory can be found by considering three qubits in the entangled GHZ state

$$|GHZ\rangle = \frac{|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle}{\sqrt{2}}$$

(Explored in final Q^{n} of final sheet)