Institute of Physics
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Quantum Mechanics I

PGF5001
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Mathematics of QM in Finite Dimension

Hilbert space: vector space ⊕ scalar product positive definite

actually it is called an inner product and $\mathcal{H}$ must be complete as a metric space

$\mathcal{H}$, $\dim \mathcal{H} = n$, $\mathbb{C}$

Dirac notation: $\vec{v} \in \mathcal{H}$, $\underbrace{|v\rangle}_{\text{ket}} \in \mathcal{H}$

$\lambda \in \mathbb{C}$: $|\lambda v) = \lambda |v\rangle$

for now, we shall use
|) when there is a number or operator alongside the vector

Scalar product

$\vec{v}^{\dagger} \cdot \vec{w} = v_i^* w_i$ Einstein's convention

$\updownarrow$ Dirac

$\underbrace{\langle v|}_{\text{bra}}\underbrace{|w\rangle}_{\text{ket}} = (v|w)$ alternate notation

Linearity

$(v|w + \lambda u) = (v|w) + \lambda (v|u)$ $\to$ $\langle v|w + \lambda u\rangle = \langle v|w\rangle + \lambda \langle v|u\rangle$

$|v\rangle, |w\rangle, |u\rangle \in \mathcal{H}$, $\lambda \in \mathbb{C}$

Consequences

i) $\langle \varphi|\varphi\rangle \geq 0$ positive definite

ii) antilinear in first argument

1st result:

$(v|w) = (w|v)^*$

$(v|w) = v_i^* w_i = (w_i^* v_i)^* = (w|v)^*$

2nd result

$(v + \lambda u|w) = (v|w) + \lambda^* (u|w)$

$(v + \lambda u|w) = (w|v + \lambda u)^* = [(w|v) + \lambda (w|u)]^*$

$= (w|v)^* + \lambda^* (w|u) = (v|w) + \lambda^* (u|w)$

$\underbrace{\{|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle\}}_{\text{basis}} \in \mathcal{H}$

basis → linearly independent vectors
span $\mathcal{H}$

↓

Gram-Schmidt Orthonormalization → we can always found an orthonormal basis

$\langle e_i | e_j \rangle = \delta_{ij}$

↓

convention: we shall always pick orthonormal bases

Vector decomposition

$$\mathcal{H} \ni |\varphi\rangle = \sum_i \varphi_i |e_i\rangle$$

$$\varphi_i = ?$$

$$\langle e_k | \varphi \rangle = \sum_i \varphi_i \underbrace{\langle e_k | e_i \rangle}^{\delta_{ki}} = \varphi_k$$

$$\langle \chi | \varphi \rangle = \sum_i \chi_i^* \varphi_i$$

$$\langle \varphi | \varphi \rangle = \sum_i |\varphi_i|^2 \geqslant 0$$

Consequence

$$\langle \varphi | \varphi \rangle = 0 \Rightarrow \varphi_i = 0, \forall i \Rightarrow |\varphi\rangle = 0$$

Schwartz Inequality → Heisenberg's Uncertainty Principle

$$|\langle \chi | \varphi \rangle|^2 \leqslant \|\chi\|^2 \|\varphi\|^2$$

Let $|\beta\rangle = |\chi\rangle + \lambda |\varphi\rangle$ → $\lambda \in \mathbb{C}$

$$\langle \beta | \beta \rangle \geqslant 0$$

$$\langle \chi | \chi \rangle + |\lambda|^2 \langle \varphi | \varphi \rangle + \lambda \langle \chi | \varphi \rangle + \lambda^* \langle \varphi | \chi \rangle \geqslant 0$$

Let $\lambda = - \dfrac{\langle \chi | \varphi \rangle}{\|\varphi\|^2}$.

Some more algebra yields the result.

Linear Operators

Let V and W be Hilbert spaces

$$\hat{A}: V \to W$$

Linear: $|\varphi\rangle \in V,\ \lambda \in \mathbb{C}$

$$|\hat{A}(\lambda\varphi)) = \lambda \hat{A}|\varphi\rangle$$
$$|\hat{A}(\chi+\varphi)) = \hat{A}|\chi\rangle + \hat{A}|\varphi\rangle$$

Example: scalar product

$$W = \mathbb{C}$$

$$\hat{A}_\chi : \mathcal{H} \to \mathbb{C}$$

$$\hat{A}_\chi|\varphi\rangle \equiv \langle\chi|\varphi\rangle$$

$\langle\chi| \in \mathcal{H}^* \to \mathcal{H}$ dual

Hermitian Conjugate

$\hat{A}$ is a linear operator

$$(\chi|\hat{A}^\dagger\varphi) \equiv (\hat{A}\chi|\varphi)$$

Hermitian or self-conjugate operators: $\hat{A} = \hat{A}^\dagger \to (\chi|\hat{A}\varphi) = (\hat{A}\chi|\varphi)$

or self-adjoint

$\langle\chi|\hat{A}|\varphi\rangle$

Matrix Representation of Linear Operators

Let $\{|e_i\rangle\}$ be an orthonormal basis in $\mathcal{H}$

$$\hat{A}_{mn} = (e_m|\hat{A}e_n)$$

$$(\hat{A}^\dagger)_{mn} = (e_m|\hat{A}^\dagger e_n) = (\hat{A}e_m|e_n) = (e_n|\hat{A}e_m)^* = \hat{A}^*_{nm}$$

Trace

$$\mathrm{tr}[\hat{A}] = \sum_i \hat{A}_{ii}$$

Determinant

$$\det \hat{A} = \frac{1}{n!}\sum \epsilon_{i_1\cdots i_n}\epsilon_{k_1\cdots k_n}\hat{A}_{i_1k_1}\cdots\hat{A}_{i_nk_n}$$

Projectors

$\hat{P}_v$ = projector along $|v\rangle$ in $\mathcal{H}$

$$\hat{P}_{v^\perp} = \mathbb{1} - \hat{P}_v$$

Properties

i) $\hat{P}_v^{\,2} = \hat{P}_v$

ii) $\hat{P}_v \hat{P}_{v^\perp} = 0$

iii) $\hat{P}_v + \hat{P}_{v^\perp} = \mathbb{1}$

Explicit Expression

$$|\varphi\rangle = \varphi_v |v\rangle + \varphi_{v^\perp} |v^\perp\rangle$$

$$\varphi_v = \frac{\langle v|\varphi\rangle}{\langle v|v\rangle}$$

$$|\varphi\rangle = \frac{\langle v|\varphi\rangle}{\langle v|v\rangle} |v\rangle + \varphi_{v^\perp} |v^\perp\rangle$$

$$= \underbrace{\boxed{\frac{|v\rangle\langle v|\varphi\rangle}{\langle v|v\rangle}}}_{\text{projector } \hat{P}_v} + \varphi_{v^\perp} |v^\perp\rangle$$

$$\hat{P}_v = \frac{|v\rangle\langle v|}{\langle v|v\rangle}$$

$$\hookrightarrow \hat{P}_{v^\perp} = \mathbb{1} - \frac{|v\rangle\langle v|}{\langle v|v\rangle}$$

$|v\rangle\langle v|$

external product or tensor product

$$\begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} (v_1^* \dots v_n^*) = \begin{pmatrix} v_1 v_1^* & v_1 v_2^* & \dots & v_1 v_n^* \\ v_2 v_1^* & v_2 v_2^* & \dots & v_2 v_n^* \\ \vdots & \vdots & \ddots & \vdots \\ v_n v_1^* & v_n v_2^* & \dots & v_n v_n^* \end{pmatrix}$$

Let $\{|e_i\rangle\} \in \mathcal{H}$ be a basis

$$|\varphi\rangle = \sum_i \varphi_i |e_i\rangle$$

we don't divide by the norm because the basis is orthonormal

$$= \sum_i \langle e_i|\varphi\rangle |e_i\rangle$$

$$= \underbrace{\left(\sum_i |e_i\rangle\langle e_i|\right)}_{\mathbb{1}} |\varphi\rangle$$

For an orthonormal basis

$$\sum_i |e_i\rangle\langle e_i| = \mathbb{1}$$

$\hookrightarrow$ resolution or decomposition of the identity also known as completeness

$$\hat{A} = \mathbb{1}\hat{A}\mathbb{1}$$
$$= \left(\sum_i |e_i\rangle\langle e_i|\right)\hat{A}\left(\sum_k |e_k\rangle\langle e_k|\right)$$
$$= \sum_{i,k} \hat{A}_{ik} |e_i\rangle\langle e_k|$$

Gram-Schmidt Orthonormalization Procedure

$\{|a_i\rangle\}_{i=1}^{n}$ linearly independent

$$|e_1\rangle = \frac{|a_1\rangle}{\sqrt{\langle a_1|a_1\rangle}}$$
$$|E_2\rangle = |a_2\rangle - \langle e_1|a_2\rangle|e_1\rangle$$
$$|e_2\rangle = \frac{|E_2\rangle}{\sqrt{\langle E_2|E_2\rangle}}$$
$$|E_3\rangle = |a_3\rangle - \langle e_1|a_3\rangle|e_1\rangle - \langle e_2|a_3\rangle|e_2\rangle$$
$$|e_3\rangle = \frac{|E_3\rangle}{\sqrt{\langle E_3|E_3\rangle}}$$

Unitary Operators

both orthonormal

Let $\{|e_i\rangle\}$ and $\{|e'_k\rangle\}$ be bases in $\mathcal{H}$

$$|e_m\rangle = \sum_{k} U^*_{mk} |e'_k\rangle$$

I can interpret U_{mk} as the matrix elements of some operator in some sense

$\cancel{U_{mk} = (e_k|\hat{U}e'_m)}$

$U_{mk} = (e_k|e'_m)$

Einstein's convention

$$|e'_m\rangle = |e_k\rangle\underbrace{\langle e_k|e'_m\rangle}_{U^*_{mk}}$$

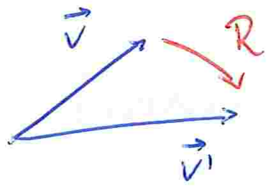
$$\underbrace{U^*_{mk}U_{kn}}_{(\hat{U}^\dagger U)_{mn}} = \langle e_k|e'_m\rangle\langle e'_n|e_k\rangle = \langle e'_n|e_k\rangle\langle e_k|e'_m\rangle = \langle e'_n|e'_m\rangle = \delta_{nm}$$

$(\hat{U}^\dagger U)_{mn} = \delta_{mn} \Rightarrow \hat{U}^\dagger\hat{U} = \mathbb{1} \rightarrow$ operators that satisfy this condition are said to be unitary

Exercise: show that unitary operators preserve the norm of vectors.

Eigenvalue problem

$|v\rangle, \quad \hat{A}|v\rangle$



in general, they are not parallel

There are special vectors, for a given operator $\hat{A}$, such that $\hat{A}|v\rangle \parallel |v\rangle$

eigenvalue

$$\hat{A}|a\rangle = a|a\rangle$$ eigenvector

$$(\hat{A}-a)|a\rangle = 0, \quad \underbrace{(\hat{A}-a)}_{\hat{B}}$$

suppose $\exists\, \hat{B}^{-1}$

$$\hat{B}|a\rangle = 0$$

$$\underbrace{\hat{B}^{-1}\hat{B}}_{\mathbb{1}}|a\rangle = \hat{B}^{-1}0$$

$$|a\rangle = 0$$

$\nexists\, \hat{B}^{-1}$

Unless $\det(\hat{A}-a)=0$, $\underbrace{|a\rangle = 0}_{\text{not interesting}}$

$$\det(\hat{A}-a)=0$$

dim $\mathcal{H}$ solutions

↓

they don't need to be different

↓

degeneracy

Hermitian operators → $\hat{A}^{\dagger} = \hat{A}$

Properties

i) all eigenvalues are real

ii) the eigenvectors compose an orthogonal basis for $\mathcal{H}$

Proofs

i) $|a\rangle$, a, $\hat{A}|a\rangle = a|a\rangle$

$$\langle a|\hat{A}|a\rangle = a\langle a|a\rangle$$

$$\hat{A}|a\rangle = a|a\rangle \Rightarrow \langle a|\hat{A}^{\dagger} = \langle a|a^{*}$$ $\hat{A}$ is hermitian

$$\langle a|\hat{A} = \langle a|a^{*}$$

$$\langle a|\hat{A}|a\rangle = a^{*}\langle a|a\rangle$$

$$\therefore \quad a\langle a|a\rangle = a^{*}\langle a|a\rangle$$

$$a = a^{*}$$

ii) a, a' eigenvalues (we suppose $a \neq a'$)

$$\hat{A}|a\rangle = a|a\rangle$$

$$\hat{A}|a'\rangle = a'|a'\rangle \xrightarrow{\text{hermitian} + \text{real number}} \langle a'|\hat{A} = a'\langle a'|$$

~~$\hat{A}|a\rangle a$~~

$$\hat{A}|a\rangle = a|a\rangle \Rightarrow \langle a'|\hat{A}|a\rangle = a\langle a'|a\rangle$$

$$a'\langle a'|a\rangle = a\langle a'|a\rangle$$

$$\underbrace{(a'-a)}_{\neq 0}\langle a'|a\rangle = 0$$

$$\langle a'|a\rangle = 0$$

For the non-degenerate case, the eigenvectors form a basis

↳ dim $\mathcal{H}$ different eigenvalues ⇒ dim $\mathcal{H}$ orthogonal eigenvectors

For the degenerate case, I might choose eigenvectors ~~such~~ that orthonormalize the bases

↳ pick a basis for the degenerated subspace and apply Gram-Schmidt's algorithm within the subspace

Unitary operators → $\hat{U}^\dagger \hat{U} = \mathbb{1} = \hat{U}\hat{U}^\dagger$ ⇔ $(\hat{U}a|\hat{U}b) = (a|b)$

$(\hat{U}\hat{U}^\dagger a|b) = (a|b)$

Properties

i) all eigenvalues are pure phases $e^{i\alpha}$

ii) the eigenvectors compose an orthogonal basis for $\mathcal{H}$

Proofs.

i) $\hat{U}|u\rangle = u|u\rangle$

$(u|\hat{U}u) = u(u|u)$ → always happens

$$(u|u) = (\hat{U}u|\hat{U}u) = u(\hat{U}u|u) = u^* u(u|u)$$

$$(1 - u^* u)(u|u) = 0$$

$$|u|^2 = u^* u = 1 \Rightarrow u = e^{i\alpha}$$

ii) Analogous to the proof for Hermitian operators

Remarks

i) on the eigenvector basis, an operator is diagonal

ii) $\hat{U} = \underbrace{\{|u_1\rangle, \dots, |u_n\rangle\}}_{\text{eigenvector for an operator}}$, $\hat{U}^\dagger \hat{U} = \mathbb{1}$

Spectral Decomposition

$\hat{O}$ operator, $\{|o_n\rangle\}$ → $\hat{O}$ is hermitian or unitary

$$\hat{O} = \hat{O}\,\mathbb{1} = \hat{O}\sum_n |o_n\rangle\langle o_n|$$

$$= \sum_n \hat{O}|o_n\rangle\langle o_n|$$

$$= \sum_n o_n |o_n\rangle\langle o_n|$$

Compatible Operators → Second ingredient for Heisenberg's uncertainty

Commutator: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

Compatible operators: $[\hat{A}, \hat{B}] = 0$

Claim: $[\hat{A}, \hat{B}] = 0 \Leftrightarrow \exists$ set of eigenvectors common to $\hat{A}$ and $\hat{B}$

Proof:

$\Rightarrow$) non-degenerate eigenvalues

eigenvector with eigenvalue a

$\hat{A}|a\rangle = a|a\rangle$

$\hat{A}\hat{B}|a\rangle = \hat{B}\hat{A}|a\rangle = a\hat{B}|a\rangle \Rightarrow \hat{A}(\hat{B}|a\rangle) = a(\hat{B}|a\rangle)$

Not-degenerate: $\hat{B}|a\rangle = b_a|a\rangle$, for some b_a

↳ $|a\rangle$ is also an eigenvector for $\hat{B}$

degenerate eigenvalues

suppose a has k-fold degeneracy → k-dimensional eigenspace

$$\hat{B}|a,j\rangle = \sum_{i=1}^{k} \underbrace{C^a_{ij}}_{k\times k \text{ matrix}} |a,i\rangle$$

Let $C^a\vec{\beta} = b_a\vec{\beta}$ with $(\vec{\beta})_i = \beta_i$ and consider $\sum_i \beta_i |a,i\rangle$

$$\hat{B}\sum_i \beta_i |a,i\rangle = \sum_i \beta_i \hat{B}|a,i\rangle$$ $\hat{B}|a,i\rangle = \sum_{l=1}^{k} C^a_{li}|a,l\rangle$

$$= \sum_{i,l} C^a_{li}\beta_i |a,l\rangle$$ $C^a\vec{\beta} = b_a\vec{\beta}$

$$= \sum_l b_a \beta_l |a,l\rangle$$

$$= b_a \underbrace{\sum_l \beta_l |a,l\rangle}$$ eigenvector for $\hat{A}$ and $\hat{B}$

$\Leftarrow$:

$$\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle$$
$$\hat{B}|\varphi_n\rangle = b_n|\varphi_n\rangle$$

$$|\varphi\rangle = \sum_n c_n|\varphi_n\rangle$$

$$(\hat{A}\hat{B}-\hat{B}\hat{A})|\varphi\rangle = \sum_n c_n(\hat{A}\hat{B}-\hat{B}\hat{A})|\varphi_n\rangle$$
$$= \sum_n c_n(a_nb_n - b_na_n)|\varphi_n\rangle$$
$$= \sum_n 0|\varphi_n\rangle = 0, \quad \forall\ |\varphi\rangle$$

$$\therefore [\hat{A},\hat{B}] = 0$$

Functions of Operators

$$f(x) = \sum_{n=0}^{+\infty} \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n \longrightarrow f(\hat{A}) = \sum_{n=0}^{+\infty} \frac{f^{(n)}(x_0)(\hat{A}-x_0)^n}{n!}$$

If $\hat{A}$ has spectral decomposition

$$\hat{A} = \sum_n a_n |a_n\rangle\langle a_n|$$

$$f(\hat{A}) = \sum_n f(a_n) |a_n\rangle\langle a_n|$$

sum over eigenvalues } n goes from 1 up to the number of eigenvalues

$$\hat{A}^n = \prod_{j=1}^{n} \left(\sum_{i_j=1}^{m} a_{i_j} |a_{i_j}\rangle\langle a_{i_j}| \right)$$

$$= \sum_{i_1, i_2, \dots, i_n} \prod_{j=1}^{n} a_{i_j} |a_{i_1}\underbrace{\rangle\langle a_{i_1}|a_{i_2}}_{\delta_{i_1 i_2}}\underbrace{\rangle\langle a_{i_2}|a_{i_3}}_{\delta_{i_2 i_3}}\rangle\langle a_{i_3}| \cdots \langle a_{i_n}|$$

$$= \sum_{i_1, i_2, \dots, i_n} \prod_{j=1}^{n} a_{i_j} \delta_{i_1 i_2}\delta_{i_2 i_3}\cdots\delta_{i_{n-1} i_n} |a_{i_1}\rangle\langle a_{i_n}|$$

$$= \sum_i a_i^n |a_i\rangle\langle a_i|$$

$$f(\hat{A}) = \sum_n \frac{f^{(n)}(0)}{n!} \hat{A}^n$$

$$= \sum_n \sum_i \frac{f^{(n)}(0)}{n!} a_i^n |a_i\rangle\langle a_i|$$

$$= \sum_i \left(\sum_n \frac{f^{(n)}(0)}{n!} a_i^n \right) |a_i\rangle\langle a_i|$$

$$= \sum_i f(a_i) |a_i\rangle\langle a_i|$$

Postulates of Quantum Mechanics

one can't derive a postulate, but can guess whether they are right and then check through experiment if they work

STATES I. The state of a system is defined by a ray of vectors in the Hilbert space $\mathcal{H}$

$$|\tilde{\varphi}\rangle = \{ e^{i\alpha}|\varphi\rangle ;\ \alpha \in (0, 2\pi] \}$$

OBSERVABLES II. Observables are represented by hermitian operators acting on the Hilbert space $\mathcal{H}$. If one measure an observable, the obtained value will be one of the observable's eigenvalues.

III. BORN RULE: given a state $|\tilde{\varphi}\rangle$, a measurement of a given observable will return the eigenvalue x with probability

$$P = \frac{|\langle x|\varphi\rangle|^2}{\langle x|x\rangle\langle\varphi|\varphi\rangle}$$

due to Born's Rule, we might simply choose $|\varphi\rangle$ to do the calculations

debatable and controversial

IV. COLAPSE OF STATE AFTER MEASUREMENT: given a state $|\tilde{\varphi}\rangle$ and an observable $\hat{A}$ with eigenvectors $\{|a_n\rangle\}$, so that $|\varphi\rangle = \sum \varphi_n |a_n\rangle$, $\varphi_n = \langle a_n|\varphi\rangle$, if a measurement of $\hat{A}$ returns a result a_i, the state $|\varphi\rangle$ collapses to the state $|a_i\rangle$. → instantaneously

V. TIME EVOLUTION: time evolution is unitary: $\hat{\mathcal{U}}(t, t_0)$

$$|\varphi(t)\rangle = \hat{\mathcal{U}}(t, t_0)|\varphi(t_0)\rangle.$$

For consistency, we need that $\hat{\mathcal{U}}(t_2, t_0) = \hat{\mathcal{U}}(t_2, t_1)\hat{\mathcal{U}}(t_1, t_0)$. Furthermore, $\hat{\mathcal{U}}$ must obey the differential equation

$$i\hbar \frac{\partial \hat{\mathcal{U}}(t,t_0)}{\partial t} = \hat{H}\,\hat{\mathcal{U}}(t,t_0).$$

hermitian Hamiltonian

however, how do we compute the operator $\hat{U}(t,t_0)$?

$$i\hbar \frac{\partial|\varphi(t)\rangle}{\partial t} = i\hbar \frac{\partial}{\partial t}\left(\hat{U}(t,t_0)|\varphi(t_0)\rangle\right)$$
$$= i\hbar \frac{\partial \hat{U}}{\partial t}(t,t_0)|\varphi(t_0)\rangle$$
$$= \hat{H}\hat{U}(t,t_0)|\varphi(t_0)\rangle$$
$$= \hat{H}|\varphi(t)\rangle$$

Schrödinger Equation

Obtaining $\hat{U}(t,t_0)$

i) Time-independent $\hat{H}$

$$i\hbar \frac{\partial \hat{U}}{\partial t} = \hat{H}\hat{U} \Rightarrow \hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$$

time translation is the exponential of an hermitian operator (times i)

$\hat{H}$ is hermitian, $\hbar$ and $(t-t_0)$ are real

$$\hat{U}^\dagger\hat{U} = e^{\frac{i}{\hbar}\hat{H}(t-t_0)}\, e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$$

$[\hat{H},\hat{H}]=0$

$$= e^{\frac{i}{\hbar}\hat{H}(t-t_0) - \frac{i}{\hbar}\hat{H}(t-t_0)}$$
$$= \mathbb{1}$$

ii) Time-dependent $\hat{H}$

NAIVELY

$$i\hbar \frac{d\hat{U}}{\hat{U}} = \hat{H}\,dt$$

$$i\hbar\int_{t_0}^{t_0}\frac{d\hat{U}}{\hat{U}} = \int_{t_0}^{t}\hat{H}\,dt \Rightarrow \hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(\tau)\,d\tau}$$

I would like

$$e^{-\frac{i}{\hbar}\int_{t_1}^{t_2}\hat{H}(\tau)d\tau}\, e^{-\frac{i}{\hbar}\int_{t_0}^{t_1}\hat{H}(\tau)d\tau} \neq e^{-\frac{i}{\hbar}\int_{t_0}^{t_2}\hat{H}(\tau)d\tau}$$

in general

$$i\hbar\frac{\partial \hat{U}(t,t_0)}{\partial t} = \hat{H}(t)\,\hat{U}(t,t_0)$$

$$\hat{U}(t,t_0) - \hat{U}(t_0,t_0) = \frac{1}{i\hbar}\int_{t_0}^{t}\hat{H}(\tau)\,\hat{U}(\tau,t_0)\,d\tau$$

$$\hat{U}(t,t_0) = \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{H}(\tau)\,\hat{U}(\tau,t_0)\,d\tau$$

iterate

$$= \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t}d\tau\,\hat{H}(\tau)\left(\mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{\tau}d\tau'\,\hat{H}(\tau')\left(\mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{\tau'}d\tau''\,\hat{H}(\tau'')\left(\mathbb{1} + \dots\right.\right.\right.$$

to make sense of this, we need $\hat{H}(t)$ to be small for the series to be valid at least in the perturbative sense

Dyson Series

Time Evolution of an Energy Eigenstate

stationary states

$$\hat{H}|E_n\rangle = E_n|E_n\rangle$$

$$\hat{U}(t,t_0)|E_n\rangle = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} = e^{-\frac{i}{\hbar}E_n(t-t_0)}|E_n\rangle$$

Expectation Value

Classical: A measured, N-times, A_n obtained with frequency p_n

$$\langle A\rangle = \sum_n p_n A_n$$

Quantum: $\hat{A}$ measured, outcome a_n with probability $p_n = |\langle a_n|\varphi\rangle|^2$

$$\langle \hat{A} \rangle_\varphi = \sum_n p_n a_n$$

$$= \sum_n |\langle a_n | \varphi \rangle|^2 a_n$$

$$= \sum_n a_n \langle \varphi | a_n \rangle \langle a_n | \varphi \rangle$$

$$= \langle \varphi | \left(\sum_n a_n | a_n \rangle \langle a_n | \right) | \varphi \rangle$$

$$= \langle \varphi | \hat{A} | \varphi \rangle$$

Time Evolution

$$\langle \hat{A}(t) \rangle_\varphi = \langle \varphi(t) | \hat{A} | \varphi(t) \rangle$$

$$= \langle \varphi(t_0) | \hat{U}^\dagger(t,t_0) \hat{A} \hat{U}(t,t_0) | \varphi(t_0) \rangle$$

↳ two pictures:

Schrödinger picture: $|\varphi(t)\rangle$, $\hat{A}$ is constant
$|\varphi(t)\rangle = \hat{U}(t,t_0)|\varphi(t_0)\rangle$
$\hat{A} = cte$
} Schrödinger Equation

Heisenberg picture: $\hat{A}(t)$, $|\varphi\rangle$ is constant
$\hat{A}(t) = \hat{U}^\dagger(t,t_0)\hat{A}\hat{U}(t,t_0)$
$|\varphi\rangle = cte$
} Heisenberg's Equation of Motion

Show that:

$$i\hbar \frac{\partial \hat{A}(t)}{\partial t} = [\hat{A}(t), \hat{H}]$$

Heisenberg Inequalities

$$\Delta_\varphi \hat{A} = \hat{A} - \langle \hat{A} \rangle_\varphi$$

$$(\Delta_\varphi \hat{A})^2 = \hat{A}^2 + \langle \hat{A} \rangle^2 - 2\hat{A}\langle \hat{A} \rangle$$

↳ dispersion or variance

$$\langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2 \equiv \sigma_A^2$$

$$\sigma_A^2\sigma_B^2 \geq \frac{|\langle[\hat{A},\hat{B}]\rangle|^2}{4}$$

Anti-commutator

$$\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

Proof

$$\left.\begin{aligned}|\varphi_A\rangle &\equiv \Delta\hat{A}|\varphi\rangle \\ |\varphi_B\rangle &\equiv \Delta\hat{B}|\varphi\rangle\end{aligned}\right\} \quad \begin{aligned}\sigma_A^2 &= \langle\varphi_A|\varphi_A\rangle \\ \sigma_B^2 &= \langle\varphi_B|\varphi_B\rangle\end{aligned}$$

$$\sigma_A^2\sigma_B^2 = \langle\varphi_A|\varphi_A\rangle\langle\varphi_B|\varphi_B\rangle \geq |\langle\varphi_A|\varphi_B\rangle|^2 = \underbrace{\mathrm{Re}(\langle\varphi_A|\varphi_B\rangle)}_{\frac{1}{2}\langle\{\Delta\hat{A},\Delta\hat{B}\}\rangle_\varphi}{}^2 + \underbrace{\mathrm{Im}(\langle\varphi_A|\varphi_B\rangle)}_{\frac{1}{2}\langle[\hat{A},\hat{B}]\rangle_\varphi}{}^2$$

$$= \frac{1}{4}\langle\{\Delta\hat{A},\Delta\hat{B}\}\rangle^2 + \frac{1}{4}\langle[\hat{A},\hat{B}]\rangle^2$$

$$\geq \frac{1}{4}\langle[\hat{A},\hat{B}]\rangle^2$$

Temporal Heisenberg Inequalities

↳ something is odd: time is not an operator

Let $\hat{A}$ be any observable and $\hat{H}$ be the hamiltonian

$$\sigma_A^2\sigma_H^2 \geq \frac{\langle\varphi|[\hat{A},\hat{H}]|\varphi\rangle^2}{4} \underset{\text{Heisenberg picture}}{=} \frac{\hbar^2}{4}\left|\langle\varphi|\frac{\partial\hat{A}}{\partial t}|\varphi\rangle\right|^2$$

uncertainty on energy

$$\Delta E\,\tau \geq \frac{\hbar}{2}$$

"typical time for the process to occur"

$$\frac{1}{\tau_A} \equiv \frac{\left|\langle\frac{\partial\hat{A}}{\partial t}\rangle\right|}{\sigma_A} \Rightarrow \tau_A\,\sigma_H \geq \frac{\hbar}{2}$$

Malus' Law

Polarized EM wave $\hat{E}$, polarimeter $\hat{n}$

direction of polarization

$$I_{after} = I_{before}\underbrace{(\hat{E}\cdot\hat{n})^2}_{\cos^2(\theta_{\hat{E},\hat{n}})}$$

QM: polarization has 2 independent states

↳ let $|E_x\rangle$, $|E_y\rangle$

↳ $\mathcal{H} = \mathbb{C}^2$

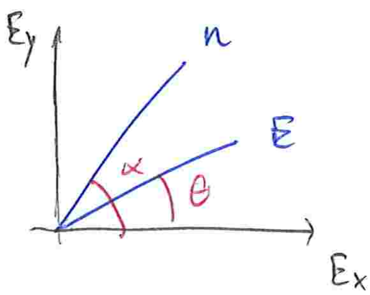
$$\left.\begin{aligned}\hat{P}|E_x\rangle &= |E_x\rangle \\ \hat{P}|E_y\rangle &= |E_y\rangle\end{aligned}\right\}$$ $\hat{P}$ is the polarization observable

Polarimeter $\hat{n}$: $\hat{P} = |\hat{n}\rangle\langle\hat{n}|$ → $|n\rangle = \cos\alpha\,|E_x\rangle + \sin\alpha\,|E_y\rangle$

Polarized photon: $|E\rangle = \cos\theta\,|E_x\rangle + \sin\theta\,|E_y\rangle$

photon → polarimeter ⟨ passes / doesn't pass } we can only compute the probability of passing or not

$$p = |\langle E|n\rangle|^2$$
$$= |(\cos\theta\,\langle E_x| + \sin\theta\,\langle E_y|)(\cos\alpha\,|E_x\rangle + \sin\alpha\,|E_y\rangle)|^2$$
$$= |\cos\theta\cos\alpha + \sin\theta\sin\alpha|^2$$
$$= |\cos(\theta-\alpha)|^2$$
$$= \cos^2(\theta-\alpha)$$



↳ Malus' Law → the postulates are explaining nature so far

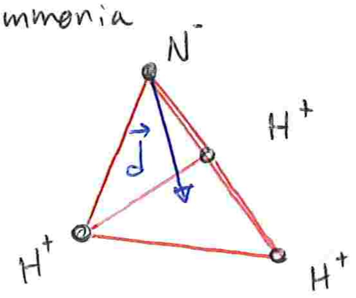
Systems With Finite Number of States

NH_3 Ammonia → 4 nuclei and 3·1+7 electrons → very hard

C_6H_6 Benzene

Nevertheless, we can describe some properties of the molecule

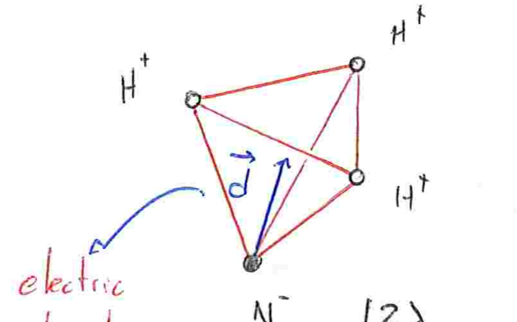
Ammonia



$|1\rangle$

state one

nitrogen is above the H plane



$|2\rangle$

state two

$\vec{E} = \vec{0}$ (no electric field) - Can we obtain a hamiltonian?

$$\begin{cases} \langle 1|\hat{H}|1\rangle = E_0 \\ \langle 2|\hat{H}|2\rangle = E_0 \\ \langle 1|\hat{H}|2\rangle = -A \quad , \quad A > 0 \\ \langle 2|\hat{H}|1\rangle = -A \end{cases}$$

symmetry

N can jump to beneath the plane for reasons we will see on the future and it is observed experimentally

follows from $\langle 1|\hat{H}|2\rangle = -A$ due to symmetry or hermiticity of $\hat{H}$

$$\hat{H} = \begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix}$$

Time evolution: $|\psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}} |\psi(0)\rangle$

spectral decomp.

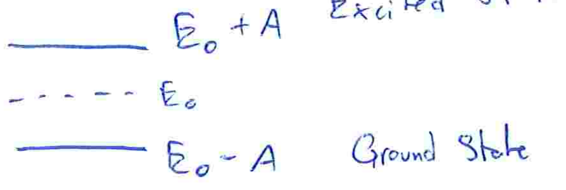
expand in stationary states

Spectral Decomposition of $\hat{H}$

i) eigenvalues

$\det(\hat{H} - \lambda) = 0$

$\lambda_{\pm} = E_0 \pm A$



ii) eigenvectors

$$|E_0 - A\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ +1 \end{pmatrix}, \quad |E_0 + A\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} +1 \\ 1 \end{pmatrix}$$

$\boxed{\text{ERRATA: the eigenvectors are swapped}}$

$$\hat{H} = (E_0 - A)\,|E_0 - A\rangle\langle E_0 - A| + (E_0 + A)\,|E_0 + A\rangle\langle E_0 + A|$$

$$|E_0 - A\rangle\langle E_0 - A| = \frac{1}{2}\begin{pmatrix} -1 \\ 1 \end{pmatrix}\begin{pmatrix} -1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$|E_0 + A\rangle\langle E_0 + A| = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\hat{H} = \frac{E_0 - A}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + \frac{E_0 + A}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\therefore\ e^{-\frac{i\hat{H}t}{\hbar}} = \frac{1}{2}\, e^{-\frac{i(E_0 - A)t}{\hbar}}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + \frac{1}{2}\, e^{-\frac{i(E_0 + A)t}{\hbar}}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$= e^{-\frac{iE_0 t}{\hbar}}\begin{bmatrix} \cos\left(\frac{At}{\hbar}\right) & i\sin\left(\frac{At}{\hbar}\right) \\ -i\sin\left(\frac{At}{\hbar}\right) & \cos\left(\frac{At}{\hbar}\right) \end{bmatrix}$$

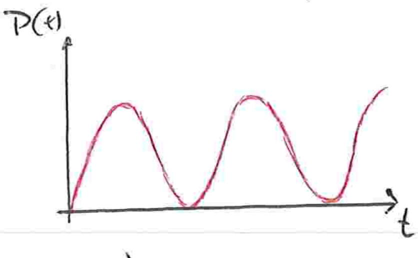
Suppose $|\psi(0)\rangle = |1\rangle$

$$P(t) = |\langle 2|\psi(t)\rangle|^2$$

$$= \left|(0,\ 1)\, e^{-\frac{iE_0 t}{\hbar}}\begin{pmatrix} \cos & i\sin \\ -i\sin & \cos \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right|^2$$

$$= \left|(0\ \ 1)\begin{pmatrix} \cos \\ -i\sin \end{pmatrix}\right|^2$$

$$= \sin^2\left(\frac{At}{\hbar}\right)$$

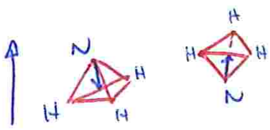


measuring the oscillation period allows us to obtain the parameter A

$\vec{E} \neq \vec{0}$ (presence of an electric field)

$$\Delta H = -\vec{d}\cdot\vec{E}$$

$\vec{E}$



→ we suppose $\vec{E}$ is perpendicular to the hidrogen plane

$|1\rangle$: $E_0 + d\mathcal{E}$

$|2\rangle$: $E_0 - d\mathcal{E}$

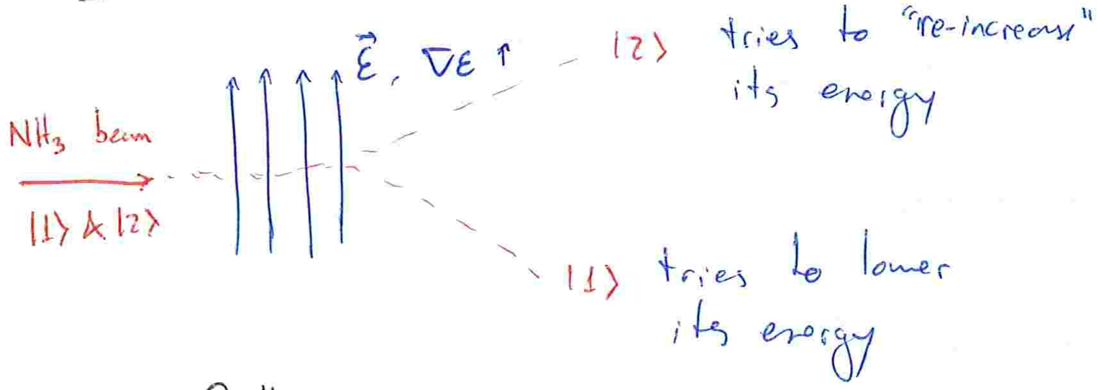
$$\hat{H} = \begin{bmatrix} E_0 + d\mathcal{E} & -A \\ -A & E_0 - d\mathcal{E} \end{bmatrix}$$

→ we lost the symmetry

↳ a new computation is necessary

$\vec{\mathcal{E}} \neq \vec{0}$ can be used to seperate $|1\rangle$ from $|2\rangle$!

$$\Delta H = -d\mathcal{E} \rightarrow \vec{F} = d\,\nabla\mathcal{E}$$



Ethylene C_2H_4

$H_2C=CH_2$

Bonds

σ-electrons
→ skeleton of the bond
→ "fixed"

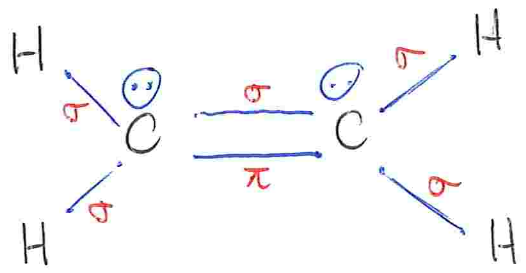
π-electrons
→ can jump from on atom to the next one

Pauli Principle: at most two electrons for all states

Electron Structure of C_2H_4

	C	H
2p	↑↑	
2s	↑↓	
1s	↑↓	↑

secluded (don't participate in bond)



$|\varphi_1\rangle$ π-electron on the left

$|\varphi_2\rangle$ π-electron on the right

$$\hat{H} = \begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix}$$

for every π-electron

Same as for the ammonia molecule

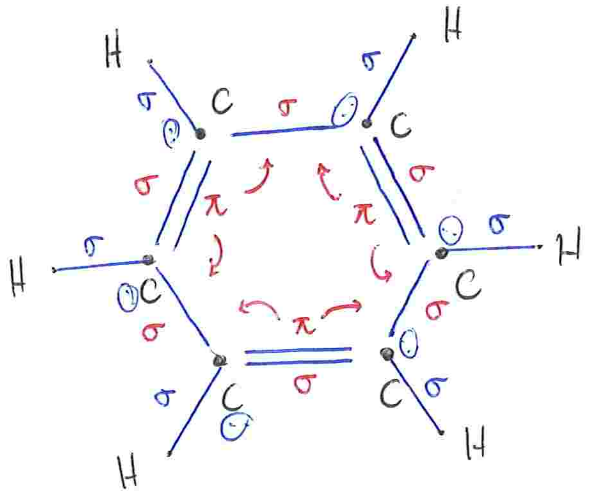
Complete hamiltonian of 2 π-electrons

$$\hat{H}_{tot} = \underbrace{\hat{H}}_{e^- 1} + \underbrace{\hat{H}}_{e^- 2} + \cancel{\hat{H}_{int}}$$

we assume the interaction hamiltonian is small

$$\underbrace{E^{tot}_{GS}}_{\text{ground state}} \simeq 2(E_0 - A)$$

Benzene C_6H_6



since π-electrons can jump around, the location of the double bonds changes over time

6 π-electrons

non-interacting: $E^{tot}_{GS} \simeq 6(E_0 - A)$ however...

$$E^{exp}_{GS} \simeq 6E_0 - 8A$$

we are neglecting the chain structure

N-atom chain

π-electrons: $|\varphi_0\rangle, |\varphi_1\rangle, \ldots, |\varphi_{N-1}\rangle$

Hamiltonian:

$$\langle\varphi_m|\hat{H}|\varphi_n\rangle = E_0\delta_{mn} - A(\delta_{m+1,n} + \delta_{m,n+1})$$

$$\hat{H} = E_0 \mathbb{1} - A(\hat{U} + \hat{U}')$$

$$\langle \varphi_i | \hat{U} | \varphi_k \rangle = \delta_{i,k+1} \Rightarrow \hat{U}|\varphi_i\rangle = |\varphi_{i+1}\rangle$$

$$\langle \varphi_i | \hat{U}' | \varphi_k \rangle = \delta_{i+1,k} \Rightarrow \hat{U}'|\varphi_i\rangle = |\varphi_{i-1}\rangle$$

$$\langle \varphi_i | \varphi_i \rangle = \langle \varphi_{i-1} | \underbrace{\hat{U}^\dagger \hat{U}}_{\text{has to be } \mathbb{1}} | \varphi_{i-1} \rangle = 1 = \langle \varphi_{i-1} | \varphi_{i-1} \rangle$$

$$\hat{U}' |\varphi_i\rangle = |\varphi_{i-1}\rangle$$

$$\underbrace{\hat{U}\hat{U}'}_{\mathbb{1}} |\varphi_i\rangle = |\varphi_i\rangle$$

$$\hat{U}' = \hat{U}^\dagger$$

NOTATION ERRATA.
From now on,
$\hat{U}^\dagger$ raises
$\hat{U}$ lowers

Periodicity: $|\varphi_{i+N}\rangle = |\varphi_i\rangle$
$$= \underbrace{\hat{U}^N}_{\mathbb{1}} |\varphi_{i+N}\rangle$$

for every unitary operator

$$[\hat{U}, \hat{U}^\dagger] = 0$$

$$\Downarrow \quad \hat{H} = E_0 \mathbb{1} - A(\hat{U} + \hat{U}^\dagger)$$

$$[\hat{U}, \hat{H}] = 0$$

common eigenbasis

$\downarrow$

study $\hat{U}$

$\hat{U}$ is unitary: $\lambda = e^{i\alpha_n}$

$\hat{U}^N = \mathbb{1}$: $\left(e^{i\alpha_n}\right)^N = 1$

$$\alpha_n = \frac{2n\pi}{N}$$

eigenvectors

$$|\alpha_n\rangle = \sum_{m=0}^{N-1} C_m^n |\varphi_m\rangle$$

$$\hat{U}|\alpha_n\rangle = e^{i\alpha_n}|\alpha_n\rangle$$

$$\hat{U}\sum_{m=0}^{N-1} C_m^n |\varphi_m\rangle = e^{i\frac{2\pi n}{N}} \sum_{m=0}^{N-1} C_m^n |\varphi_m\rangle$$

$$= \sum_m C_m^n |\varphi_{m-1}\rangle$$

$$= \sum_m C_{m+1}^n |\varphi_m\rangle$$

$$C_{m+1}^n = e^{i\frac{2\pi n}{N}} C_m^n$$

$$C_{m+1}^n = \left(e^{i\frac{2\pi n}{N}}\right)^{m+1} C_0^n$$

$$|\alpha_n\rangle = \sum_m \left(e^{i\frac{2\pi n}{N}}\right)^m C_0^n |\varphi_m\rangle$$

normalization: $C_0^n = \frac{1}{\sqrt{N}}$

common eigenvectors for $\hat{U}$ and $\hat{H} = E_0 \mathbb{1} - A(\hat{U} + \hat{U}^\dagger)$

$$\hat{H}|\alpha_n\rangle = \left[E_0 - A\left(e^{i\frac{2\pi n}{N}} + e^{-i\frac{2\pi n}{N}}\right)\right]|\alpha_n\rangle$$

$$= \underbrace{\left[E_0 - 2A\cos\left(\frac{2\pi n}{N}\right)\right]}_{\text{energy}}|\alpha_n\rangle$$

Benzene $N = 6$

	$n=0$	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
energy	$E_0 - 2A$	$E_0 - A$	$E_0 + A$	$E_0 + 2A$	$E_0 + A$	$E_0 - A$
π-electrons	↑↓	↑↓				↑↓

$$E = 2\cdot(E_0 - 2A) + 4\cdot(E_0 - A) = 6E_0 - 8A$$

Time - Independent Perturbation Theory

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{unperturbed Hamiltonian}} + \underbrace{\epsilon}_{\text{small adimensionless parameter}} \hat{V}$$

we want to make a Taylor expansion

$$\hat{H}_0 |n_0\rangle = \underbrace{E_n^0 |n_0\rangle}_{\text{known}}$$

$$\hat{H}|n\rangle = E_n |n\rangle$$

$$\left.\begin{cases} E_n = E_n^0 + \epsilon E_n^1 + \epsilon^2 E_n^2 + \cdots \\ |n\rangle = |n_0\rangle + \epsilon |n_1\rangle + \epsilon^2 |n_2\rangle + \cdots \end{cases}\right\} \text{ansatz}$$

$$(\hat{H}_0 + \epsilon \hat{V})(|n_0\rangle + \epsilon |n_1\rangle + \cdots) = (E_n^0 + \epsilon E_n^1 + \cdots)(|n_0\rangle + \epsilon |n_1\rangle + \cdots)$$

$\mathcal{O}(\epsilon^0)$: $\hat{H}_0 |n_0\rangle = E_n^0 |n_0\rangle$ unperturbed equation → already solved

$\mathcal{O}(\epsilon^1)$: $\hat{H}_0 \underbrace{|n_1\rangle}_{\text{unknown}} + \hat{V}|n_0\rangle = E_n^0 \underbrace{|n_1\rangle}_{\text{unknown}} + \underbrace{E_n^1}_{\text{unknown}} |n_0\rangle$

$\mathcal{O}(\epsilon^2)$: we need to consider all of the terms of order ϵ^2, and our initial expression doesn't contain them → list of exercises

↳ we should write
$$E = E_n^0 + \epsilon E_n^1 + \epsilon^2 E_n^2 + \cdots$$
instead of
$$E = E_n^0 + \epsilon E_n^1 + \cdots$$

$$|n_1\rangle = \sum_m C_m^1 |m_0\rangle$$ → $|n_1\rangle \in \mathcal{H}$ and $\{|m_0\rangle\}$ is a basis for the Hilbert space

$$(\hat{H}_0 - E_n^0)|n_1\rangle = (E_n^1 - \hat{V})|n_0\rangle$$

$$\sum_m C_m^1 (\hat{H}_0 - E_n^0)|m_0\rangle = (E_n^1 - \hat{V})|n_0\rangle$$

$$\sum_m C_m^1 (E_m^0 - E_n^0)|m_0\rangle = (E_n^1 - \hat{V})|n_0\rangle$$

$\langle n_0|$

$$\sum_m C_m^1 (E_m^0 - E_n^0)\langle n_0|m_0\rangle = (E_n^1 - \langle n_0|\hat{V}|n_0\rangle)$$

$$C_n^1 (E_n^0 - E_n^0) = 0 = E_n^1 - \langle n_0|\hat{V}|n_0\rangle$$

$$E_n^1 = \langle n_0|\hat{V}|n_0\rangle$$

$\langle k_0|$, $k \neq n$

$$\sum_m C_m^1 (E_m^0 - E_n^0)\overbrace{\langle k_0|m_0\rangle}^{\delta_{km}} = E_n^1 \overbrace{\langle k_0|n_0\rangle}^{0} - \langle k_0|\hat{V}|n_0\rangle$$

$$C_k^1 (E_k^0 - E_n^0) = -\langle k_0|\hat{V}|n_0\rangle$$

$$C_k^1 = -\frac{\langle k_0|\hat{V}|n_0\rangle}{E_k^0 - E_n^0}$$

$$= \frac{\langle k_0|\hat{V}|n_0\rangle}{E_n^0 - E_k^0}, \quad k \neq n$$

We still don't know C_n^1.

$$|n\rangle = |n_0\rangle + \epsilon \sum_{k\neq n} \frac{\langle k_0|\hat{V}|n_0\rangle}{E_n^0 - E_k^0} |k_0\rangle + \epsilon C_n^1 |n_0\rangle .$$

we demand

normalization up to first order

$$\langle n|n\rangle = 1 + \Theta(\epsilon^2)$$

$$= 1 + \epsilon \underbrace{\left(C_n^1 + C_n^{1*}\right)}_{0} + \Theta(\epsilon^2)$$

always possible, for states are defined up to a phase

If we choose the phase of $|n_0\rangle$ in a manner such that $C_n^1 \in \mathbb{R}$, it follows that $C_n^1 = 0$.

$$\begin{cases} E_n = E_n^0 + \epsilon \langle n_0|\hat{V}|n_0\rangle + \dots \\ |n\rangle = |n_0\rangle + \epsilon \sum_{m\neq n} \frac{\langle m_0|\hat{V}|n_0\rangle}{E_n^0 - E_m^0} |m_0\rangle + \dots \end{cases}$$

what about the degenerate case?

Degenerate Spectrum

Suppose $\hat{H}_0$ has a degenerate subspace $\mathcal{H}_Q$, $|n_{Q_1}\rangle, \dots, |n_{Q_d}\rangle$ all with eigenvalue E_Q^0

$$\hat{H} = \hat{H}_0 + \epsilon \hat{V} = \underbrace{\left(\hat{H}_0 + \epsilon \hat{V}_Q\right)}_{\hat{H}_0'} + \epsilon \hat{V}'$$

$$\hat{V} = \sum_{m,n} \hat{V}_{mn} |m_0\rangle\langle n_0|$$

solve analytically for $\hat{H}_0'$ and do perturbation theory for $\hat{V}'$

$$\hat{V}_Q = \sum_{m,n\in Q} V_{mn} |m_0\rangle\langle n_0| , \qquad \hat{V}' = \hat{V} - \hat{V}_Q$$

Example

$$\hat{H} = \underbrace{\begin{bmatrix} A_0 & & \\ & A_0 & \\ & & B_0 \end{bmatrix}}_{\hat{H}_0} + \epsilon \underbrace{\begin{bmatrix} 0 & \xi_1 & \xi_2 \\ \xi_1 & 0 & 0 \\ \xi_2 & 0 & 0 \end{bmatrix}}_{\hat{V}}$$

$\hookrightarrow |A_0^1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

$|A_0^2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

$|B_0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$$\hat{V}_Q = \begin{bmatrix} 0 & \xi_1 & 0 \\ \xi_1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \Rightarrow \hat{V}' = \hat{V} - \hat{V}_Q = \begin{bmatrix} 0 & 0 & \xi_2 \\ 0 & 0 & 0 \\ \xi_2 & 0 & 0 \end{bmatrix}$$

New unperturbed Hamiltonian

$$\hat{H}_0 = \hat{H}_0 + \epsilon \hat{V}_Q = \begin{bmatrix} A_0 & \epsilon\xi_1 & 0 \\ \epsilon\xi_1 & A_0 & 0 \\ 0 & 0 & B_0 \end{bmatrix}$$

$|A_0 + \epsilon\xi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$

$|A_0 - \epsilon\xi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$

$|B_0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

no longer degenerate

$\hookrightarrow$ If still degenerate due to B_0, perturbation theory won't work

Time Dependent Perturbation Theory

sometimes called interaction $\rightarrow$ common in QFT

$$\hat{H} = \hat{H}_0 + \epsilon \hat{V}(t)$$

$\hookrightarrow \hat{H}_0 |n_0\rangle = E_n^0 |n_0\rangle$

$\{|n_0\rangle\}$ is an orthonormal basis for $\mathcal{H}$

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

Interaction Picture $\rightarrow$ AKA Dirac Picture

$$|\psi(t)\rangle = \sum_n c_n(t)|n_0\rangle$$

$\downarrow \epsilon \to 0$

$$c_n(t) \to e^{-\frac{iE_n^0 t}{\hbar}} c_n(0)$$

Idea:

$$c_n(t) \equiv e^{-\frac{iE_n^0 t}{\hbar}} \gamma_n(t) = e^{-i\omega_n^0 t}\gamma_n(t)$$

$$\omega_n^0 \equiv \frac{E_n^0}{\hbar}$$

$$|\psi_S(t)\rangle = \sum_n e^{-i\omega_n^0 t}\, \gamma_n(t)\, |n_0\rangle$$

S stands for Schrödinger

$$= \sum_n e^{-\frac{i\hat{H}_0 t}{\hbar}}\, \gamma_n(t)\, |n_0\rangle$$

$$= \underbrace{e^{-\frac{i\hat{H}_0 t}{\hbar}}}_{\hat{U}_0} \underbrace{\sum_n \gamma_n(t)\, |n_0\rangle}_{|\psi_I(t)\rangle}$$

I stands for interaction

States Interaction Picture: $|\psi_S(t)\rangle = \hat{U}_0\, |\psi_I(t)\rangle$

Operators Interaction Picture:

$$\langle \hat{A}(t)\rangle_\varphi = \langle \varphi_S(t)|\, \hat{A}_S\, |\varphi_S(t)\rangle$$

$$= \langle \varphi_I(t)|\, \underbrace{\hat{U}_0^\dagger\, \hat{A}_S\, \hat{U}_0}_{\hat{A}_I(t)}\, |\varphi_I(t)\rangle$$

$$\hat{A}_I(t) = \hat{U}_0^\dagger\, \hat{A}_S\, \hat{U}_0$$

Equation of Motion in the Interaction Picture (Exercise)

$$i\hbar \frac{\partial |\psi_I(t)\rangle}{\partial t} = \epsilon\, \hat{V}_I(t)\, |\psi_I(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \hat{A}_I(t) = [\hat{A}_I(t), \hat{H}_0]$$

Therefore, we have

$$\begin{cases} |\psi_I(t)\rangle = \sum_n \gamma_n(t)\, |n_0\rangle \\ i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = \epsilon\, \hat{V}_I(t)\, |\psi_I(t)\rangle \end{cases}$$

$$i\hbar \sum_n \dot{\gamma}_n(t)\, |n_0\rangle = \epsilon\, \hat{V}_I(t) \sum_m \gamma_m(t)\, |m_0\rangle$$

$\langle k_0|$

$$i\hbar\, \dot{\gamma}_k = \epsilon \sum_m \gamma_m\, \langle k_0|\, \underbrace{\hat{V}_I(t)}_{\hat{U}_0^\dagger \hat{V}(t) \hat{U}_0}\, |m_0\rangle$$

$$\hat{U}_0 |m_0\rangle = e^{-\frac{i\hat{H}_0 t}{\hbar}} |m_0\rangle = e^{-i\omega_m^0 t} |m_0\rangle$$

$$\langle k_0 | \hat{U}_0^\dagger = e^{i\omega_k^0 t} \langle k_0 | \quad \dagger$$

$$i\hbar \dot{\gamma}_k = \epsilon \sum_m \gamma_m e^{i(\omega_k^0 - \omega_m^0)t} \langle k_0 | \hat{V}(t) | m_0 \rangle$$

Example

$\underbrace{\text{Spin } 1/2 \text{ particle}}_{\text{magnetic moment}}$ in a periodic $\vec{B}$ field

$$\vec{\mu} = \frac{1}{2} \hat{\gamma} \hbar \vec{\sigma}$$

gyromagnetic factor

electron $\hat{\gamma}_e = -\frac{e}{2m_e}$ $\quad$ ${}^{13}C$ $\hat{\gamma}_c = 1.40 \frac{e}{2m_p}$

proton $\hat{\gamma}_p = 5.59 \frac{e}{2m_e}$ $\quad$ ${}^{19}F$ $\hat{\gamma}_F = 5.26 \frac{e}{2m_p}$

$$\hat{H} = -\vec{\mu} \cdot \vec{B}$$

$$\vec{B} = b_0 \hat{z} + b_1 (\cos\omega t\, \hat{x} - \sin\omega t\, \hat{y})$$

$\omega_0 = \hat{\gamma}_e b_0$ Larmor frequency

$\omega_1 = \hat{\gamma}_e b_1$ Rabi frequency

$$\hat{H} = -\frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_0 \end{pmatrix}$$

$$= -\frac{\hbar}{2} \begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix} - \frac{\hbar}{2}\omega_1 \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}$$

$$E \equiv \frac{\hbar \omega_0}{2}$$

$$\begin{cases} \hat{H}_0 = -\frac{\hbar\omega_0}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} -E & 0 \\ 0 & E \end{pmatrix} \\ \epsilon \hat{V} = -\frac{\hbar\omega_1}{2} \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \end{cases}$$

$$\hat{H}_0 : \quad |-E\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |E\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

From the time evolution ODE system for γ_k we have

$$i\hbar \dot{r}_1 = r_1 \underbrace{\cancel{e^{i(\omega_1^0-\omega_1^0)t}}}_{1} \underbrace{\cancel{\langle -E|e\hat{V}(t)|-E\rangle}}_{0} + r_2\, e^{\overbrace{i(\omega_1^0-\omega_2^0)}^{-\frac{2E}{\hbar}=-\omega_0}t} \overbrace{\langle -E|e\hat{V}(t)|+E\rangle}^{-\frac{\hbar\omega_1}{2}e^{i\omega t}}$$

$$i\hbar \dot{r}_2 = r_1\, e^{\underbrace{i(\omega_2^0-\omega_1^0)}_{\frac{2E}{\hbar}=\omega_0}t} \underbrace{\langle +E|e\hat{V}(t)|-E\rangle}_{-\frac{\hbar\omega_1}{2}e^{-i\omega t}} + r_2 \overbrace{\cancel{e^{i(\omega_2^0-\omega_2^0)}}}^{1} \overbrace{\cancel{\langle +E|e\hat{V}(t)|+E\rangle}}^{0}$$

$$-\frac{\hbar\omega_1}{2} = i\hbar A$$

$$\begin{cases} i\hbar\dot{r}_1 = i\hbar A\, e^{i(\omega-\omega_0)t}\, r_2 \\ i\hbar\dot{r}_2 = i\hbar A\, e^{-i(\omega-\omega_0)t}\, r_1 \end{cases}$$

$$\begin{cases} \dot{r}_1 = A\, e^{i(\omega-\omega_0)t}\, r_2 \\ \dot{r}_2 = A\, e^{-i(\omega-\omega_0)t}\, r_1 \end{cases}$$

$$z_{1,2} = \frac{i}{2}\left(\omega-\omega_0 \pm \Omega\right)$$

$$\Omega = \sqrt{(\omega-\omega_0)^2+\omega_1^2}$$

$$\begin{cases} r_1(t) = \alpha_1 e^{z_1 t} + \beta_1 e^{z_2 t} \\ r_2(t) = \dfrac{e^{-i(\omega-\omega_0)t}}{A}\left(\alpha_1 z_1 e^{z_1 t} + \beta_1 z_2 e^{z_2 t}\right) \end{cases}$$

Suppose $|\Psi(0)\rangle = |-E\rangle$. What is the probability of finding $|E\rangle$ after time t?

$$|\Psi(0)\rangle = r_1(0)\,|-E\rangle + r_2(0)\,|+E\rangle = |-E\rangle$$

$$\begin{cases} r_1(0) = 1 \\ r_2(0) = 0 \end{cases} \Rightarrow \begin{cases} \alpha_1 = \dfrac{\Omega-(\omega-\omega_0)}{2\Omega} \\ \beta_1 = \dfrac{\Omega+(\omega-\omega_0)}{2\Omega} \end{cases}$$

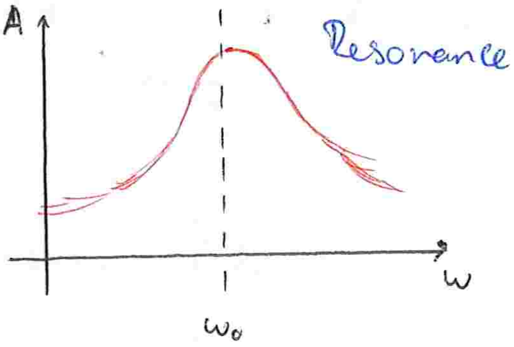
$$\begin{cases} r_1(t) = e^{\frac{i(\omega-\omega_0)t}{2}}\left[\cos\left(\frac{\Omega t}{2}\right) - i\,\frac{\omega-\omega_0}{\Omega}\sin\left(\frac{\Omega t}{2}\right)\right] \\ r_2(t) = e^{-\frac{i(\omega-\omega_0)t}{2}}\left[\frac{i\omega_1}{\Omega}\sin\left(\frac{\Omega t}{2}\right)\right] \end{cases}$$

FGFS001

$$P(t) = |\langle E|\psi(t)\rangle|^2 = \left|\langle E|\Big(\underbrace{r_1 e^{\frac{iEt}{\hbar}}|-E\rangle}_{0} + r_2 e^{-\frac{iEt}{\hbar}}|E\rangle\right|^2$$

$$= \frac{|r_2(t)|^2}{\langle\psi|\psi\rangle} = \frac{\omega_1^2}{\Omega^2\langle\psi|\psi\rangle}\sin^2\left(\frac{\Omega t}{2}\right)$$

$$= \frac{\omega_1^2}{(\omega-\omega_0)^2+\omega_1^2}\sin^2\left(\frac{\Omega t}{2}\right)\frac{1}{\langle\psi|\psi\rangle}$$



↳ applied in NMR

Nuclear Magnetic Resonance

Example 2

$$\hat{V}(t) = \hat{V}_0\ \theta(t)$$

Heaviside's θ

$$\theta(t) = \int_{-\infty}^{t}\delta(\tau)\,d\tau$$

↳ Dirac's delta

Perturbation Theory

$$i\hbar\dot{r}_n = \epsilon\sum_m r_m e^{i(\omega_n^0-\omega_m^0)t}\langle n_0|\hat{V}(t)|m_0\rangle$$

$$r_m(t) = r_m^0(t) + \epsilon r_m^1(t) + \epsilon^2 r_m^2(t) + \dots$$

$$i\hbar(\dot{r}_n^0 + \epsilon\dot{r}_n^1 + \dots) = \epsilon\sum_m(r_m^0 + \epsilon r_m^1 + \dots)e^{i(\omega_n^0-\omega_m^0)t}\langle n_0|\hat{V}(t)|m_0\rangle$$

$O(\epsilon^0)$: $\quad i\hbar\dot{r}_n^0 = 0 \Rightarrow r_n^0(t) = r_n^0(t_0)$

$O(\epsilon)$: $\quad i\hbar\dot{r}_n^1 = \sum_m r_m^0 e^{i(\omega_n^0-\omega_m^0)t}\langle n_0|\hat{V}(t)|m_0\rangle$

$$\begin{cases}\hat{V}(t) = \hat{V}_0\,\theta(t)\\ |\psi(0)\rangle = |n_0\rangle\end{cases}\qquad |\psi(t)\rangle = \sum_m r_m e^{-i\omega_m^0 t}|m_0\rangle$$

What is the probability of finding the system at $|m_0\rangle$, with $m\neq n$

Initial conditions $\begin{cases}r_m(0) = 0 & \text{when}\\ r_n(0) = 1 & m\neq n\end{cases} \Rightarrow r_m(0) = \delta_{mn}$

$$P(t) = |\gamma_m(t)|^2, \qquad \gamma_m(t) = \gamma_m^0(t_0) + \epsilon\, \gamma_m^1(t) + \dots$$

Integrating the ODE with $O(\epsilon)$

$$i\hbar\left(\gamma_m^1(t) - \gamma_m^1(t_0)\right) = \sum_k \gamma_k^0(t_0) \int_{t_0}^{t} e^{i(\omega_m^0 - \omega_k^0)\tau} \langle m_0|\hat{V}(\tau)|k_0\rangle \, d\tau$$

$$\gamma_m^1(t) = \gamma_m^1(t_0) + \frac{1}{i\hbar}\sum_k \gamma_k^0(t_0) \int_{t_0}^{t} e^{i(\omega_m^0 - \omega_k^0)\tau} \langle m_0|\hat{V}(\tau)|k_0\rangle \, d\tau$$

$$\gamma_m(t) = \gamma_m^0(t_0) + \epsilon\, \gamma_m^1(t_0) + \frac{\epsilon}{i\hbar}\sum_k \gamma_k^0(t_0) \int_{t_0}^{t} e^{i(\omega_m^0 - \omega_k^0)\tau} \langle m_0|\hat{V}(\tau)|k_0\rangle \, d\tau$$

Initial condition: $\gamma_m(0) = 0$ → I've already chosen that $m \neq n$

$$\gamma_m(0) = \gamma_m^0(0) + \epsilon\, \gamma_m^1(0) + \cancel{\frac{\epsilon}{i\hbar}\sum_k \gamma_k^0(0) \int_{0}^{0} e^{i(\omega_m^0 - \omega_k^0)\tau} \langle m_0|\hat{V}(\tau)|k_0\rangle \, d\tau} \to 0 \quad = 0$$

$$\therefore\ \gamma_m^0(0) + \epsilon\, \gamma_m^1(0) = 0$$

$$\gamma_m(t) = \frac{\epsilon}{i\hbar}\sum_k \gamma_k^0(0) \int_{0}^{t} e^{i(\omega_m^0 - \omega_k^0)\tau} \underbrace{\langle m_0|\hat{V}_0|k_0\rangle}_{\theta(\tau) = 1 \text{ for } \tau > 0} \, d\tau$$

$\theta(0)$ makes no difference

Notice that

$$\begin{aligned} \epsilon\, \gamma_m(0) &= \epsilon\left(\gamma_m^0(0) + \epsilon\, \gamma_m^1(0) + \dots\right) \\ &= \epsilon\, \gamma_m^0(0) \quad \text{up to order } \epsilon^2 \end{aligned}$$

$$\begin{aligned} \gamma_m(t) &= \frac{\epsilon}{i\hbar}\sum_k \gamma_k(0) \int_0^t e^{i(\omega_m^0 - \omega_k^0)\tau} d\tau \, \langle m_0|\hat{V}_0|k_0\rangle \\ &= \frac{\epsilon}{i\hbar}\sum_k \delta_{kn} \int_0^t e^{i(\omega_m^0 - \omega_k^0)\tau} d\tau \, \langle m_0|\hat{V}_0|n_0\rangle \end{aligned}$$

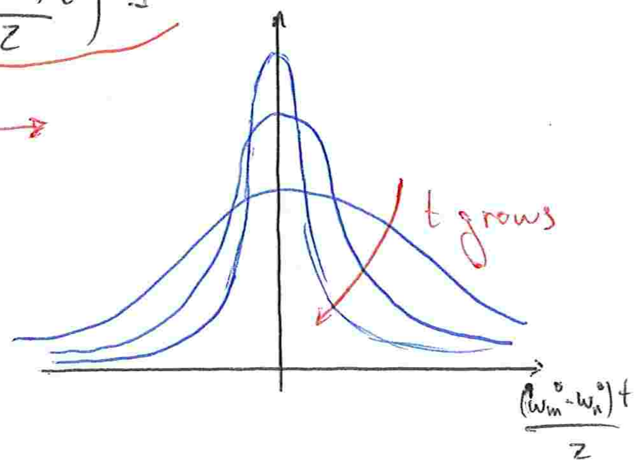
$$\gamma_m(t) = \frac{e}{i\hbar}\langle m_0|\hat{V}_0|n_0\rangle \int_0^t e^{i(\omega_m^0-\omega_n^0)\tau}\, d\tau$$

$$= \frac{\epsilon}{i\hbar}\langle m_0|\hat{V}_0|n_0\rangle \frac{e^{i(\omega_m^0-\omega_n^0)t}-1}{i(\omega_m^0-\omega_n^0)}$$

$$P(t) = |\gamma_m(t)|^2 = \frac{\epsilon^2}{\hbar^2}|\langle m_0|\hat{V}_0|n_0\rangle|^2 \left|\frac{e^{i(\omega_m^0-\omega_n^0)t}-1}{i(\omega_m^0-\omega_n^0)}\right|^2$$

$$= \frac{\epsilon^2}{\hbar^2}|\langle m_0|\hat{V}_0|n_0\rangle|^2 \left|\frac{2e^{i\frac{(\omega_m^0-\omega_n^0)t}{2}}}{(\omega_m^0-\omega_n^0)} \underbrace{\frac{\left(e^{\frac{i(\omega_m^0-\omega_n^0)t}{2}}-e^{-\frac{i(\omega_m^0-\omega_n^0)t}{2}}\right)}{2i}}_{\sin\left(\frac{(\omega_m^0-\omega_n^0)t}{2}\right)}\right|^2$$

$$= \frac{2\pi}{\hbar^2}|\langle m_0|\epsilon\hat{V}_0|n_0\rangle|^2 \underbrace{\left[\frac{1}{2\pi}\frac{\sin^2\left(\frac{(\omega_m^0-\omega_n^0)t}{2}\right)}{\left(\frac{(\omega_m^0-\omega_n^0)t}{2}\right)^2}t\right]}\, t$$



$$\xrightarrow{\text{large time}} \frac{2\pi}{\hbar^2}|\langle m_0|\epsilon\hat{V}_0|n_0\rangle|^2\,\delta(\omega_m^0-\omega_n^0)\,t$$

$$\Gamma = \lim_{t\to+\infty}\frac{P(t)}{t} = \frac{2\pi}{\hbar^2}|\langle m_0|\epsilon\hat{V}_0|n_0\rangle|^2\,\delta(\omega_m^0-\omega_n^0)$$

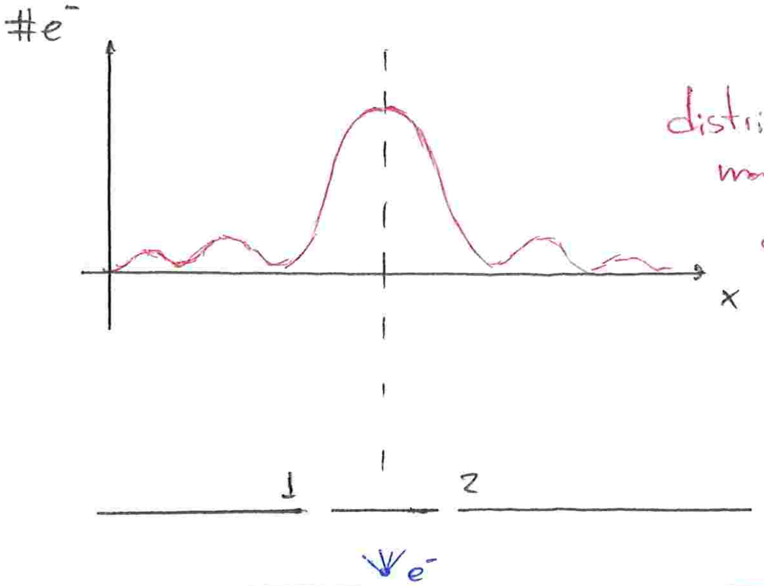
↳ Fermi's Golden Rule

Path Integral Formalism → $\boxed{\text{Finitistic Math}}$

↳ we'll follow Feynman-Hibbs → from PI to Schrödinger's

↳ other options: Gottfried, Weinberg, Sakurai

Double Slit Experiment



distribution of many electrons over a large time

diffraction pattern

$I(x) \propto |E_1(x) + E_2(x)|^2$

the pattern comes from the interference

QM: probability density

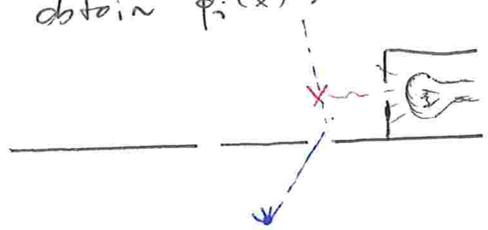
$\#e^- \propto P(x)$

$P(x) = |\phi_1(x) + \phi_2(x)|^2$

$\phi_i(x)$ are probability amplitudes

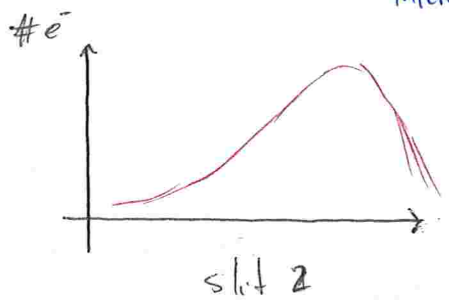
complex

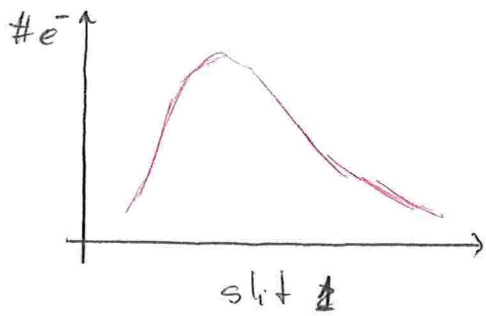
How do we obtain $\phi_i(x)$?



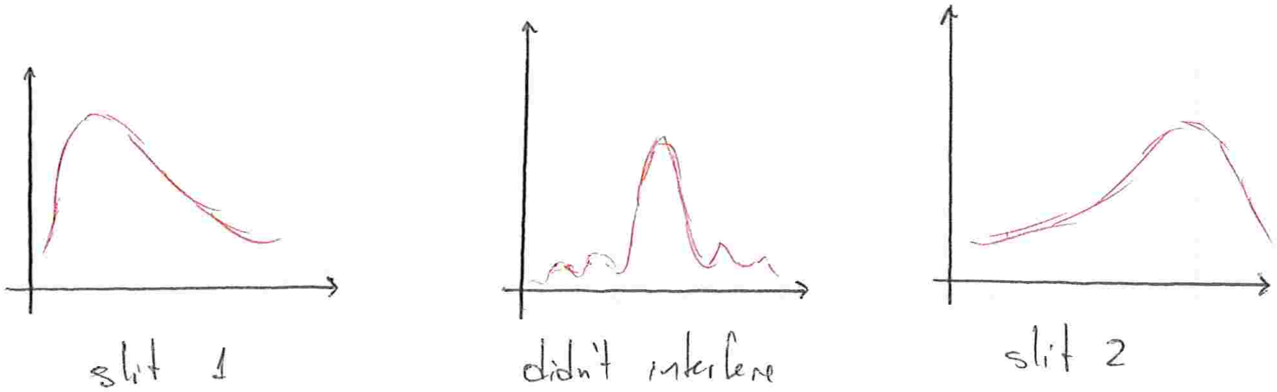
we measure the positions of the electrons so we know the probability amplitudes

Strong Lamp every electron is ~~hit~~ intercepted by a photon





Weak Lamp $\rightsquigarrow$ some electrons are not intercepted



Conclusion: probability must be computed summing the $\phi_i(x)$ of all the possible paths that are not experimentally resolved

↳ must sum over all possible interfering probabilities

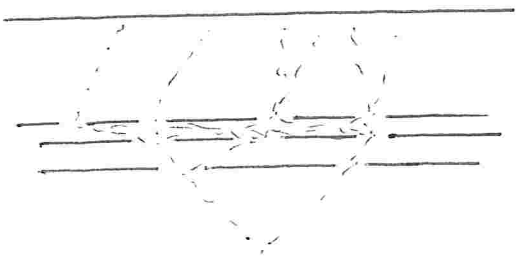
$\{\phi_i(x)\}_i$ probability amplitudes not resolved

$$P(x) = \left|\sum_i \phi_i(x)\right|^2$$

If I know the trajectory sum only over that trajectory

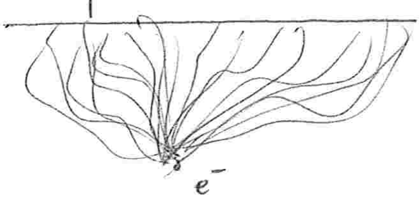
If I don't sum over all the possible paths

More Slits



the idea still holds

We can keep on adding screens and slits, we eventually have effectively no slits and no screens



→ sum over all possible paths the electron can take

$$\sum_{\text{paths}} \phi(x(t)) \equiv K(b|a)$$

→ ends at b

→ starts at a

↳ propagator/kernel/Green function

$$P(a\to b) = |K(b|a)|^2$$

what is the probability amplitude?

$$\phi(x) = \text{cte}\cdot e^{\frac{iS[x]}{\hbar}}$$

stands as a postulate for the Path Integral formulation

$$S[x] = \int_{t_a}^{t_b} L(\dot{x}(\tau), x(\tau))\, d\tau$$

Take a path for which $S[x] \gg \hbar$

Saddle Point / Steepest-descent

$$\int e^{if(x)/\epsilon} dx, \quad \epsilon \ll 1$$

$$\int e^{if(x)/\epsilon} dx \sim I(x_0)$$

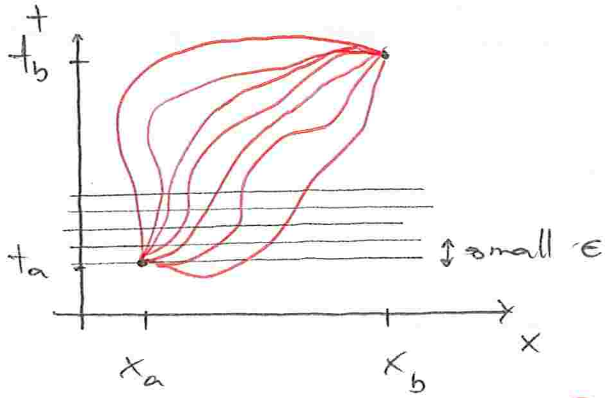
integral close to $f'(x_0)=0$ is all the relevance

The sum will leave as relevant only the region in which $S[x]$ is stationary $\Rightarrow$ classical path

↳ paths with $S[x]$ small contribute very little to the sum

How to sum over paths

$d=1$



calculate from a time slice to the next one and sum over all possibilities

$K(x_{i+1}, t_i+\epsilon \mid x_i, t_i)$

Suppose we can compute $K(i+1|i)$

$$\lim_{\epsilon\to 0} \int K(b|b-1)\dots K(a+2|a+1)\,K(a+1|a)\,dx_{a+1}\dots dx_{b-1} = K(b|a)$$

How to get $K(i+1|i)$?

$$K(i+1|i) = A\, e^{\frac{i}{\hbar}\int_{t_i}^{t_i+\epsilon} L(\dot{x},x)\,d\tau} = A\, e^{\frac{i}{\hbar}\epsilon L\left[\frac{x_{i+1}-x_i}{\epsilon},\ \frac{x_{i+1}+x_i}{2}\right]}$$

A ↳ constant

↳ to be determined

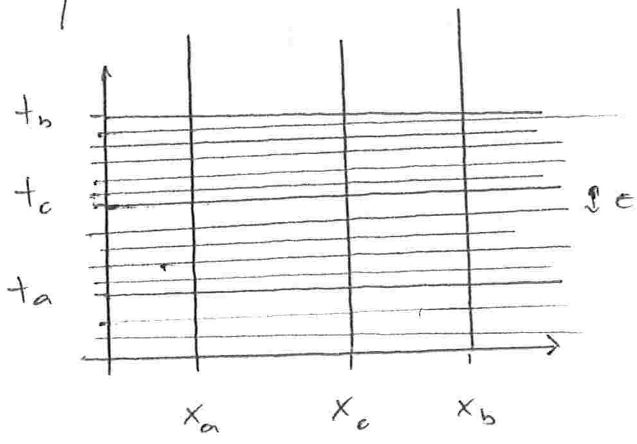
$$K(b|a) = \lim_{\epsilon\to 0}\int A^N \underbrace{e^{\frac{i}{\hbar}\epsilon L_{a+1,a}}\, e^{\frac{i}{\hbar}\epsilon L_{a+2,a+1}} \dots e^{\frac{i}{\hbar}\epsilon L_{b,b-1}}}_{e^{\frac{i}{\hbar}\int_{t_a}^{t_b} L\,dt}}\, dx_{a+1}\dots dx_{b-1}$$

$$= \underbrace{\int e^{\frac{i}{\hbar}S[x(t)]}\,\mathcal{D}x(t)}_{\text{path integral}}$$

weird measure in which we hide all the mathematical problems

General Properties

01. Composition Property



$$K(c|a) = \int K(a+1|a) \cdots K(c|c-1)\, dx_{a+1} \cdots dx_{c-1}$$

$$K(b|c) = \int K(c+1|c) \cdots K(b|b-1)\, dx_{c+1} \cdots dx_{b-1}$$

$$K(b|a) = \int K(a+1|a) \cdots K(b|b-1)\, dx_{a+1} \cdots dx_{c-1}\, dx_c\, dx_{c+1} \cdots dx_{b-1}$$

$$= \int K(c|a)\, K(b|c)\, dx_c$$

Wave function

Total amplitude to get to point (x,t) from the past

→ usually denoted as $\psi(x,t)$

→ also a kernel

$$\psi(b) = \int_{\mathbb{R}} K(b|c)\, \psi(c)\, dx_c$$

→ it is also indeed a Green function and a ~~propagator~~

→ as in QFT

→ the kernel is actually a kernel

Schrödinger Equation

$\psi(x, t+\epsilon)$, $\frac{\epsilon}{t} \ll 1$

mechanical system

$$L = \frac{m\dot{x}^2}{2} - V$$

$$\psi(x, t+\epsilon) = \int \underbrace{K(x,t+\epsilon | y,t)}_{A e^{\frac{i}{\hbar}\epsilon L\left(\frac{x-y}{\epsilon}, \frac{x+y}{2}\right)} = A e^{\frac{i}{\hbar}\epsilon\left[\frac{m(x-y)^2}{2\epsilon^2} - V\left(\frac{x+y}{2}\right)\right]}} \psi(y)\, dy$$

$$\psi(x,t) + \epsilon \frac{\partial \psi}{\partial t} = \int A e^{\frac{i}{\hbar}\left[\frac{m(x-y)^2}{2\epsilon} - \epsilon V\left(\frac{x+y}{2}\right)\right]} \psi(y,t)\, dy$$

change of variables: $y = x + \eta$

$$\psi(x,t) + \epsilon \frac{\partial \psi}{\partial t} = \int A\, e^{\frac{i}{\hbar}\left[\frac{m\eta^2}{2\epsilon} - \epsilon V\left(x + \frac{\eta}{2}\right)\right]} \psi(x+\eta, t)\, d\eta$$

$$\psi(x,t) + \epsilon \frac{\partial \psi}{\partial t} = \int A\, \underbrace{e^{\frac{i}{\hbar}\frac{m\eta^2}{2\epsilon}}}_{\text{averages to zero, except when } \eta^2 \sim \epsilon} e^{-\frac{i}{\hbar}\epsilon V\left(x + \frac{\eta}{2}\right)} \psi(x+\eta, t)\, d\eta$$

→ we may expand in η

$$\psi(x,t) + \epsilon \frac{\partial \psi}{\partial t} = A \int e^{\frac{im\eta^2}{2\epsilon}} \left(1 - \epsilon \frac{i}{\hbar} V\right)\left(\psi(x,t) + \eta \frac{\partial \psi}{\partial x} + \eta^2 \frac{\partial^2 \psi}{\partial x^2}\right) d\eta$$

Solve order by order in ϵ (equiv η^2)

$\mathcal{O}(\epsilon^0)$: $\quad \psi(x,t) = A \int e^{\frac{im\eta^2}{2\epsilon}} d\eta\, \psi(x,t)$

$$A = \sqrt{\frac{m}{2\pi i \epsilon \hbar}}$$

$\mathcal{O}(\epsilon)$: $\quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi$

Schrödinger Equation

Wave function → kernel

$$P = \int_{\mathbb{R}} |\psi(x,t)|^2 dx$$

$\hookrightarrow \psi \in L^2(\mathbb{R})$ → $L^2(\mathbb{R})$ is a Hilbert space

Path integral for the free-particle

$$L = \frac{m\dot{x}^2}{2}$$

$$K(b|a) = \lim_{N \to +\infty} \int A^N e^{\frac{i}{\hbar}\frac{(x_{a+1}-x_a)^2}{\epsilon}} e^{\frac{i}{\hbar}\frac{(x_{a+2}-x_{a+1})^2}{\epsilon}} \cdots e^{\frac{i}{\hbar}\frac{(x_b-x_{b-1})^2}{\epsilon}} dx_{a+1} \cdots dx_{b-1}$$

$$= \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}}\; e^{\frac{i m (x_b - x_a)^2}{2\hbar (t_b - t_a)}}$$

Continuum Quantum Mechanics

We are going to ignore mathematical problems, but for a more formal approach see

→ Le Bellac, chap. 7
→ Jordan, "Linear Operators for QM"
→ João Barata

Position & Momentum Operators → $\psi \in L^2(\mathbb{R})$

$$i\hbar \frac{\partial \psi}{\partial t}(x,t) = \underbrace{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)}_{\text{to make sense with our present theory, this should be the Hamiltonian}} \psi(x,t)$$

Position Operator

wishlist $\begin{cases} \hat{X} \text{ hermitian} \\ \text{eigenvalues} \in \mathbb{R} \\ \text{eigenvectors are a basis} \end{cases}$

position ($x \in \mathbb{R}$)

$$\hat{X}|x\rangle = x|x\rangle$$

$\langle x'|$ suppose $x = x'$

$$\underbrace{\langle x'|\hat{X}}_{x'\langle x'|}|x\rangle = x\langle x'|x\rangle$$

$$(x-x')\langle x'|x\rangle = 0$$

$$\Downarrow$$

$$\langle x'|x\rangle = \delta(x-x')$$

orthogonality in the continuous sense

$$|x'\rangle\langle x'|x\rangle = \delta(x-x')|x'\rangle$$

$$\int |x'\rangle\langle x'|x\rangle dx' = \int \delta(x-x')|x'\rangle dx'$$

$$\int |x'\rangle\langle x'| dx' |x\rangle = |x\rangle$$

resolution of identity for the continuous case

$$\int |x'\rangle\langle x'| dx' = \mathbb{1}$$

Let $|\psi\rangle$ be an arbitrary state (same for $|\varphi\rangle$)

$$|\psi\rangle = \mathbb{1}|\psi\rangle$$
$$= \int |x\rangle\langle x|\psi\rangle dx$$

$$\langle \psi | \varphi \rangle = \langle \psi | \mathbb{1} | \varphi \rangle$$

$$= \int \langle \psi | x \rangle \langle x | \varphi \rangle \, dx$$

suppose I call
$\langle x | \varphi \rangle = \varphi(x)$
$\langle \psi | x \rangle = \psi^*(x)$

inner product in $\mathcal{H}$

$$= \int \psi^*(x)\, \varphi(x)\, dx$$

inner product in $L^2(\mathbb{R})$ → we've found the wavefunctions in $\mathcal{H}$

Eigenfunction of eigenket of $\hat{X}$

$$\psi_{x'}(x) = \langle x | x' \rangle = \delta(x - x')$$

wavefunction of an eigenket of $\hat{X}$ does not belong to $L^2(\mathbb{R})$

states are rays of vectors in $\mathcal{H}$, but $|x\rangle \notin \mathcal{H}$. Thus, $|x\rangle$ is not a physical state

↳ physical states are combinations of $|x\rangle$ that lies in $L^2(\mathbb{R})$ → wavepackets

Action of $\hat{X}$ on a general state $|\psi\rangle$

$$\left.\begin{aligned} \langle x | \hat{X} | \psi \rangle &= [\hat{X}\psi](x) \\ x \langle x | \psi \rangle &= x\,\psi(x) \end{aligned}\right\}$$

$\hat{X}$ is a multiplication operator on the wavefunction

$$\langle x | f(\hat{X}) | \psi \rangle = f(x) \langle x | \psi \rangle = f(x)\, \psi(x)$$

Schrödinger Equation: $V(x)\psi(x) = [\hat{V}(\hat{X})\psi](x)$

Propagator

$$\underbrace{\psi(x,t)}_{\langle x|\psi(t)\rangle} = \int K(x,t|y,t')\underbrace{\psi(y,t')}_{\langle y|\psi(t')\rangle}\,dy$$

$$|\psi(t)\rangle = \hat{U}(t,t')\,|\psi(t')\rangle$$

$$\langle x|\downarrow$$

$$\langle x|\psi(t)\rangle = \langle x|\hat{U}(t,t')|\psi(t')\rangle$$

$$\langle x|\psi(t)\rangle = \int \langle x|\hat{U}(t,t')|y\rangle\langle y|\psi(t')\rangle\,dy$$

$$K(x,t|y,t') = \langle x|\hat{U}(t,t')|y\rangle$$

we know that

$$a<c<b$$

$$K(b|a) = \int K(c|a)\,K(b|c)\,dx_c.$$

with this new formalism

$$K(b|a) = \langle x_b|\hat{U}(t_b,t_a)|x_a\rangle$$

$$= \langle x_b|\hat{U}(t_b,t_c)\,\hat{U}(t_c,t_a)|x_a\rangle$$

$$= \int \langle x_b|\hat{U}(t_b,t_c)|x_c\rangle\langle x_c|\hat{U}(t_c,t_a)|x_a\rangle\,dx_c$$

$$= \int K(b|c)\,K(c|a)\,dx_c$$

How to measure momentum?

Time of flight

if we have no forces,

$$p = \frac{my}{T} + \mathcal{O}\left(\frac{mb}{T}\right)$$

$\hookrightarrow$ bigger T means less error

Probability of having a particle with momentum between p and $p+dp$

$$P(p)\,dp = \lim_{T\to+\infty} P(y)\,dy$$

$$= \lim_{T\to+\infty} dy \left| \int \underbrace{K_{free}(y,T|x,0)}_{\sqrt{\frac{m}{2\pi i\hbar T}}\, e^{\frac{im(y-x)^2}{2\hbar T}}} \psi(x,0)\,dx \right|^2$$

$$= \lim_{T\to+\infty} \frac{dy\, m}{2\pi\hbar T} \left| \int \psi(x,0)\, \underbrace{e^{\frac{im(y-x)^2}{2\hbar T}}}_{e^{\frac{imy^2}{2\hbar T}}\, e^{\frac{imx^2}{2\hbar T}}\, e^{-\frac{imxy}{\hbar T}}} dx \right|^2 \to \frac{m\,dy}{T} = dp$$

$\frac{my}{T} \to p$

$e^{\frac{imy^2}{2\hbar T}}$: vanishes with the absolute value

$e^{\frac{imx^2}{2\hbar T}} \to$ goes to 1 as $T\to+\infty$

$$P(p)\,dp = \lim_{T\to+\infty} \frac{dp}{2\pi\hbar} \left| \int e^{-\frac{ipx}{\hbar}} \psi(x,0)\,dx \right|^2$$

Introduce a wave function depending on p

$$P(p) = |\psi(p)|^2$$

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{ipx}{\hbar}} \psi(x)\,dx$$

$\to$ the position and momentum spaces are related by a Fourier Transform

Momentum Operator

wish list $\begin{cases} \hat{p}, \text{ hermitian} \\ \text{eigenvalues } \in \mathbb{R} \\ \text{eigenvectors are a basis} \end{cases}$

$$\hat{P}|p\rangle = p|p\rangle$$

déjà-vu

$$\langle p' | p \rangle = \delta(p' - p)$$

$$\int |p\rangle\langle p| \, dp = \mathbb{1}$$

$$\psi(p) = \langle p | \psi \rangle$$

$$\psi(p) = \langle p | \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{ipx}{\hbar}} \langle x | \psi \rangle \, dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \iint e^{-\frac{ipx}{\hbar}} \langle x | p' \rangle \underbrace{\langle p' | \psi \rangle}_{\psi(p')} \, dp' \, dx$$

We need $\displaystyle \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{ipx}{\hbar}} \langle x | p' \rangle \, dx = \delta(p - p')$.

Fourier transform

$$\delta(k - k') = \frac{1}{2\pi} \int e^{-i(k-k')x} \, dx$$

we identify $k = \frac{p}{\hbar}$, $k' = \frac{p'}{\hbar}$

$$\delta\left(\frac{p}{\hbar} - \frac{p'}{\hbar}\right) = \frac{1}{2\pi} \int e^{-\frac{i(p-p')x}{\hbar}} \, dx$$

$$\hbar \, \delta(p - p') = \frac{1}{2\pi} \int e^{-\frac{i(p-p')x}{\hbar}} \, dx$$

$$\delta(p - p') = \frac{1}{2\pi\hbar} \int e^{-\frac{i(p-p')x}{\hbar}} \, dx = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{ipx}{\hbar}} \langle x | p' \rangle \, dx$$

$$\langle x | p' \rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$$

also not physical states, for these functions are not square integrable

↳ not on $L^2(\mathbb{R})$

Momentum Operator

$$\langle x | \hat{p} | \psi \rangle = [\hat{p}\psi](x)$$

$$\langle x|\hat{P}|\psi\rangle = \int \langle x|\hat{P}|x'\rangle\langle x'|\psi\rangle dx'$$

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

$$\langle x|\hat{P}|x'\rangle = \int \langle x|\hat{P}|p\rangle\langle p|x'\rangle dp$$

$$= \int p \langle x|p\rangle\langle p|x'\rangle dp$$

$$= \frac{1}{2\pi\hbar}\int p\, e^{\frac{ip(x-x')}{\hbar}} dp$$

$$= -i\hbar \frac{d}{dx}\left(\frac{1}{2\pi\hbar}\int e^{\frac{ip(x-x')}{\hbar}} dp\right)$$

$$= -i\hbar \frac{d}{dx}\,\delta(x-x')$$

$$[\hat{P}\psi](x) = \int -i\hbar \frac{d}{dx}\,\delta(x-x')\,\psi(x')\,dx'$$

$$= -i\hbar\frac{d}{dx}\int \delta(x-x')\,\psi(x')\,dx'$$

$$= -i\hbar\frac{d\psi}{dx}(x)$$

$$\hat{P}^2 = -\hbar^2\frac{\partial^2}{\partial x^2} \Rightarrow \hat{H} = \frac{\hat{P}^2}{2m} + \hat{V}(\hat{x})$$

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}(x)\right)\psi(x)$$

Counting Momentum States → trick: put the system in a box

Periodic boundary conditions

$$\langle x|p\rangle = \langle x+L|p\rangle$$

$$\frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}} = \frac{e^{\frac{ip(x+L)}{\hbar}}}{\sqrt{2\pi\hbar}} \Rightarrow \frac{pL}{\hbar} = 2\pi \cdot n$$

integer

$$p = \frac{2\pi n}{\hbar L}$$

now it is discrete

General Properties of 1-dimensional Systems

$$\int |\psi(x)|^2 dx = 1$$

conservation law

can be expressed as a continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$$

$$\rho(x,t) = |\psi(x,t)|^2$$

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}(\psi^* \psi) = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}$$

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

$$-i\hbar \frac{\partial \psi^*}{\partial t} = \hat{H}\psi^*$$

$$= \frac{i}{\hbar}(\hat{H}\psi^*)\psi - \frac{i}{\hbar}\psi^*(\hat{H}\psi)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*\right)\psi - \frac{i}{\hbar}\psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi\right)$$

$$= \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\right)\left[\frac{\partial^2 \psi^*}{\partial x^2}\psi - \psi^*\frac{\partial^2 \psi}{\partial x^2}\right]$$

$$= -\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right]$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left[\underbrace{\frac{i\hbar}{2m}\left(\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right)}_{\text{probability current}}\right] = 0$$

General Property of $\langle \psi | H | \psi \rangle$

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{x})$$

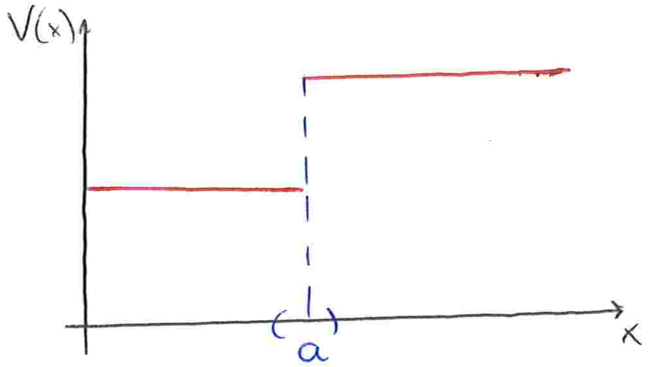
$$\langle \psi | \hat{H} | \psi \rangle \geq \langle \psi | V | \psi \rangle$$

$$\frac{\langle \psi | \hat{P}^2 | \psi \rangle}{2m} = \left\| \frac{\hat{P}}{\sqrt{2m}} | \psi \rangle \right\|^2 \geq 0$$

$\therefore$

$$\langle \psi | \hat{H} | \psi \rangle = \langle \psi | \frac{\hat{P}^2}{2m} | \psi \rangle + \langle \psi | V | \psi \rangle \geq \langle \psi | V | \psi \rangle$$

Conditions $\psi(x)$ must satisfy



$\psi(a) = ?$

↳ ψ has to be continuous if we want the probability to be well-defined

Is $\frac{\partial \psi}{\partial x}$ continuous?

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x,t)$$

$\frac{\epsilon}{a} \ll 1$ ←
$$\underbrace{i\hbar \int_{a-\epsilon}^{a+\epsilon} \frac{\partial \psi}{\partial t} dx}_{i\hbar \cdot 2\epsilon \left.\frac{\partial \psi}{\partial t}\right|_a \to 0} = \underbrace{-\frac{\hbar^2}{2m} \int_{a-\epsilon}^{a+\epsilon} \frac{\partial^2 \psi}{\partial x^2} dx}_{\left.\frac{\partial \psi}{\partial x}\right|_{a+\epsilon} - \left.\frac{\partial \psi}{\partial x}\right|_{a-\epsilon}} + \int_{a-\epsilon}^{a+\epsilon} \psi(x,t) V(x)\, dx$$

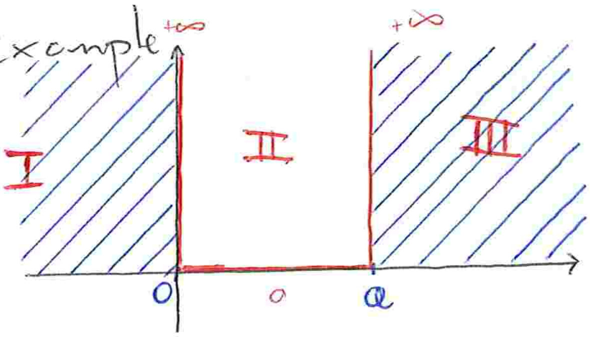
limit as $\epsilon \to 0$

$$0 = -\frac{\hbar^2}{2m}\left(\left.\frac{\partial \psi}{\partial x}\right|_{a+\epsilon} - \left.\frac{\partial \psi}{\partial x}\right|_{a-\epsilon} \right) + \underbrace{\int_{a-\epsilon}^{a+\epsilon} V(x)\, \psi(x,t)\, dx}_{2\epsilon V(a)\psi(a,t) \to 0}$$

if V has a finite discontinuity

If V has a finite discontinuity, then $\frac{\partial \psi}{\partial x}$ is continuous. However, if V has an infinite discontinuity, $\frac{\partial \psi}{\partial x}$ is not continuous.

Example



$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\,\psi(x,t)$$

separable

$$\psi(x,t) = \alpha(t)\,\phi(x)$$

$$i\hbar \frac{\dot{\alpha}\cancel{\phi}}{\alpha\cancel{\phi}} = -\frac{\hbar^2}{2m}\frac{\cancel{\alpha}\,\phi''}{\cancel{\alpha}\,\phi} + V\frac{\cancel{\alpha\phi}}{\cancel{\alpha\phi}}$$

$$\underbrace{i\hbar\frac{\dot{\alpha}}{\alpha}}_{\text{only } t} = \underbrace{-\frac{\hbar^2}{2m}\frac{\phi''}{\phi} + V}_{\text{only } x}$$

$$i\hbar\frac{\dot{\alpha}}{\alpha} = \underbrace{E = -\frac{\hbar^2}{2m}\frac{\phi''}{\phi} + V}_{\text{time-independent}}$$

eigenvalue equation

though for a differential operator

$$-\frac{\hbar^2}{2m}\phi'' + V\phi = E\phi$$

solve in each region

Region II

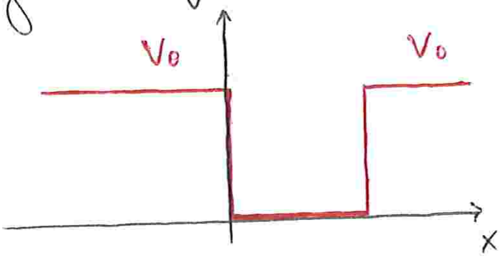
$V(x) = 0$

$$-\frac{\hbar^2}{2m}\phi'' = E\phi$$

$$\phi''(x) = -\frac{2mE}{\hbar^2}\phi(x) \quad \longrightarrow \quad k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

$$\phi(x) = A\cos kx + B\sin kx$$

Regions I & III: $\phi(x) = 0$



We'll solve the problem for a finite well and take the limit as $V_0 \to +\infty$

$$-\frac{\hbar^2}{2m}\phi''(x) = (E - V_0)\phi(x)$$

$E < V_0$, for we will take the limit as $V_0 \to +\infty$

$$\phi''(x) = -\frac{2m(E-V_0)}{\hbar^2}\phi(x) \quad \longrightarrow \quad \frac{2m(V-E_0)}{\hbar^2} = \lambda^2$$

$$\phi(x) = \alpha_* e^{\lambda x} + \beta_* e^{-\lambda x}$$

Region I:

$$\phi_I(x) = \alpha_* e^{\lambda x}$$

$\downarrow$

goes to zero as $V_0 \to +\infty$ (and thus $\lambda \to +\infty$), for $x < 0$

Region III:

$$\phi_{III}(x) = \beta e^{-\lambda x}$$

$\downarrow$

goes to zero as $V_0 \to +\infty$ (and thus $\lambda \to +\infty$), for $x > 0$

Continuity of $\phi(x)$:

$x = 0$: $\quad \phi_{II}(0) = 0 = A \Rightarrow \phi_{II}(x) = B\sin kx$

$x = a$: $\quad \phi_{II}(a) = 0 = B\sin ka \Rightarrow ka = n\pi \Rightarrow k = \frac{n\pi}{a}, \quad n \in \mathbb{N}$

$$\therefore \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{a}$$

$$E = \left(\frac{\hbar \pi n}{a}\right)^2 \frac{1}{2m}$$

quantization of energy

$$\phi_{II}(x) = B \sin\left(\frac{n\pi x}{a}\right)$$

Quantum Harmonic Oscillator

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{k}{2}\hat{X}^2 \qquad (1\text{-dim})$$

we'll deal with 3D in ~~the~~ following lectures

Two options

i) Position representation

Frobenius Method

ii) Algebraic Method

Frobenius Method

Time-independent Schrödinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{k}{2}x^2\psi(x) = E\,\psi(x)$$

Fuch's Theorem: at least one of the solutions is of the form of a power series

if we write it in an adimensional form, it gets clearer

Out of $\hbar$, m, k and x, only one adimensional quantity can be defined

$$k = m\omega^2, \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x$$

ε also adimensional

$$\psi''(\xi) - \xi^2\psi(\xi) + \frac{2E}{\hbar\omega}\psi(\xi) = 0$$

$$\psi''(\xi) = (\xi^2 - \epsilon)\,\psi(\xi)$$

If $\xi \to \pm\infty$, then $\psi''(\xi) \sim \xi^2 \psi(\xi)$, and the only allowed solution is $\psi(\xi) \sim e^{-\xi^2/2}$

positive sign is not square integrable

$$\psi(\xi) = u(\xi)\, e^{-\xi^2/2}$$

Schrödinger Equation

$$u''(\xi) - 2\xi u'(\xi) + (\epsilon - 1)\,u(\xi) = 0$$

Hermite's Differential Equation

Write $u(\xi) = \sum_{n=0}^{+\infty} c_n \xi^n$.

inserting this ansatz on HDE we get:

$$c_{n+2} = \frac{2n - (\epsilon - 1)}{(n+1)(n+2)}\, c_n\,, \quad n \geq 0$$

Problem: $n \gg 1$

$$\frac{c_{n+2}}{c_n} \sim \frac{n}{n^2} \sim \frac{1}{n} \longrightarrow u(\xi) = e^{\xi^2}$$

$$\psi(\xi) = e^{\xi^2} e^{-\xi^2/2} = e^{\xi^2/2}$$

not square integrable !!

Solution: truncate the series

after all, finite sums can't diverge

$$u_N(\xi) = \sum_{n=0}^{N} c_n \xi^n$$

Hermite polynomial of order N

$$\Downarrow$$

$$c_{N+2} = 0 \Rightarrow 2N = \epsilon + 1$$

energy of harmonic oscillator is quantized!

$$\frac{2E}{\hbar\omega} = \epsilon = 2N + 1 \Rightarrow E_N = \hbar\omega\left(N + \tfrac{1}{2}\right)$$

Summary

Eigenfunctions: $\psi_n(\xi) = H_n(\xi)\, e^{-\xi^2/2}$

Hermite polynomials

Eigenvalues: $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$

$n \geq 0$

Algebraic Method

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m\omega^2}{2}\hat{X}^2 = \frac{\hbar\omega}{2}\left(\hat{q}^2 + \hat{Q}^2\right)$$

adimensional variables

$$\begin{cases} \hat{q} = \sqrt{\frac{m\omega}{\hbar}}\,\hat{X} \\ \hat{Q} = \frac{1}{\sqrt{\hbar m\omega}}\,\hat{P} \end{cases}$$

If $\hat{q}$ and $\hat{Q}$ were numbers, $\hat{H}$ could be factorized as

$$H = \frac{\hbar\omega}{2}(q + iQ)(q - iQ)$$

no hats, for it ain't so trivial for operators

$$\hat{a} \equiv \frac{\hat{q} + i\hat{Q}}{\sqrt{2}}, \quad \hat{a}^\dagger \equiv \frac{\hat{q} - i\hat{Q}}{\sqrt{2}}$$

$$[\hat{a}, \hat{a}^\dagger] = 1$$

$$\hat{H} = \hbar\omega\left(\underbrace{\hat{a}^\dagger\hat{a}}_{\hat{N}} + \frac{1}{2}\right)$$

$[\hat{H}, \hat{N}] = 0$

$\hat{N}|n\rangle = n|n\rangle$

studying $\hat{N}$ will teach us about $\hat{H}$

Properties

i) $n \geq 0$

$$\langle n|\hat{N}|n\rangle = n\langle n|n\rangle$$

$$n = \langle n|\hat{N}|n\rangle$$
$$= \langle n|\hat{a}^{\dagger}\hat{a}|n\rangle$$
$$= \| \hat{a}|n\rangle \|^2 \geq 0$$

$|0\rangle$ ain't the null vector, but the eigenvector associated to $n=0$

ii) $n=0 \Rightarrow \hat{a}|0\rangle = 0$

$$n = \| \hat{a}|n\rangle \|^2$$
$$0 = \| \hat{a}|0\rangle \|^2 \Rightarrow \hat{a}|0\rangle = 0$$

iii) $n \neq 0 \Rightarrow \hat{a}|n\rangle$ is an eigenstate of $\hat{N}$

$[\hat{a}, \hat{a}^{\dagger}] = 1$

$$N\hat{a}|n\rangle = \hat{a}^{\dagger}\hat{a}\hat{a}|n\rangle$$
$$= (\hat{a}\hat{a}^{\dagger} - 1)\hat{a}|n\rangle$$
$$= \hat{a}(\hat{a}^{\dagger}\hat{a} - 1)|n\rangle$$
$$= \hat{a}(\hat{N} - 1)|n\rangle$$
$$= (n-1)\hat{a}|n\rangle$$

↳ $\hat{a}|n\rangle$ is an eigenvector of $\hat{N}$ associated with the eigenvalue $n-1$

$$\hat{a}|n\rangle = c|n-1\rangle$$

I suppose $\hat{N}$ has a non-degenerate spectrum. If I get to something ridiculous, then perhaps we should consider another possibility

$$\langle n|\hat{a}^{\dagger}\hat{a}|n\rangle = |c|^2\langle n-1|n-1\rangle$$

$$|c|^2 = \langle n|\hat{N}|n\rangle = n \Rightarrow c = \sqrt{n}$$

↳ phase is arbitrary

$$\therefore \hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

iv) $\hat{a}^{+}|n\rangle$ is an eigenstate of $\hat{N}$

$$\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

can be proven by the same arguments used in iii

v) n is an integer

$n \geq 0$

if n was not an integer, we could simply apply $\hat{a}$ until we had $n' < 0$, which would be a contradiction

discrete states
$$\begin{cases} n=0 \rightarrow |0\rangle \\ n=1 \rightarrow |1\rangle = \hat{a}^{+}|0\rangle \\ n=2 \rightarrow |2\rangle = \dfrac{\hat{a}^{+}}{\sqrt{2}}|1\rangle \\ \vdots \end{cases}$$

For $\hat{H}$

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$

$$\hat{H}|n\rangle = \underbrace{\hbar\omega\left(n + \frac{1}{2}\right)}_{E_n}|n\rangle$$

Eigenfunctions

$$|n\rangle = \frac{(\hat{a}^{+})^n}{\sqrt{n!}}|0\rangle$$

$$\langle x|\hat{a}|0\rangle = 0$$

$$\hat{a} = \frac{\hat{q} + i\hat{Q}}{\sqrt{2}} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,\hat{X} + i\frac{1}{\sqrt{\hbar\omega m}}\hat{P}\right)$$

$$\langle x|\sqrt{\frac{m\omega}{2\hbar}}\,\hat{X} + i\frac{1}{\sqrt{2\hbar\omega m}}\hat{P}|0\rangle = 0$$

$$\sqrt{\frac{m\omega}{2\hbar}}\,x\underbrace{\langle x|0\rangle}_{\psi_0(x)} + \frac{i}{\sqrt{2\hbar\omega m}}\underbrace{\langle x|\hat{P}|0\rangle}_{-i\hbar\frac{\partial}{\partial x}\psi_0(x)} = 0$$

$$\sqrt{\frac{m\omega}{2\hbar}} \times \psi_0(x) + \sqrt{\frac{\hbar}{2m\omega}} \frac{\partial \psi_0}{\partial x} = 0$$

$$\frac{\partial \psi_0}{\partial x} = -\frac{m\omega}{\hbar} \times \psi_0(x)$$

$$\psi_0(x) = C e^{-\frac{m\omega x^2}{2\hbar}} \rightarrow \frac{m\omega x^2}{\hbar} = \xi^2$$

both methods agree for the ground state

Look at $\psi_1(x)$

$$\psi_1(x) = \langle x | 1 \rangle$$
$$= \langle x | \hat{a}^\dagger | 0 \rangle$$
$$= \frac{1}{\sqrt{2}} \langle x | \sqrt{\frac{m\omega}{\hbar}} \hat{X} - \frac{i}{\sqrt{\hbar\omega m}} \hat{P} | 0 \rangle$$
$$= \sqrt{\frac{m\omega}{2\hbar}} \times \langle x | 0 \rangle - \frac{i}{\sqrt{\hbar m\omega}} \langle x | \hat{P} | 0 \rangle$$
$$= \sqrt{\frac{m\omega}{2\hbar}} \times \psi_0(x) - \sqrt{\frac{\hbar}{2m\omega}} \frac{\partial \psi_0}{\partial x}$$

$\rightarrow$ coincides with Frobenius

$$E_{n+1} - E_n = \hbar\omega\left(n+1+\tfrac{1}{2}\right) - \hbar\omega\left(n+\tfrac{1}{2}\right) = \hbar\omega$$

annihilation of particles

$\hat{a}^\dagger$	0 particles	$\uparrow \hat{a}$	$E_0 \rightarrow$ vacuum
	1 particle (at rest)		$E_0 + mc^2$
$\hat{a}^\dagger$	2 particles (at rest)	$\uparrow \hat{a}$	$E_0 + 2mc^2$
	$\vdots$		$\vdots$

creation of particles

Quantum Field Theory

Path Integral Resolution of the Harmonic Oscillator

If the Lagrangian has the form

$$L_0 = \frac{m\dot{x}^2}{2} + b(t)\, x\dot{x} + c(t)\, x^2 + d(t)\, \dot{x} + e(t)\, x + f(t)$$

then (see Shulman or Feynman)

$$K(b|a) = e^{iS_{cl}(t_b,t_a)/\hbar} \left(\frac{m}{2\pi i \hbar \, f(t_b,t_a)} \right)^{1/2}$$

(x_b, t_b) (x_a, t_a) classical action

time only

$$m \frac{\partial^2 f}{\partial t_b^2} - 2c(t) f = 0$$

$$f(t_a, t_a) = 0$$

$$\left. \frac{\partial f}{\partial t}(t, t_a) \right|_{t=t_b} = 1$$

For the harmonic oscillator

$$c(t) = -\frac{m\omega^2}{2}$$

solve for $f(t, t_a)$

$$f(t, t_a) = \frac{\sin(\omega(t - t_a))}{\omega}$$

$T \equiv t_b - t_a$

$$S_{cl}(t_b, t_a) = \frac{m\omega}{2\sin(\omega T)} \left((x_a^2 + x_b^2)\cos\omega T - 2x_a x_b \right)$$

Thus, the kernel for the quantum harmonic oscillator is

$$K(b|a) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega T)}} \; e^{\frac{im\omega}{2\hbar \sin(\omega T)} \left[(x_a^2 + x_b^2)\cos\omega T - 2x_a x_b \right]}$$

how can we extract useful information from this expression?

Another general property of path integrals

$$K(b|a) = \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle$$

$\hat{H}$ is time-independent

$$= \langle x_b | e^{-i\frac{\hat{H}T}{\hbar}} | x_a \rangle$$

$\mathbb{1} = \sum_n |E_n\rangle\langle E_n|$

if E_n was continuous, we would simply use an integral

$$= \sum_n \langle x_b | e^{-\frac{i\hat{H}T}{\hbar}} | E_n \rangle \langle E_n | x_a \rangle$$

$$K(b|a) = \sum_n e^{-\frac{iE_nT}{\hbar}} \underbrace{\langle x_b | E_n \rangle}_{\psi_n(x_b)} \underbrace{\langle E_n | x_a \rangle}_{\psi_n^*(x_a)}$$

same position, different times

$$K(x,t_b|x,t_a) = \sum_n e^{-\frac{iE_nT}{\hbar}} \underbrace{\langle x | E_n \rangle\langle E_n | x \rangle}_{\langle E_n | x \rangle\langle x | E_n \rangle}$$

$$\int K(x,t_b|x,t_a)\,dx = \sum_n \int e^{-\frac{iE_nT}{\hbar}} \langle E_n | x \rangle\langle x | E_n \rangle\, dx$$

$$= \sum_n e^{-\frac{iE_nT}{\hbar}} \langle E_n | E_n \rangle$$

$$= \sum_n e^{-\frac{iE_nT}{\hbar}}$$

For the QHO, we have

$$\int K(x,t_b|x,t_a)\,dx = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} \int e^{\frac{im\omega}{2\hbar\sin(\omega T)}2x^2(\cos\omega T - 1)}\,dx$$

Gaussian Integral

$$= \frac{1}{\sqrt{2(\cos\omega T - 1)}}$$

$$= \frac{1}{\sqrt{-4\sin^2\left(\frac{\omega T}{2}\right)}}$$

$$= \frac{1}{2i}\csc\left(\frac{\omega T}{2}\right)$$

$$= \frac{1}{2i}\frac{2i}{e^{\frac{i\omega T}{2}} - e^{-\frac{i\omega T}{2}}}$$

$$= \frac{e^{-\frac{i\omega T}{2}}}{1 - e^{-i\omega T}}$$

$$\int K(x,t_b|x,t_a)\,dx = e^{-\frac{i\omega T}{2}} \sum_n e^{-in\omega T}$$

$$= \sum_n e^{-i\omega T(n+\frac{1}{2})}$$

$$= \sum_n e^{-i\hbar\omega T(n+\frac{1}{2})/\hbar} = \sum_n e^{-iE_nT/\hbar}$$

$$\Downarrow$$

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right)$$

Coherent States

↳ or Glauber States

↳ eigenstates of the annihilation operator $\hat{a}$

$$\hat{a}|\alpha\rangle = \alpha \underbrace{|\alpha\rangle}_{\text{coherent state}} \rightarrow \alpha \in \mathbb{C} \text{ in general}$$

↳ $\hat{a}$ is not an hermitian operator

Basis $\{|n\rangle\}_{n\in\mathbb{N}}$

$\hat{N}|n\rangle = n|n\rangle$ → $\hat{N}$: number operator

$\hat{N} = \hat{a}^\dagger\hat{a}$

$|\alpha\rangle = \sum_n |n\rangle\langle n|\alpha\rangle$ → must satisfy $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$

$$\hat{a}\sum_{n=0}^{+\infty}\langle n|\alpha\rangle|n\rangle = \alpha\sum_{n=0}^{+\infty}|n\rangle\langle n|\alpha\rangle$$

$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$

$$\sum_{n=1}^{+\infty}\sqrt{n}\,|n-1\rangle\langle n|\alpha\rangle = \sum_{n=0}^{+\infty}\alpha\,|n\rangle\langle n|\alpha\rangle$$

↳ $n=0$ yields 0

$$\sum_{n=0}^{+\infty} \underbrace{\left[\sqrt{n+1}\,\langle n+1|\alpha\rangle - \alpha\langle n|\alpha\rangle\right]}_{\sqrt{n+1}\,\langle n+1|\alpha\rangle - \alpha\langle n|\alpha\rangle = 0} |n\rangle = 0$$

$$\langle n+1|\alpha\rangle = \frac{\alpha}{\sqrt{n+1}}\langle n|\alpha\rangle$$

$n=0$: $\langle 1|\alpha\rangle = \alpha\langle 0|\alpha\rangle$

$n=1$: $\langle 2|\alpha\rangle = \frac{\alpha}{\sqrt{2}}\langle 1|\alpha\rangle = \frac{\alpha^2}{\sqrt{2}}\langle 0|\alpha\rangle$

$n=2$: $\langle 3|\alpha\rangle = \frac{\alpha}{\sqrt{3}}\langle 2|\alpha\rangle = \frac{\alpha^3}{\sqrt{3!}}\langle 0|\alpha\rangle$

$\vdots$

$$\langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}}\langle 0|\alpha\rangle$$

$$|\alpha\rangle = \sum_{n=0}^{+\infty} \frac{\alpha^n}{\sqrt{n!}} \underbrace{\langle 0|\alpha\rangle}_{?} |n\rangle$$

Normalization

$$1 = \langle\alpha|\alpha\rangle = \sum_m \frac{\alpha^{*m}}{\sqrt{m!}}\langle m|\langle\alpha|0\rangle \sum_n \frac{\alpha^n}{\sqrt{n!}}\langle 0|\alpha\rangle|n\rangle$$

$$1 = |\langle 0|\alpha\rangle|^2 \sum_{m,n} \frac{\alpha^{*m}\alpha^n}{\sqrt{m!\,n!}} \overbrace{\langle m|n\rangle}^{\delta_{mn}}$$

$$= |\langle 0|\alpha\rangle|^2 \underbrace{\sum_n \frac{|\alpha|^{2n}}{n!}}_{e^{|\alpha|^2}} = |\langle 0|\alpha\rangle|^2 e^{|\alpha|^2} = 1 \Rightarrow \langle 0|\alpha\rangle = e^{-|\alpha|^2/2}$$

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

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Time Evolution

$$|\alpha(t)\rangle = e^{-i\omega(\hat{N}+\frac{1}{2})t}|\alpha\rangle$$

$$= e^{-i\omega(\hat{N}+\frac{1}{2})t}\sum_n e^{-|\alpha|^2/2}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

$$= \sum_n e^{-\frac{|\alpha|^2}{2}}\frac{\alpha^n}{\sqrt{n!}}e^{-i\omega(n+\frac{1}{2})t}|n\rangle$$

$$= e^{-\frac{i\omega t}{2}}e^{-\frac{|\alpha|^2}{2}}\sum_n \frac{\alpha^n}{\sqrt{n!}}e^{-in\omega t}|n\rangle$$

$$= e^{-\frac{i\omega t}{2}}e^{-\frac{|\alpha|^2}{2}}\sum_n \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}|n\rangle$$

$$|\alpha(t)\rangle = e^{-\frac{i\omega t}{2}}|\alpha e^{-i\omega t}\rangle$$

also a coherent state!

Stationary states

$$\langle\hat{X}(t)\rangle_{st} = \langle n(t)|\hat{X}|n(t)\rangle$$

$$= \langle n|e^{\frac{iE_nt}{\hbar}}\hat{X}e^{-\frac{iE_nt}{\hbar}}|n\rangle$$

$$= \langle n|\hat{X}|n\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\langle n|\hat{a}+\hat{a}^\dagger|n\rangle$$

$$\sqrt{n}\underbrace{\langle n|n-1\rangle}_{0} + \sqrt{n+1}\underbrace{\langle n|n+1\rangle}_{0}$$

$$= 0$$

Coherent States

$$\langle\hat{X}(t)\rangle_{coh} = \langle\alpha(t)|\hat{X}|\alpha(t)\rangle$$

$$= \langle\alpha e^{-i\omega t}|e^{i\omega t/2}\hat{X}e^{-i\omega t/2}|\alpha e^{-i\omega t}\rangle$$

$$= \langle\alpha e^{-i\omega t}|\hat{X}|\alpha e^{-i\omega t}\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha e^{-i\omega t}|\hat{a}+\hat{a}^\dagger|\alpha e^{-i\omega t}\rangle$$

$$\langle \hat{x}(t) \rangle_{coh} = \sqrt{\frac{\hbar}{2m\omega}} \left(\alpha e^{-i\omega t} + \alpha^* e^{i\omega t} \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \cdot 2\,\mathrm{Re}\left[\alpha e^{-i\omega t} \right] \qquad \alpha = |\alpha| e^{-i\varphi}$$

$$= \sqrt{\frac{2\hbar}{m\omega}} |\alpha| \cos(\omega t + \varphi)$$

Coherent states: mimic classical states

Stationary states: don't

terms similar to this appear when you couple EM to the hamiltonian

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right) + \underbrace{\hbar\left(f(t)\,\hat{a} + f^*(t)\,\hat{a}^\dagger \right)}_{\text{classical source}}$$

quantizing EM

suppose small

Interaction Picture

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = \hat{V}_I(t) |\psi(t)\rangle_I$$

$\Downarrow$ for this case, the time-evolution operator can be written as the exponential of an integral

can be seen through excruciatingly boring computation

solution

$$|\psi(t)\rangle_I = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} |\psi(0)\rangle_I \qquad \alpha = -i f_0 t\, e^{-i\omega t}$$

Suppose $|\psi(0)\rangle_I = |0\rangle$

$$|\psi(t)\rangle_I = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} |0\rangle$$

$$= e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n (\hat{a}^\dagger)^n}{n!} |0\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle$$

$|n\rangle$

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$$|\psi(t)\rangle_I = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle = |\alpha\rangle$$

classical sources create coherent states

Creation and annihilation of photons induce electromagnetic waves

next step: laser physics (but not on this course)

3D Quantum Mechanics

$$\hat{P}|p\rangle = p|p\rangle \xrightarrow{\text{I want}} \hat{P}_i |\vec{p}\rangle = p_i |\vec{p}\rangle$$

$i = 1, 2, 3$

Which mathematical entity can give us this?

tensor product of Hilbert Spaces

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$$

$\dim \mathcal{H} = (\dim \mathcal{H}_1)(\dim \mathcal{H}_2)$

$|\varphi_1\rangle \in \mathcal{H}_1$, $|\chi_2\rangle \in \mathcal{H}_2$

$$|\varphi_1\rangle \otimes |\chi_2\rangle = \underbrace{\begin{pmatrix} (\varphi_1)_1 (\chi_2)_1 \\ (\varphi_1)_1 (\chi_2)_2 \\ \vdots \\ (\varphi_1)_1 (\chi_2)_{\dim \mathcal{H}_2} \\ (\varphi_1)_2 (\chi_2)_1 \\ \vdots \\ (\varphi_1)_{\dim \mathcal{H}_1} (\chi_2)_{\dim \mathcal{H}_2} \end{pmatrix}}_{\dim \mathcal{H} \text{ entries}}$$

does not need to be finite

What about operators?

$$A \otimes B = \begin{bmatrix} A_{11} B & A_{12} B & A_{13} B & \cdots \\ A_{21} B & A_{22} B & A_{23} B & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$(A \otimes \mathbb{1})|\varphi_1\rangle \otimes |\chi_2\rangle = (A|\varphi_1\rangle) \otimes |\chi_2\rangle$$

Therefore, we could define

$$|\vec{p}\rangle = |p_x\rangle \otimes |p_y\rangle \otimes |p_z\rangle$$

$$\hat{\underline{P}}_x = \hat{P}_x \otimes \mathbb{1} \otimes \mathbb{1}$$

$$\hat{\underline{P}}_y = \mathbb{1} \otimes \hat{P}_y \otimes \mathbb{1}$$

we shall write simply $\hat{P}_x$ and $\hat{P}_y$ in a while

$$\hat{\underline{P}}_x|\vec{p}\rangle = (\hat{P}_x|p_x\rangle) \otimes |p_y\rangle \otimes |p_z\rangle$$

$$= p_x\, |p_x\rangle \otimes |p_y\rangle \otimes |p_z\rangle$$

$$= p_x\, |\vec{p}\rangle$$

as desired

Determinant and Trace with tensor products

$$\det(A \otimes B) = (\det A)^{\dim \mathcal{H}_1} (\det B)^{\dim \mathcal{H}_2}$$

$$\operatorname{tr}(A \otimes B) = (\operatorname{tr} A)(\operatorname{tr} B)$$

$$(A_1 \otimes \mathbb{1})(A_2 \otimes \mathbb{1}) = (A_1 A_2) \otimes \mathbb{1}$$

$$A_1 \otimes A_2 = (A_1 \otimes \mathbb{1})(\mathbb{1} \otimes A_2) = (\mathbb{1} \otimes A_2)(A_1 \otimes \mathbb{1})$$

Scalar Products

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$$

$$|\chi\rangle = |\chi_1\rangle \otimes |\chi_2\rangle$$

$$\longrightarrow \langle \chi|\psi\rangle = \langle \chi_1|\psi_1\rangle \cdot \langle \chi_2|\psi_2\rangle$$

Thus,

$$\langle \vec{x} | \vec{p} \rangle = \langle x | p_x \rangle \cdot \langle y | p_y \rangle \cdot \langle z | p_z \rangle$$

$$= \frac{e^{\frac{i p_x x}{\hbar}}}{\sqrt{2\pi\hbar}} \cdot \frac{e^{\frac{i p_y y}{\hbar}}}{\sqrt{2\pi\hbar}} \cdot \frac{e^{\frac{i p_z z}{\hbar}}}{\sqrt{2\pi\hbar}}$$

$$= \frac{e^{\frac{i \vec{p} \cdot \vec{x}}{\hbar}}}{(2\pi\hbar)^{3/2}}$$

$$\hat{\vec{P}}^2 = \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2$$

$$\hat{P}_x^2 \otimes \mathbb{1} \otimes \mathbb{1} \qquad \mathbb{1} \otimes \hat{P}_y^2 \otimes \mathbb{1} \qquad \mathbb{1} \otimes \mathbb{1} \otimes \hat{P}_z^2$$

Hamiltonian

$d=1$: $$\hat{H} = \frac{\hat{P}_x^2}{2m} + V(\hat{x})$$

$d=3$: $$\hat{H} = \frac{\hat{\vec{P}}^2}{2m} + V(\hat{\vec{x}})$$

Wave functions:

$$\hat{P}_i = -i\hbar \frac{\partial}{\partial x_i}$$

$$\hat{p}^2 = -\hbar^2 \nabla^2$$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\hat{\vec{x}})$$

Free particle in 3D:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{x}) = E\, \psi(\vec{x})$$

time independent Schrödinger - Equation

Separation of variables

$$\psi(\vec{x}) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

$$\underbrace{\mathcal{H} = \mathcal{H}_x \otimes \mathcal{H}_y \otimes \mathcal{H}_z}$$

I could choose other factorizations for $\mathcal{H}$ as well

→ e.g. spherical coordinates

→ the factorization is not unique

Ehrenfest Theorem

$$\frac{d\langle\vec{\hat{p}}\rangle}{dt} = -\langle\nabla V\rangle$$

→ expectation values obey classical laws

Proof [Heisenberg Picture]:

→ expectation values are picture-independent

$$i\hbar\frac{d\hat{p}_i}{dt} = [\hat{p}_i, H]$$

→ $\hat{p}(t)$ in Heisenberg's Picture

$$= \left[\hat{p}_i, \frac{\hat{p}^2}{2m} + V(\hat{x})\right]$$

$$= \left[\hat{p}_i, \frac{\hat{p}^2}{2m}\right]_{\to 0} + [\hat{p}_i, V(\hat{x})]$$

$$\frac{1}{2m}\left[\hat{p}_x \otimes 1\!\!1 \otimes 1\!\!1,\ \hat{p}_x^2 \otimes 1\!\!1 \otimes 1\!\!1 + \cancel{1\!\!1 \otimes \hat{p}_y^2 \otimes 1\!\!1}_{\to 0} + \cancel{1\!\!1 \otimes 1\!\!1 \otimes \hat{p}_z^2}_{\to 0}\right]$$

$$= \frac{1}{2m}\left[\hat{p}_x \otimes 1\!\!1 \otimes 1\!\!1,\ \hat{p}_x^2 \otimes 1\!\!1 \otimes 1\!\!1\right]$$

$$= \frac{1}{2m}\left[\hat{p}_x, \hat{p}_x^2\right] = 0$$

We still have to obtain $[\hat{p}_i, V(\vec{x})]$

$$[\hat{P}_i, V(\hat{\vec{x}})] = [\hat{P}_i, V_0 + \frac{\partial V}{\partial x_k} \hat{x}_k + \frac{1}{2} \frac{\partial^2 V}{\partial x_k \partial x_m} \hat{x}_k \hat{x}_m + \dots]$$

$$[\hat{P}_i, V_0] = 0$$

↳ $V_0 \mathbb{1}$

$$\frac{\partial V}{\partial x_k} \underbrace{[\hat{P}_i, \hat{X}_k]}_{-i\hbar \delta_{ik}} = -i\hbar \frac{\partial V}{\partial x_i}$$

↳ proven by bruteforce (test function and explicit calculation) or symmetries (next week)

$$[\hat{P}_i, \hat{X}_k \hat{X}_m] = \hat{X}_k [\hat{P}_i, \hat{X}_m] + [\hat{P}_i, \hat{X}_k] \hat{X}_m$$

$$= \hat{X}_k(-i\hbar \delta_{im}) + (-i\hbar \delta_{ik}) \hat{X}_m$$

$$\frac{\partial^2 V}{\partial x_k \partial x_m} [\hat{P}_i, \hat{X}_k \hat{X}_m] = -i\hbar \frac{\partial^2 V}{\partial x_k \partial x_i} \hat{X}_k - i\hbar \frac{\partial^2 V}{\partial x_i \partial x_m} \hat{X}_m$$

$$= -i\hbar \cdot 2 \frac{\partial^2 V}{\partial x_i \partial x_k} \hat{X}_k$$

$$[\hat{P}_i, V(\hat{\vec{x}})] = -i\hbar \frac{\partial V}{\partial x_i} - i\hbar \frac{\partial^2 V}{\partial x_i \partial x_k} \hat{X}_k + \dots$$

$$= -i\hbar \frac{\partial V}{\partial x_i}(\hat{\vec{x}})$$

↳ in general,

$$[\hat{P}_i, f(\hat{\vec{x}})] = -i\hbar \frac{\partial f}{\partial x_i}(\hat{\vec{x}})$$

Therefore,

$$i\hbar \frac{d\hat{P}_i}{dt} = -i\hbar \frac{\partial V}{\partial x_i}$$

$$\frac{d\hat{P}_i}{dt} = -\frac{\partial V}{\partial x_i}$$

$$\frac{d\vec{P}}{dt} = -\nabla V$$

$$\left\langle \frac{d\vec{P}}{dt} \right\rangle = -\langle \nabla V \rangle$$

in Heisenberg picture, states are time-independent

$$\frac{d\langle \vec{P} \rangle}{dt} = -\langle \nabla V \rangle$$

even if we don't know what to do with operators, we know that the expectation values must obey classical laws

A Conundrum on Hermite Polynomials

$H_0 = 1$

$H_1 = x$

$H_2 = x^2 - 1$

$H_3 = x^3 - 3x$

$H_4 = x^4 - 6x^2 + 3$

$H_5 = x^5 - 10x^3 + 15x$

odd index $\Rightarrow$ odd polynomial

even index $\Rightarrow$ even polynomial

in fact, there is a hidden symmetry on our problem

parity

Parity - Classical Level

$\vec{X} \rightarrow -\vec{X}$

$\vec{P} \rightarrow -\vec{P}$

$\vec{p} = c \cdot \frac{d\vec{x}}{dt}$

What about QM?

Unitary operator $\hat{\Pi}$ parity operator

non-trivial result

$$\hat{\Pi}|\alpha\rangle = |\alpha'\rangle$$

How to implement parity in QM?

we know what to do with expectation values

$$\langle \hat{\vec{X}} \rangle \longrightarrow -\langle \hat{\vec{X}} \rangle$$

$$\langle \hat{\vec{P}} \rangle \xrightarrow{\text{parity}} -\langle \hat{\vec{P}} \rangle$$

$$\langle \alpha'|\hat{\vec{X}}|\alpha'\rangle = -\langle \alpha|\hat{\vec{X}}|\alpha\rangle$$

$$\langle \alpha'|\hat{\vec{P}}|\alpha'\rangle = -\langle \alpha|\hat{\vec{P}}|\alpha\rangle$$

$$\langle \alpha|\hat{\Pi}^\dagger\hat{\vec{X}}\hat{\Pi}|\alpha\rangle = -\langle \alpha|\hat{\vec{X}}|\alpha\rangle \quad \forall\, |\alpha\rangle \in \mathcal{H}$$

$$\hat{\Pi}^\dagger\hat{\vec{X}}\hat{\Pi} = -\hat{\vec{X}}$$

$\hat{\Pi}$ is unitary

$$\hat{\vec{X}}\hat{\Pi} + \hat{\Pi}\hat{\vec{X}} = 0$$

$$\hat{\vec{P}}\hat{\Pi} + \hat{\Pi}\hat{\vec{P}} = 0$$

same arguments

Consider $\hat{\Pi}|\vec{x}\rangle$

$$\begin{aligned}\hat{\vec{X}}(\hat{\Pi}|\vec{x}\rangle) &= -\hat{\Pi}(\hat{\vec{X}}|\vec{x}\rangle)\\ &= -\hat{\Pi}(\vec{x}|\vec{x}\rangle)\\ &= -\vec{x}(\hat{\Pi}|\vec{x}\rangle)\end{aligned}$$

$\hat{\Pi}|\vec{x}\rangle = |-\vec{x}\rangle$

up to a phase, which I can absorb on the operator $\hat{\Pi}$ → Wigner Theorem next week

$$\underbrace{\langle \vec{x} | \hat{\Pi} | \psi \rangle}_{(\hat{\Pi}\psi)(\vec{x})} = \underbrace{\langle -\vec{x} | \psi \rangle}_{\psi(-\vec{x})}$$

$$(\hat{\Pi}\psi)(\vec{x}) = \psi(-\vec{x})$$

Eigenvalues of $\hat{\Pi}$

$\hat{\Pi}^\dagger \hat{\Pi} = \mathbb{1} = \hat{\Pi}\hat{\Pi}^\dagger$ → eigenvalues are pure phases

$\hat{\Pi}^2 |\vec{x}\rangle = \hat{\Pi} |-\vec{x}\rangle = |\vec{x}\rangle$

$\hat{\Pi}^2 = \mathbb{1} = \hat{\Pi}^\dagger \hat{\Pi} \Rightarrow \hat{\Pi}^\dagger = \hat{\Pi}$ → eigenvalues are real

→ ± 1

Eigenkets

$$\hat{\Pi} |\pm\rangle = \pm |\pm\rangle$$

$$\underbrace{\langle \vec{x} | \hat{\Pi} | \pm \rangle}_{\underbrace{\langle -\vec{x} | \pm \rangle}_{\psi_\pm(-\vec{x})}} = \pm \underbrace{\langle \vec{x} | \pm \rangle}_{\psi_\pm(\vec{x})} \Rightarrow \psi_\pm(-\vec{x}) = \pm \psi(\vec{x})$$

Apply $\hat{\Pi}$ to $\hat{H}$

$$\hat{\Pi}^\dagger \hat{H} \hat{\Pi} = \hat{\Pi}^\dagger \left(\frac{\hat{p}^2}{2m} + \frac{k\hat{x}^2}{2} \right) \hat{\Pi}$$

$$= \frac{\hat{\Pi}^\dagger \hat{p}^2 \hat{\Pi}}{2m} + \frac{k}{2} \hat{\Pi}^\dagger \hat{x}^2 \hat{\Pi} = \hat{H}$$

→ $\hat{\Pi}^\dagger \hat{p} \hat{\Pi} = -\hat{p}$

$$\hat{\Pi}^\dagger \hat{p}^2 \hat{\Pi} = \hat{\Pi}^\dagger \hat{p} \hat{\Pi} \hat{\Pi}^\dagger \hat{p} \hat{\Pi} = (-\hat{p})(-\hat{p}) = \hat{p}^2$$

→ same for $\hat{x}^2$

$$\hat{\Pi}^\dagger \hat{H} \hat{\Pi} = \hat{H}$$

$$\hat{H}\hat{\Pi} = \hat{\Pi}\hat{H}$$

$$[\hat{H}, \hat{\Pi}] = 0$$

Readings for Next Class (Symmetries on Classical Physics):

- Noether's Theorem (Lemos 2.7)
- Canonical Infinitesimal Transformations (Lemos 8.1, 8.4, 8.5)
- "Symmetries in Fundamental Physics" (K. Sundermeyer)

Symmetries

Canonical Quantization → Dirac

Poisson Brackets (Hamiltonian Mechanics):

$$\{f, g\} = \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i}\frac{\partial f}{\partial p_i} \quad \rightarrow \text{implicit summation}$$

$$\frac{dA}{dt} = \{A, \mathcal{H}\}$$

$\mathcal{H}$ → hamiltonian

$A(q,p)$ → no explicit time dependence

$$\{x_i, p_k\} = \delta_{ik}$$

In QM, we have (on Heisenberg Picture):

$$\frac{d\hat{A}_H}{dt} = \frac{1}{i\hbar}[\hat{A}_H, \hat{H}] \xrightarrow{\text{similar to}} \frac{dA}{dt} = \{A, \mathcal{H}\}$$

$$[\hat{x}_i, \hat{p}_k] = i\hbar\, \delta_{ik} \longrightarrow \{x_i, p_k\} = \delta_{ik}$$

$$[\hat{p}_i, f(\vec{x})] = -\frac{\partial f}{\partial x_i} i\hbar$$

$$\{p_i, f(x)\} = \underbrace{\frac{\partial p_i}{\partial x_k}\frac{\partial f}{\partial p_k}}_{0} - \underbrace{\frac{\partial p_i}{\partial p_k}}_{\delta_{ik}}\frac{\partial f}{\partial x_k} = -\frac{\partial f}{\partial x_k}$$

Canonical Quantization:

To go from CM to QM, just promote functions to hermitian operators and change

$$\{\cdot, \cdot\} \longrightarrow \frac{[\cdot, \cdot]}{i\hbar}$$

Symmetries in QM

Classical level

Q: symmetry generator — continuous symmetry

$$\begin{cases} \delta x_i = \{x_i, Q\} \\ \delta p_i = \{p_i, Q\} \end{cases} \xrightarrow{\text{canonical quantization}} \begin{cases} \delta \hat{x}_i = \dfrac{[\hat{x}_i, \hat{Q}]}{i\hbar} \\ \delta \hat{p}_i = \dfrac{[\hat{p}_i, \hat{Q}]}{i\hbar} \end{cases}$$

quantum symmetry transformations (for symmetries that depend on continuous parameters up to first order on the parameter)

example: translation

$$\vec{x} \to \vec{x} + \vec{a}$$

Finite form of transformations

$$\hat{X}_i' = e^{\frac{i\hat{Q}}{\hbar}} \hat{X}_i \, e^{-\frac{i\hat{Q}}{\hbar}}$$

$$= \left[\mathbb{1} + \frac{i\hat{Q}}{\hbar} + \dots \right] \hat{X}_i \left[\mathbb{1} - \frac{i\hat{Q}}{\hbar} + \dots \right]$$

$$= \hat{X}_i + \frac{i\,\hat{Q}\,\hat{X}_i}{\hbar} - \frac{i\,\hat{X}_i\,\hat{Q}}{\hbar} + \dots$$

$$= \hat{X}_i + \frac{1}{i\hbar}\left(\hat{X}_i \hat{Q} - \hat{Q}\hat{X}_i \right) + \dots$$

$$\hat{X}_i' - \hat{X}_i = \frac{[\hat{X}_i, \hat{Q}]}{i\hbar}$$

$$\hat{P}_i' = e^{\frac{i\hat{Q}}{\hbar}} \hat{P}_i \, e^{-\frac{i\hat{Q}}{\hbar}}$$

Remark

Q real $\longrightarrow$ $\hat{Q}$ hermitian $\rightarrow$ $e^{-\frac{i\hat{Q}}{\hbar}}$ unitary

Generalization

$$\hat{A}' = e^{\frac{i\hat{Q}}{\hbar}} \hat{A} \, e^{-\frac{i\hat{Q}}{\hbar}}$$

↳ states?

↳ require $\langle \hat{A} \rangle$ to be the same before and after symmetry transformation

$$\langle \hat{A} \rangle = \langle \varphi | \hat{A}' | \varphi \rangle = \langle \varphi | e^{\frac{i\hat{Q}}{\hbar}} \hat{A} \, e^{-\frac{i\hat{Q}}{\hbar}} | \varphi \rangle = \langle \varphi' | \hat{A} | \varphi' \rangle$$

On kets,

$$|\varphi'\rangle = e^{-\frac{i\vec{Q}}{\hbar}}|\varphi\rangle$$ → there is a caveat

General Properties of Symmetries

↳ Symmetry: transformation that leaves the Physics invariant

QM: symmetries must leave probabilities invariant

↳ symmetries must act on rays of vectors

↳ $|\langle\varphi|\chi\rangle|^2 = |\langle\varphi_g|\chi_g\rangle|^2$

$$g: \underbrace{\|\varphi\rangle}_{\{e^{i\alpha}|\varphi\rangle\}} \to \|\varphi_g\rangle$$

Conditions on g

i) e ($ge = eg = g$) is a symmetry

ii) if g is a symmetry, so is g^{-1}

iii) if g_1 and g_2 is a symmetry, so is their composition

iv) composition is associative

↳ description of symmetries in terms of Group Theory

If $[g_1, g_2] = 0$, the group is Abelian. Otherwise, non-Abelian.

Representations

$$g \to U(g)$$ $\to$ operator $\to$ must satisfy all the properties of a group

$$\begin{cases} U(e) = \mathbb{1} \\ U(g)^{-1} \text{ is a symmetry} \\ U(g_2)U(g_1) \text{ is a symmetry} \end{cases}$$

when the space on which $U(g)$ is acting is N-dimensional, we talk about a N-dimensional representation

Given two representations of the same group $U(g)$ and $U'(g)$, both N-dimensional, we say they are equivalent iff $\exists\, S$

$$U(g) = S\,U'(g)\,S^{-1}.$$

If the representation is equivalent to a representation of the form $\begin{bmatrix} U_1(g) & A(g) \\ 0 & U_2(g) \end{bmatrix}$, we say it is reducible. When $A(g)=0$, the representation is fully reducible. When it is not possible to block-diagonalize further the operators, each block is said to be an irreducible representation

Wigner Theorem: here stated without proof

If $g : \|\varphi\rangle \to \|\varphi_g\rangle$ is a symmetry, then it can be implemented by an operator $\hat{U}(g)$ that acts on kets of the ray

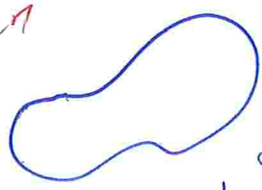
$$|\varphi\rangle \to \hat{U}(g)|\varphi\rangle.$$ $|\varphi\rangle$ representative of $\|\varphi\rangle$

Furthermore, $\hat{U}(g)$ is either unitary or antiunitary and is fixed up to a phase. □

Unitary: $\langle \hat{U}\varphi | \hat{U}\chi \rangle = \langle \varphi | \chi \rangle$

Anti-unitary: $\langle \hat{U}\varphi | \hat{U}\chi \rangle = \langle \varphi | \chi \rangle^*$

simply connected



can be deformed continuously to a point

Let $g = g_1 g_2$

$\hat{U}(g)|\varphi\rangle \in \| \varphi_g \rangle$

$\hat{U}(g_1 g_2)|\varphi\rangle \in \| \varphi_{g_1 g_2} \rangle$

$$\hat{U}(g)|\varphi\rangle = e^{i\alpha} \hat{U}(g_1)\hat{U}(g_2)|\varphi\rangle$$

$$\hookrightarrow \hat{U}(g) = e^{i\alpha}\hat{U}(g_1)\hat{U}(g_2)$$

Projective Representation

Weinberg QFT Vol. 1

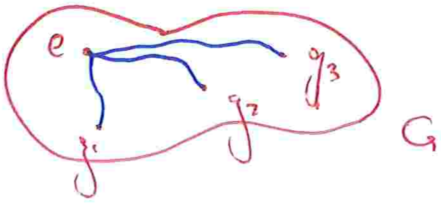
i) α can be absorbed in the definition of $\hat{U}(g)$ when the group is simply connected

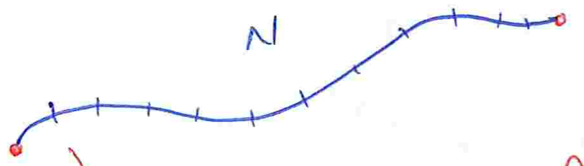
ii) when the group is not simply connected, we find a group $\tilde{G}$ that is simply connected and for which $\exists$ homomorphism $\tilde{G} \to G$ and we work with the unitary representation of $\tilde{G}$

$\hookrightarrow$ $\tilde{G}$ is said to be the universal covering of G

Lie Groups

Each element can be connected to e by a continuous path inside the group





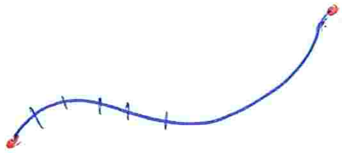
α: continuous parameter

$g(0) = e$

$$g(\alpha) = \lim_{N\to+\infty}\left(e + i\frac{\alpha}{N}t\right)^N \equiv e^{i\alpha t}$$

t → generator → Lie Algebra

For unitary or anti-unitary representations



$$\hat{U}(g) = e^{i\alpha\hat{t}}$$

$\hat{t}$ is a hermitian operator

Translations in Space & in Time

Classical Mechanics: linear momentum generates translations in space

$Q = \vec{\epsilon}\cdot\vec{p}$

$$\delta x_i = \{x_i, Q\} = \epsilon_k\{x_i, p_k\} = \epsilon_i$$

$$\delta p_i = \{p_i, Q\} = \epsilon_k\{p_i, p_k\} = 0$$

Canonical Quantization

$$\{x_i, p_k\} = \delta_{ik} \longrightarrow [\hat{x}_i, \hat{p}_k] = i\hbar\,\delta_{ik}$$

$$\{p_i, p_k\} = 0 \longrightarrow [\hat{p}_i, \hat{p}_k] = 0$$

the different components of momentum are compatible

$$\delta x_i = \{x_i, \vec{\epsilon}\cdot\vec{p}\} \longrightarrow \hat{X}_i' = e^{\frac{i\vec{\epsilon}\cdot\hat{\vec{P}}}{\hbar}} \hat{X}_i \, e^{\frac{-i\vec{\epsilon}\cdot\hat{\vec{P}}}{\hbar}} = \hat{X}_i + e_i$$

$$\delta p_i = \{p_i, \vec{\epsilon}\cdot\vec{p}\} \longrightarrow \hat{P}_i' = \underbrace{e^{\frac{i\vec{\epsilon}\cdot\hat{\vec{P}}}{\hbar}} \hat{P}_i \, e^{\frac{-i\vec{\epsilon}\cdot\hat{\vec{P}}}{\hbar}}}_{\text{commute}} = \hat{P}_i$$

$$e^{\frac{-i\vec{\epsilon}\cdot\hat{\vec{P}}}{\hbar}} |\vec{x}\rangle = \int e^{\frac{-i\vec{\epsilon}\cdot\hat{\vec{P}}}{\hbar}} |\vec{p}\rangle\langle\vec{p}|\vec{x}\rangle \, d^3p$$

$$= \int e^{-\frac{i\vec{\epsilon}\cdot\vec{p}}{\hbar}} |\vec{p}\rangle \cdot \frac{e^{-\frac{i\vec{p}\cdot\vec{x}}{\hbar}}}{(2\pi\hbar)^{3/2}} \, d^3p$$

$$= \int |\vec{p}\rangle \cdot \frac{1}{\sqrt{2\pi\hbar}^{\,3}} \, e^{-\frac{i\vec{p}\cdot(\vec{x}+\vec{\epsilon})}{\hbar}} \, d^3p$$

$$= \int |\vec{p}\rangle\langle\vec{p}|\vec{x}+\vec{\epsilon}\rangle \, d^3p = |\vec{x}+\vec{\epsilon}\rangle$$

Classical Mechanics: the Hamiltonian generates translations in space $\rightarrow$ $Q = \Delta t H$

$$\hat{A}' = e^{\frac{i\Delta t\hat{H}}{\hbar}} \hat{A} \, e^{-\frac{i\Delta t\hat{H}}{\hbar}}$$ $\rightarrow$ Heisenberg picture

in CM, observables evolve in time, and it is thus natural that the analogy between CM and QM comes from HP, given that the state evolution of SP is new

Symmetries of the Hamiltonian

$$\hat{U}^\dagger \hat{H} \hat{U} = \hat{H}$$
$$\hat{H}\hat{U} = \hat{U}\hat{H} \quad \Rightarrow \quad \hat{H}(\hat{U}|E_n\rangle) = \hat{U}(\hat{H}|E_n\rangle) = E_n(\hat{U}|E_n\rangle)$$
$$[\hat{U}, \hat{H}] = 0$$

$\hat{U}|E_n\rangle$ are eigenstates with eigenvalue E_n

there may be a degeneracy

if there is degeneracy, it is possible and plausible that there is a symmetry somewhere

e.g. hydrogen atom

as we shall see

Suppose $\hat{U}$ is a unitary representation of a Lie group

$$\hat{U} = e^{-i\alpha\hat{T}} \approx \mathbb{1} - i\alpha\hat{T}$$

hermitian

$$[\hat{U}, \hat{H}] = 0 = [\mathbb{1} - i\alpha\hat{T}, \hat{H}]$$
$$= -i\alpha[\hat{T}, \hat{H}] \Rightarrow [\hat{T}, \hat{H}] = 0$$
$$\Downarrow$$
$$\frac{d\hat{T}}{dt} = 0$$

quantum version of Noether's Theorem

Rotations in $\mathbb{R}^n$

transformations that preserve the scalar product

$$\vec{v}' = R\vec{v}$$
$$\vec{v}' \cdot \vec{w}' = \vec{v} \cdot \vec{w}$$

and therefore preserve angles, norms, et cetera

$$\vec{v}^{\,T} R^T R \vec{w} = \vec{v}^{\,T} \vec{w}$$

$$R^T R = \mathbb{1}$$

defines a group

$$O(n) = \{ R \in M_n(\mathbb{R}) ;\ R^T R = \mathbb{1} \}$$

orthogonal group

$$\det(R^T R) = \det \mathbb{1} = 1$$

$$(\det R)^2 = 1 \implies \det R = \pm 1$$

proper rotations

Lie group $SO(n)$

special orthogonal

space inversions

not a group

$(-\mathbb{1})(-\mathbb{1}) = \mathbb{1}$

what is the Lie algebra of $SO(n)$?

$$R = e^{i\theta T}$$

generator of rotations

$$R = \sum_n e^{i\theta T_n} |T_n\rangle\langle T_n|$$

eigenvalues of T

$$1 = \det R = \prod_n e^{i\theta T_n}$$

$$= e^{i\theta \sum_n T_n} = e^{i\theta \,\mathrm{tr}(T)} \implies \mathrm{tr}(T) = 0$$

$$R^T R = \mathbb{1}$$

$$(\mathbb{1} + i\theta T^T)(\mathbb{1} + i\theta T) = \mathbb{1}$$

$$\mathbb{1} + i\theta(T^T + T) = \mathbb{1}$$

$$T^T = -T$$

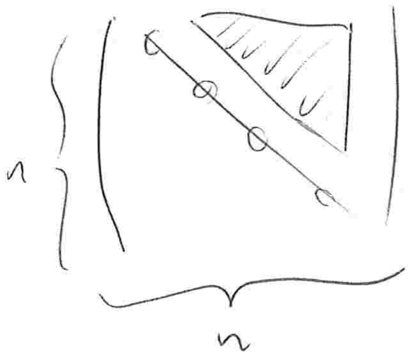
antisymmetric matrix

$$T = \begin{bmatrix} 0 & n_1 & n_2 & \cdots \\ -n_1 & 0 & n_3 & \cdots \\ -n_2 & -n_3 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$T = \sum_i n_i T_i$$

↳ generators

↳ how many are there?



$$= \frac{n^2 - n}{2} = \frac{n(n-1)}{2}$$

→ number of generators of $SO(n)$

↳ the representation of dim $= n$ is called fundamental representation

e.g.

$n=2$: 1 trivial

$n=3$: 3 Euler angles

$n=4$: 6

Closure of $SO(n)$

$$R R' = R''$$

$$R = e^{i\theta T} = e^{i\theta n_i T_i} = e^{i\theta_i T_i}$$

$$e^{i\theta_i T_i} e^{i\theta_i' T_i} = e^{i\theta_i'' T_i}$$

$$i\theta_i'' T_i = \log\left(e^{i\theta_i T_i} e^{i\theta_i' T_i}\right) = \log\Big(\mathbb{1} + \overbrace{e^{i\theta_i T_i} e^{i\theta_i' T_i} - \mathbb{1}}^{K}\Big)$$

$$i\theta_i'' T_i \simeq K - \frac{1}{2}K^2$$

$$= i(\theta_i + \theta_i')T_i + \frac{1}{2}\theta_i\theta_j'\left(T_j T_i - T_i T_j\right)$$

$$\theta_i\theta_j'[T_i, T_j] = i\,\underbrace{2(\theta_k + \theta_k' - \theta_k'')}_{\gamma_k \,=\, \theta_i\theta_j' f_{ijk}} T_k$$

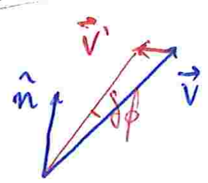
↳ I impose so the relation holds $\forall\, \theta_i, \theta_j'$

$$[T_i, T_j] = i \underbrace{f_{ijm}}_{\text{structure constants}} T_m$$

$[T_i, T_j] = 0 \Rightarrow$ Abelian

$[T_i, T_j] = i f_{ijk} T_k \Rightarrow$ non-abelian

SO(3)



$$\vec{v}' = \vec{v} + \delta\phi\, \hat{n}\times\vec{v} = R\vec{v}$$

$$= (\mathbb{1} + i\delta\phi T)\vec{v}$$

$$= \vec{v} + i\delta\phi T\vec{v}$$

$$iT\vec{v} = \hat{n}\times\vec{v}$$

$$T_{ik} v_k = -i\epsilon_{ijk} n_j v_k$$

$$T_{ik} = -i\epsilon_{ijk} n_j$$

$$T = i\begin{bmatrix} 0 & n_3 & -n_2 \\ -n_3 & 0 & n_1 \\ n_2 & -n_1 & 0 \end{bmatrix}$$

$$T_1 = i\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$$

$$T_2 = i\begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

$$T_3 = i\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Lie Algebra of SO(3):

$$[T_i, T_j] = i\,\epsilon_{ijk}\,T_k$$

Angular Momentum

↳ classical mechanics: angular momentum is the generator of rotations

$$\delta\vec{r} = \delta\phi\,\hat{n}\times\vec{r}$$

$$\delta r_i = \delta\phi\,\epsilon_{ijk}\,n_j\,r_k$$
$$= \{r_i, Q\}$$
$$= \underbrace{\frac{\partial r_i}{\partial r_k}}_{\delta_{ik}}\frac{\partial Q}{\partial p_k} = \frac{\partial Q}{\partial p_i}$$

$$Q = \delta\phi\,\epsilon_{ijk}\,n_j\,r_k\,p_i$$
$$= \delta\phi\,n_j\,(\epsilon_{ijk}\,r_k\,p_i)$$
$$= \delta\phi\,n_j\,(\epsilon_{jki}\,r_k\,p_i)$$
$$= \delta\phi\,n_j\,(\vec{r}\times\vec{p})_j$$
$$= \delta\phi\,\hat{n}\cdot\vec{L}$$

QM

unitary representation

not fundamental

$$\hat{U}(\delta\vec{\phi}) = e^{-i\delta\vec{\phi}\cdot\vec{J}/\hbar}$$

total angular momentum

must generate rotations of SO(3)

$$[\hat{J}_i, \hat{J}_j] = i\hbar\, \epsilon_{ijk}\, \hat{J}_k$$

in order to obtain the representation, we will find the largest possible set of compatible operators and study their eigenkets

Rule of thumb

\# commuting generators = # operators that commute with all elements of the algebra

Casimir operators

pick up one element from the algebra plus the Casimir operators and diagonalize this set

$[\hat{J}_i, \hat{J}_i] = 0$

\# comuting generators = 1 = # Casimir

$$[\hat{\vec{J}}^2, \hat{J}_k] = 0$$

implicit sum

$\hat{\vec{J}}^2 = \hat{J}_k^2$

$$\{\hat{\vec{J}}^2, \hat{J}_3\}$$

set of compatible operators we are going to study

$$\hat{\vec{J}}^2 = \begin{cases} \text{hermitian} \\ \text{positive} \to \text{eigenvalues} \geq 0 \end{cases}$$

$\hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2$

Eigenket problem: $|k, m\rangle$

$$\begin{cases} \hat{\vec{J}}^2 |k, m\rangle = k^2 \hbar^2 |k, m\rangle \\ \hat{J}_3 |k, m\rangle = m\hbar |k, m\rangle \end{cases}$$

can't we use information from $\hat{J}_1$ and $\hat{J}_2$?

$$\hat{J}_\pm \equiv \hat{J}_1 \pm i \hat{J}_2$$

$$(\hat{J}_-)^\dagger = (\hat{J}_1 - i\hat{J}_2)^\dagger$$
$$= \hat{J}_1 + i\hat{J}_2 = \hat{J}_+$$

Commutation relations

$$[\hat{J}_+, \hat{J}_-] = 2\hbar \hat{J}_3$$

$$[\hat{\vec{J}}^2, \hat{J}_\pm] = 0$$

$$[\hat{J}_3, \hat{J}_\pm] = \pm\hbar \hat{J}_\pm$$

$$\therefore \hat{J}_3 \hat{J}_\pm |k,m\rangle = (\pm\hbar \hat{J}_\pm + \hat{J}_\pm \hat{J}_3)|k,m\rangle$$
$$= \hat{J}_\pm (\hat{J}_3 \pm \hbar)|k,m\rangle$$
$$= \hat{J}_\pm \hbar(m \pm 1)|k,m\rangle$$
$$= \hbar(m \pm 1)\hat{J}_\pm |k,m\rangle$$

eigenket of $\hat{J}_3$ with eigenvalue $\hbar(m\pm1)$

$$\hat{J}_\pm |k,m\rangle = A|k, m\pm1\rangle$$

$A = ?$

$$\hat{\vec{J}}^2 = \hat{J}_+ \hat{J}_- + \hat{J}_3 (\hat{J}_3 - \hbar)$$
$$= \hat{J}_- \hat{J}_+ + \hat{J}_3 (\hat{J}_3 + \hbar)$$

$$\hat{J}_\pm \hat{J}_\mp = \hat{\vec{J}}^2 - \hat{J}_3 (\hat{J}_3 \mp \hbar)$$

determined by normalization

$$|A|^2 \langle k, m\pm 1 | k, m\pm 1 \rangle = \langle k,m| \hat{J}_\mp \hat{J}_\pm |k,m\rangle$$
$$= \langle k,m| \hat{\vec{J}}^2 - \hat{J}_3 (\hat{J}_3 \pm \hbar) |k,m\rangle$$
$$= \left(k^2 \hbar^2 - \hbar m (\hbar m \pm \hbar)\right) \langle k,m|k,m\rangle$$

$$|A|^2 = \hbar^2 \left(k^2 - m(m\pm 1)\right)$$

choice of phase

$A \in \mathbb{R}_+$

$$A = \hbar \sqrt{k^2 - m(m\pm 1)}$$

$$k^2 \geq m(m\pm 1)$$

For a fixed value of k, we have

$$\underbrace{\boxed{\frac{1}{2} - \frac{\sqrt{1+4k^2}}{2}}}_{-j} \leq m \leq \underbrace{\boxed{-\frac{1}{2} + \frac{\sqrt{1+4k^2}}{2}}}_{j} \geq 0$$

solving for k^2 in terms of j

$$k^2 = j(j+1), \qquad -j \leq m \leq j$$

$$\hat{J}_{\pm} |j, m\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)}\, |j, m \pm 1\rangle$$

$$\hat{J}_{+} |j, j\rangle = 0$$

$$\hat{J}_{-} |j, -j\rangle = 0$$

$$\left.\begin{array}{l} |j, j\rangle \\ |j, j-1\rangle \\ \quad\vdots \\ |j, -j+1\rangle \\ |j, -j\rangle \end{array}\right\} \underbrace{2j+1}_{\text{integer}} \text{ states}$$

$\hat{J}_{+}$ raises and $\hat{J}_{-}$ lowers between neighbouring states.

$\to \dim \mathcal{H} = 2j+1$

$\to j \in \frac{\mathbb{N}}{2}$

$j = \frac{1}{2}$, $\dim \mathcal{H} = 2$

$$|\tfrac{1}{2}, \tfrac{1}{2}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\tfrac{1}{2}, +\rangle = |+\rangle$$

$$|\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\tfrac{1}{2}, -\rangle = |-\rangle$$

$$\left.\begin{array}{l} \hat{J}_3 |+\rangle = \frac{\hbar}{2} |+\rangle \\ \hat{J}_3 |-\rangle = -\frac{\hbar}{2} |-\rangle \end{array}\right\} \quad \hat{J}_3 = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\left.\begin{array}{l} \hat{J}_+ |+\rangle = 0 \\ \hat{J}_+ |-\rangle = \hbar |+\rangle \end{array}\right\} \quad \left.\begin{array}{l} \hat{J}_+ = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\ \hat{J}_- = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \end{array}\right\} \quad \begin{array}{l} \hat{J}_1 = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \hat{J}_2 = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \end{array}$$

For $j = \frac{1}{2}$, $\hat{J}_i = \frac{\hbar}{2} \sigma_i$ $\qquad \hat{J}^2 \propto \mathbb{1}$

$j=1, \quad \dim \mathcal{H} = 3$

$$|1,1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \hat{J}_3 = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$|1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \hat{J}_1 = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$|1,-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad \hat{J}_2 = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}$$

$$\hat{\vec{J}}^2 = 2\hbar^2 \mathbb{1}$$

Theorem

All linear operators in $\mathcal{H}$ can be written as linear combinations of products of angular momentum operators □

$j=\frac{1}{2}$: $\quad M = \alpha_0 \mathbb{1} + \vec{\alpha} \cdot \frac{\vec{\sigma}}{2}$ → proved in problem sets

$j=1$: $\quad \dim \mathcal{H} = 3$

$$\underset{9}{M} = \underset{1}{\alpha_0 \mathbb{1}} + \underset{3}{\vec{\alpha} \cdot \vec{J}} + \underset{\substack{5 \\ \text{(I want)}}}{T}$$

→ should be quadratic in $\hat{J}_i$

$\hat{J}_i \hat{J}_k$ → Seems to have 9 degrees of freedom, but

- $[\hat{J}_i, \hat{J}_j] = i\hbar \epsilon_{ijk} \hat{J}_k$ → linear 3
- $\hat{\vec{J}}^2 = 2\hbar \mathbb{1}$ → identity 1

→ do not count

Symmetric and traceless combinations

$$T_{ik} = \frac{\hat{J}_i \hat{J}_k + \hat{J}_k \hat{J}_i}{2} - \frac{2}{3}\delta_{ik}$$

$$\sum_i T_{ii} = \hat{\vec{J}}^2 - 2 = 0$$

apart from some $\hbar$'s

This leaves us with 5 degrees of freedom, and

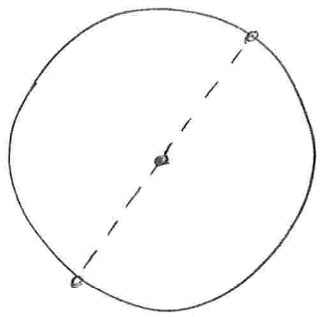
$$M = \alpha_0 \mathbb{1} + \vec{\alpha}\cdot\vec{J} + \alpha_{ij} T_{ij}$$

Connection between SO(3) and SU(2)

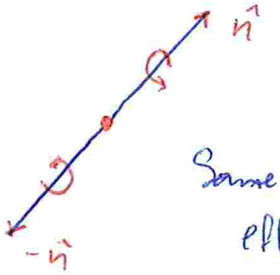
Topology = topology parameters of rotations

$$R(\vec{\theta}) = e^{i\vec{\theta}\cdot\vec{T}}$$

$$\vec{\theta} = \theta \cdot \hat{n} \qquad 0 \leq \theta \leq \pi$$



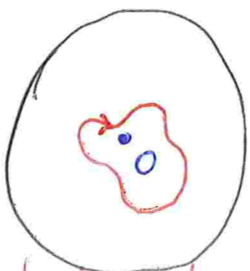
$\theta = \pi$



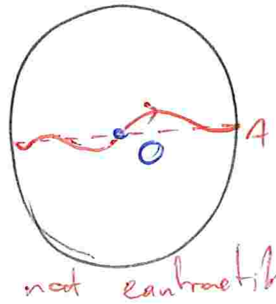
Same effect

Topology of SO(3):

ball of radius π with antipodal points identified



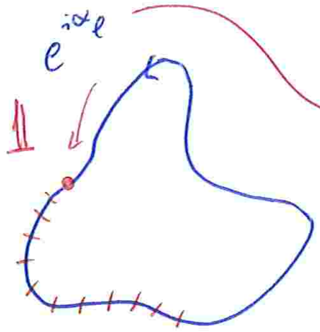
contractible to O



not contractible to O

Unitary representation

$$\hat{U}(g_1 g_2) = e^{i\alpha(g_1, g_2)}\, \hat{U}(g_1)\, \hat{U}(g_2)$$



gains a phase after walking the path

Take $\hat{U}$ to be N-dim representation and impose

$\det \hat{U} = 1$

$$\mathbb{1} \xrightarrow{\text{path } \ell} e^{i\alpha_\ell}\mathbb{1}$$

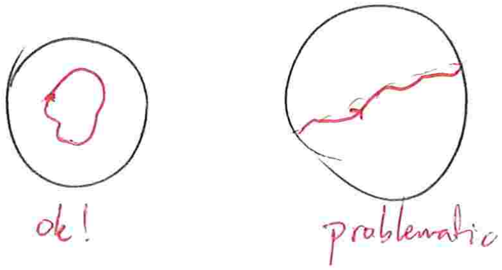
$$1 = \det\left(e^{i\alpha_\ell}\mathbb{1}\right) = e^{iN\alpha_\ell} = 1$$

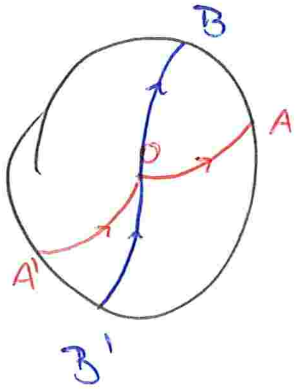
Simply Connected Space: all the paths are contractible to 0

Weinberg (QFT: I) α_ℓ can always be chosen to be 0 in simply connected spaces

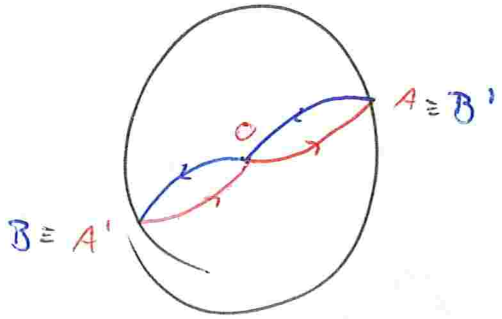
↳ only genuine unitary representations

SO(3) is not simply connected ↳ we need to worry about projective representations

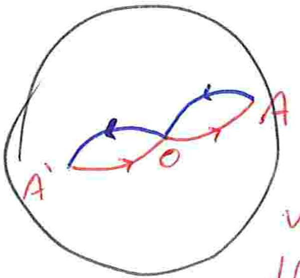




$B' \to A$



two closed paths



with two closed paths, we can now deform them to O

$(e^{i\alpha_\ell})^2 = 1$ contractible

SO(3) is doubly connected

$2\alpha_\ell = 2\pi n$

$e^{i\alpha_\ell} = \pm 1$

$(e^{i\alpha_\ell})^N = 1 \rightarrow N\alpha_\ell = 2\pi m$

$(\pm 1)^N = 1$

$N = 2j + 1$

$j = \frac{odd}{2} \Rightarrow N$ is even $\Rightarrow e^{i\alpha_\ell} = \pm 1$ → projective representations

$j = \frac{even}{2} \Rightarrow N$ is odd $\Rightarrow e^{i\alpha_\ell} = +1 \Rightarrow \alpha_\ell$

→ genuine representations

Projective representations of rotations when

$$j = \frac{\text{odd}}{2} \qquad \hat{\mathcal{U}}(g) = \pm\, \hat{\mathcal{U}}(g_1)\, \hat{\mathcal{U}}(g_2)$$

Genuine representations of rotations when

$$j = \frac{\text{even}}{2} \qquad \hat{\mathcal{U}}(g) = +\, \hat{\mathcal{U}}(g_1)\, \hat{\mathcal{U}}(g_2)$$

Example:

$$\vec{\alpha} = \alpha \hat{n}$$

$$j = \frac{1}{2}$$

$$\hat{\mathcal{U}}(\vec{\alpha}) = e^{-i\frac{\vec{\alpha}\cdot\vec{\sigma}}{2\hbar}} = \cos\left(\frac{\alpha}{2}\right) - i \sin\left(\frac{\alpha}{2}\right) \hat{n}\cdot\vec{\sigma}$$

Rotations around 3rd axis $\quad \hat{n} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$$\hat{\mathcal{U}}(\alpha\hat{z}) = \cos\left(\frac{\alpha}{2}\right) - i \sin\left(\frac{\alpha}{2}\right) \sigma_3$$

$$\alpha = \pi; \quad \hat{\mathcal{U}}(\pi\hat{z}) = -i\sigma_3$$

$$\alpha = 2\pi; \quad \hat{\mathcal{U}}(2\pi\hat{z}) = -1$$

$$\left.\begin{array}{l} \hat{\mathcal{U}}(2\pi) = -1 \\ \hat{\mathcal{U}}(\pi)\hat{\mathcal{U}}(\pi) = (-i\sigma_3)^2 = -1 \end{array}\right\} + \text{ sign in this case}$$

Covering Group of SO(3)

there is a 1:1 correspondence between vectors in $\mathbb{R}^3$ and traceless, hermitian, 2×2 matrices

$$\vec{V} \in \mathbb{R}^3 \Rightarrow \hat{V} = V_i \sigma_i = \begin{pmatrix} V_3 & V_1 - iV_2 \\ V_1 + iV_2 & -V_3 \end{pmatrix}$$

$$\det \hat{V} = -V_1^2 - V_2^2 - V_3^2 = -\|\vec{V}\|^2, \quad \mathrm{tr}\, \hat{V}^2 = 2\|\vec{V}\|^2$$

Let $\hat{U}$ be unitary

$$\hat{V} \to \hat{U}^\dagger \hat{V} \hat{U} = \hat{V}'$$ still hermitian

$$\det \hat{V}' = (\det \hat{U})^2 \underbrace{\det \hat{V}}_{-\|\vec{V}\|^2}$$

in fact, I believe $\det(\hat{U}^\dagger \hat{U}) = \|\det \hat{U}\|^2 = 1$, but we want $\det \hat{U} = 1$ for some other reason...

If $\det \hat{U} = \pm 1$, $\det \hat{V}' = \det \hat{V}$

$$\|\vec{V}'\|^2 = \|\vec{V}\|^2$$

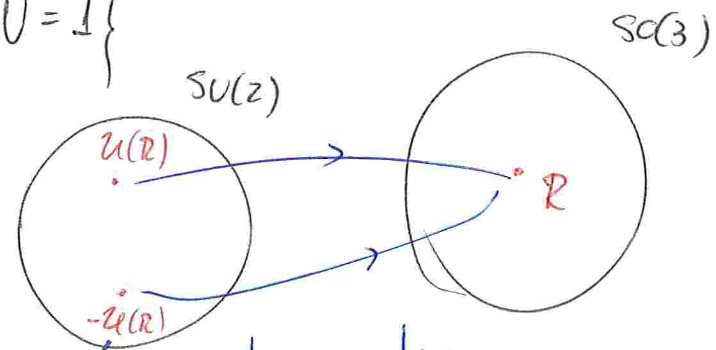
if $\det \hat{U}' = -1$, $\hat{U}' = -1\,\hat{U}$

rotations are implemented on $\hat{V}$ by $\hat{U}^\dagger \hat{V} \hat{U}$

Let us consider unitary $\hat{U}$ with $\det \hat{U} = +1$

$$SU(2) = \{\hat{U},\ \hat{U}\hat{U}^\dagger = \mathbb{1},\ \det \hat{U} = 1\}$$

special unitary



homomorphism

I guess this should be $U^\dagger(R)$

Parameters for SU(2) transformations

$$\hat{U} = \alpha_0 \mathbb{1} + \alpha_i T_i$$

$$= a_0 \mathbb{1} + \vec{\theta} \cdot \vec{\sigma}$$

around $\mathbb{1}$, $a_0 \simeq 1$

$\vec{\theta} \cdot \vec{\sigma}$ will be hermitian if $\vec{\theta} \in \mathbb{R}^3$

three parameters

just like SO(3)

$$\hat{U} = \mathbb{1} + \alpha_i T_i = \mathbb{1} + \theta_i \sigma_i$$

$\alpha_i = 2\theta_i$

$T_i = \frac{\sigma_i}{2}$ ← generators of SU(2) → Lie algebra of SU(2)

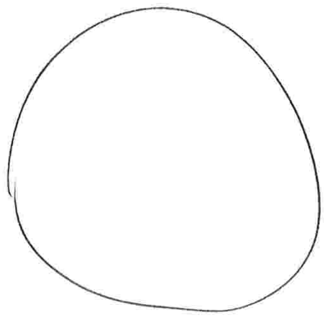
$[T_i, T_j] = i\,\epsilon_{ijk} T_k$

Topology of SU(2)

$$\hat{U} = e^{\frac{i\vec{\alpha}\cdot\vec{\sigma}}{2}} = \cos\left(\frac{\alpha}{2}\right) + i\sin\left(\frac{\alpha}{2}\right)\hat{n}\cdot\vec{\sigma}$$

$\vec{\alpha} = \alpha\hat{n} \longrightarrow$ topology

$0 \leq \alpha \leq \pi$



$\alpha = \pi$: $\hat{n} \longrightarrow \hat{U} = i\hat{n}\cdot\vec{\sigma}$; $-\hat{n} \longrightarrow \hat{U} = -i\hat{n}\cdot\vec{\sigma}$; $\neq$

the topology is a ball of radius π, without identification of antipodal points

↓

SU(2) is simply connected

Addition of Angular Momenta

$\vec{J}_1, \vec{J}_2$

→ 2 particle system

→ 1 particle system with orbital angular momentum + spin

What happens to $\vec{J} = \vec{J}_1 + \vec{J}_2$?

$\hookrightarrow \{(\vec{J}_1)^2, (J_1)_3, (\vec{J}_2)^2, (J_2)_3\}$

$\hookrightarrow |\alpha, j_1, j_2, m_1, m_2\rangle$

$\hookrightarrow$ other quantum numbers

For α, j_1, j_2 given, there are still $(2j_1+1)(2j_2+1)$ possible kets

$$\vec{J}_1 \to \mathcal{H}_1$$
$$\vec{J}_2 \to \mathcal{H}_2$$

$$\boxed{\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2}$$

$$\dim \mathcal{H}_1 = 2j_1+1$$
$$\dim \mathcal{H}_2 = 2j_2+1$$
$$\dim \mathcal{H} = (2j_1+1)(2j_2+1)$$

$$\Downarrow$$

$$\vec{J} = \vec{J}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \vec{J}_2$$

Could we use another basis to describe our system?

total

$$[\vec{J}^2, \vec{J}_1^2] = 0 \qquad [\vec{J}^2, J_3] = 0$$
$$[\vec{J}^2, \vec{J}_2^2] = 0 \qquad [\vec{J}_1^2, J_3] = 0$$
$$[\vec{J}_2^2, J_3] = 0$$

$\{\vec{J}_1^2, \vec{J}_2^2, \vec{J}^2, J_3\}$ are compatible operators

$\hookrightarrow |\alpha, j_1, j_2, J, m\rangle \equiv |j\, m\rangle$

$\hookrightarrow \alpha, j_1, j_2$ are fixed

two bases

$|\alpha, j_1, j_2, m_1, m_2\rangle \equiv |m_1\, m_2\rangle$

How can we find j and m given j_1, j_2, m_1, m_2?

$$J_3 |m_1 m_2\rangle = \left[(J_1)_3 \otimes \mathbb{1} + \mathbb{1} \otimes (J_2)_3 \right] |m_1\rangle \otimes |m_2\rangle$$
$$= (\hbar m_1 + \hbar m_2) |m_1\rangle \otimes |m_2\rangle$$
$$= \hbar(m_1 + m_2) |m_1 m_2\rangle = \hbar m |m_1 m_2\rangle$$
$$\downarrow$$
$$m = m_1 + m_2$$

Before we find j let us consider an example

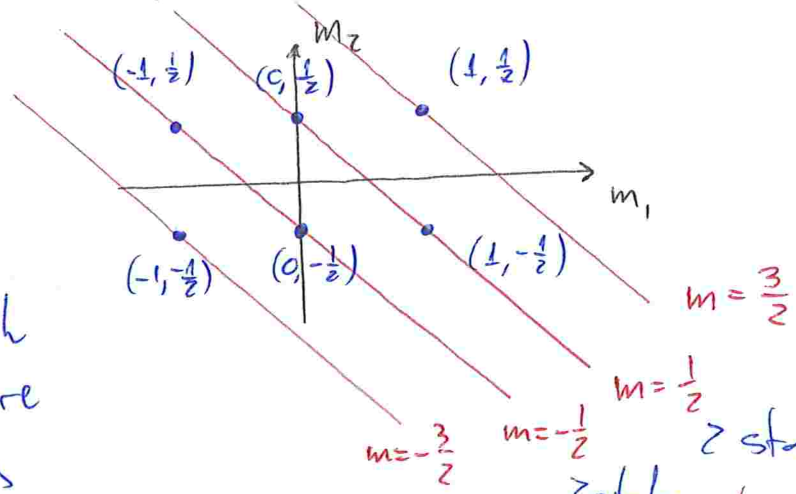
$j_1 = 1 \Rightarrow m_1 = -1, 0, 1$

$j_2 = \frac{1}{2} \Rightarrow m_2 = -\frac{1}{2}, \frac{1}{2}$

$m = m_1 + m_2$

$m_2 = m - m_1$

↳ curves with constant m are straight lines



1 state

2 states

2 states

1 state

has to be $|j = \frac{3}{2}, m = \frac{3}{2}\rangle$

has to be $|j = +\frac{3}{2}, m = -\frac{3}{2}\rangle$

how can we find these?

$|\frac{3}{2}, \frac{3}{2}\rangle$

$\downarrow J_-$

$|\frac{3}{2}, \frac{1}{2}\rangle$

$\downarrow J_-$

$|\frac{3}{2}, -\frac{1}{2}\rangle$

$\downarrow J_-$

$|\frac{3}{2}, -\frac{3}{2}\rangle$

two new states

↳ two are missing

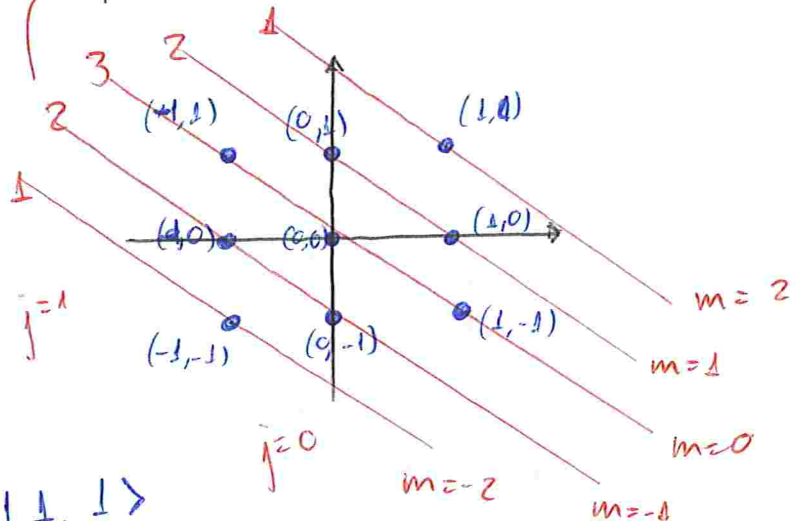
As the remaining states must have $m = \pm 1/2$, we assume they have $j = \frac{1}{2}$ (as it can't be $3/2$, for there are only 4 eigenstates with such a value) and obtain $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ and $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$.

$$j = \frac{3}{2} = j_1 + j_2$$

$$j = \frac{1}{2} = j_1 - j_2 = |j_1 - j_2|$$

Another example

$\left.\begin{matrix} j_1 = 1 \\ j_2 = 1 \end{matrix}\right\}$ 9 states



$j = 2$	$j = 1$	$j = 0$
$m=2$ $\|2, 2\rangle$		
$\downarrow$		
$m=1$ $\|2, 1\rangle$	$\|1, 1\rangle$	$\|0, 0\rangle$
$\downarrow$	$\downarrow$	
$m=0$ $\|2, 0\rangle$	$\|1, 0\rangle$	
$\downarrow$	$\downarrow$	
$m=-1$ $\|2, -1\rangle$	$\|1, -1\rangle$	
$\downarrow$		
$m=-2$ $\|2, -2\rangle$		
5	3	1

$$j = 2 = j_1 + j_2$$

$$j = 1$$

$$j = 0 = |j_1 - j_2|$$

In general, it does hold that

$$m = m_1 + m_2$$

$$|j_1 - j_2| \leq j \leq j_1 + j_2$$

$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ admits both $\{|m_1 m_2\rangle\}$ and $\{|j\, m\rangle\}$ as bases (α, j_1 and j_2 fixed)

$$|j\, m\rangle = \mathbb{1}\, |j\, m\rangle$$
$$= \sum_{m_1, m_2} |m_1\, m_2\rangle \underbrace{\langle m_1\, m_2 | j\, m\rangle}_{\text{Clebsch - Gordan coefficient}}$$

Example:

$j_1 = j_2 = \frac{1}{2}$

$\{|m_1\, m_2\rangle\} = \{|+\,+\rangle, |+\,-\rangle, |-\,+\rangle, |-\,-\rangle\}$

$\{|j\, m\rangle\} = \{|1,1\rangle, |1,0\rangle, |1,-1\rangle, |0,0\rangle\}$

How do we compute the CG coefficients?

$|1\,1\rangle \rightarrow m = 1 = \frac{1}{2} + \frac{1}{2} \rightarrow$ only satisfied by $|+\,+\rangle$

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

$|1\,0\rangle = k J_-\, |1\,1\rangle = k\hbar\sqrt{2}\,|1\,0\rangle \Rightarrow \quad k = \frac{1}{\hbar\sqrt{2}}$

$$|1,0\rangle = \frac{J_-}{\hbar\sqrt{2}}\, |1\,1\rangle$$

$$|1,0\rangle = \frac{J_-|1\,1\rangle}{\hbar\sqrt{2}} = \frac{1}{\hbar\sqrt{2}}\left(J_{1-} + J_{2-}\right)|+\,+\rangle$$

$$= \frac{1}{\hbar\sqrt{2}}\left(\hbar\,|-\,+\rangle + \hbar\,|+\,-\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\left(|-\,+\rangle + |+\,-\rangle\right)$$

If we want the basis to be orthonormal,

$$|0\,0\rangle = \frac{1}{\sqrt{2}}\left(|+\,-\rangle - |-\,+\rangle\right)$$

$$\begin{cases} |1\,1\rangle = |+\,+\rangle \\ |1\,0\rangle = \frac{1}{\sqrt{2}}\left(|+\,-\rangle + |-\,+\rangle\right) \\ |1\,-1\rangle = |-\,-\rangle \\ |0\,0\rangle = \frac{1}{\sqrt{2}}\left(|+\,-\rangle - |-\,+\rangle\right) \end{cases}$$

Explict (tensor) computation

Total angular momentum $\Leftrightarrow$ which representation of $SO(3)/SU(2)$?

$$\left[\vec{J}_1\otimes\mathbb{1},\ \mathbb{1}\otimes\vec{J}_2\right] = 0$$

Rotation: $$\mathcal{U}(R) = e^{i\vec{\alpha}\cdot\left(\vec{J}_1\otimes\mathbb{1} + \mathbb{1}\otimes\vec{J}_2\right)/\hbar}$$

$$= e^{i\vec{\alpha}\cdot(\vec{J}_1\otimes\mathbb{1})/\hbar}\; e^{i\vec{\alpha}(\mathbb{1}\otimes\vec{J}_2)/\hbar}$$

$$= \left(e^{i\vec{\alpha}\cdot\vec{J}_1/\hbar}\otimes\mathbb{1}\right)\cdot\left(\mathbb{1}\otimes e^{i\vec{\alpha}\vec{J}_2/\hbar}\right)$$

$$e^{i\vec{\alpha}\cdot(\vec{J}_1\otimes\mathbb{1})/\hbar} = \sum_n \left(\frac{i\alpha}{\hbar}\right)^n \frac{(\vec{J}_1\otimes\mathbb{1})^n}{n!}$$

$$= \sum_n \left(\frac{i\alpha}{\hbar}\right)^n \frac{(\vec{J}_1)^n\otimes\mathbb{1}}{n!}$$

$$= e^{i\vec{\alpha}\vec{J}_1/\hbar}\otimes\mathbb{1}$$

$$(A\otimes\mathbb{1})(B\otimes\mathbb{1}) = (AB)\otimes\mathbb{1}$$

$$\mathcal{U}(R) = \left(e^{-i\vec{\alpha}\cdot\vec{J}_1/\hbar} \otimes \mathbb{1}\right)\cdot\left(\mathbb{1} \otimes e^{-i\vec{\alpha}\cdot\vec{J}_2/\hbar}\right)$$

$$= \left(\mathcal{U}_1(\vec{\alpha}) \otimes \mathbb{1}\right)\cdot\left(\mathbb{1} \otimes \mathcal{U}_2(\vec{\alpha})\right)$$

$$= \mathcal{U}_1 \otimes \mathcal{U}_2$$

product representation

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\{|m_1\, m_2\rangle\} = \{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$$

$$|v\rangle \otimes |w\rangle = \begin{pmatrix} v_1 w_1 \\ \vdots \\ v_1 w_n \\ v_2 w_1 \\ \vdots \end{pmatrix}$$

$$|++\rangle = |+\rangle \otimes |+\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|+-\rangle = |+\rangle \otimes |-\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|-+\rangle = |-\rangle \otimes |+\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|--\rangle = |-\rangle \otimes |-\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$J_3 = (J_1)_3 \otimes \mathbb{1} + \mathbb{1} \otimes (J_2)_3$$

$$= \frac{\hbar}{2}\sigma_3 \otimes \mathbb{1} + \mathbb{1} \otimes \frac{\hbar}{2}\sigma_3$$

$$= \frac{\hbar}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]$$

$$= \frac{\hbar}{2}\left[\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}\right]$$

$$= \frac{\hbar}{2}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} = \hbar\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$J_+ = \hbar \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad J_- = \hbar \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

$$|1,1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad |1,0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(|+-\rangle + |-+\rangle \right)$$

$$|1,-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \qquad |0,0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(|+-\rangle - |-+\rangle \right)$$

Generators

$\vec{J}^2$

$\lambda = 2$ (for $j=1$) w/ degeneracy 3

eigenvalues

$\lambda = 0$ (for $j=0$) w/ degeneracy 1

$$\underbrace{\left(\begin{array}{c|c} 3D & 0 \\ \hline 0 & 1D \end{array}\right)}_{\text{direct sum}}$$

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

or $2 \otimes 2 = 1 \oplus 3$

dimension

thus,

$$j_1 \otimes j_2 = \bigoplus_{|j_1 - j_2|}^{j_1 + j_2} J$$

Remark: as we have been doing, from now on we shall drop the hats on operators for simplicity of notation and the difference between operators and "non-operators" should be clear from context

Orbital Angular Momentum

vector product

CM $\qquad \vec{L} = \vec{r} \wedge \vec{p}$

$\downarrow$

QM $\qquad \vec{L} = \vec{r} \wedge \vec{p}$

operators

is this definition consistent with our understanding of angular momentum from the group theory point of view?

i) hermiticity

$$L_i^\dagger = (\epsilon_{ijk} r_j p_k)^\dagger = \epsilon_{ijk} p_k r_j \qquad [r_j, p_k] = i\hbar\,\delta_{jk}$$

$$= \epsilon_{ijk}(r_j p_k - \cancel{i\hbar\,\delta_{jk}}^{\,0})$$

$$= L_i$$

ii) commutation relation $\longrightarrow$ $[L_i, L_j] = i\hbar\epsilon_{ijk} L_k$

Holds (brute force computation)

Position Representation

$$\langle \vec{r} | e^{-\frac{i\alpha L_3}{\hbar}} | \psi \rangle \approx \psi(\vec{r}) - \frac{i\alpha}{\hbar} \langle \vec{r} | L_3 | \psi \rangle$$

$$= \psi(\vec{r}) - \frac{i\alpha}{\hbar} \langle \vec{r} | x p_y - y p_x | \psi \rangle$$

$$= \psi(\vec{r}) - \frac{i\alpha}{\hbar} \left[x\left(-i\hbar \frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)\right] \psi(\vec{r})$$

$$= \psi(\vec{r}) - \alpha x \frac{\partial \psi}{\partial y} + \alpha y \frac{\partial \psi}{\partial x}$$

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases}$$

$$\approx \psi(x + \alpha y, \; y - \alpha x, \; z)$$

↳ gets clearer in spherical coordinates

$$x + \alpha y = r\sin\theta(\cos\varphi + \alpha\sin\varphi)$$

$$\simeq r\sin\theta\cos(\varphi - \alpha)$$

$$y - \alpha x \approx r\sin\theta\sin(\varphi - \alpha)$$

$$\left[e^{-\frac{i\alpha L_3}{\hbar}}\psi\right](r, \theta, \varphi) = \psi(r, \theta, \varphi - \alpha)$$

↓ Taylor expansion

$$\psi(r,\theta,\varphi) - \frac{i\alpha}{\hbar}(L_3\psi)(r,\theta,\varphi) = \psi(r,\theta,\varphi) - \alpha\frac{\partial\psi}{\partial\varphi}$$

$$L_3 \psi = -i\hbar \frac{\partial \psi}{\partial \varphi}$$

Overall result → obtained after extensive and painful computation

$$\vec{L} = i\hbar \left[\frac{\hat{e}_\theta}{\sin\theta} \frac{\partial}{\partial \varphi} - \hat{e}_\varphi \frac{\partial}{\partial \theta} \right]$$

$$\vec{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right]$$

Eigenkets of Orbital Angular Momentum

↳ $|j\, m\rangle \rightarrow |l\, m\rangle$

↳ cannot depend on r, for angular momentum is related to rotations only

lives on the unit sphere

$$\langle \theta, \varphi | l, m \rangle \equiv Y_l^m(\theta, \varphi)$$

spherical harmonics

$$[L_3 Y_l^m](\theta,\varphi) = \langle \theta, \varphi | L_3 | l, m \rangle = \hbar m \langle \theta, \varphi | l, m \rangle$$

$$\parallel$$

$$-i\hbar \frac{\partial Y_l^m}{\partial \varphi}$$

$$-i\hbar \frac{\partial Y_l^m}{\partial \varphi} = \hbar m Y_l^m$$

↳ suggests separation of variables

PGF5001

$$Y_\ell^m(\theta,\varphi) = \Theta_{\ell m}(\theta)\,\Phi_{\ell m}(\varphi)$$

$$-i\hbar \frac{\partial \Phi_{\ell m}}{\partial \varphi}\,\Theta_{\ell m}(\theta) = \hbar m\, \Theta_{\ell m}(\theta)\,\Phi_{\ell m}(\varphi)$$

$$-i \frac{\partial \Phi_{\ell m}}{\partial \varphi} = m\,\Phi_{\ell m}(\varphi)$$

$$\Phi_{\ell m}(\varphi) = e^{im\varphi}$$

$$Y_\ell^m(\theta,\varphi) = \Theta_{\ell m}(\theta)\, e^{im\varphi}$$

dependence on φ is simply a phase

$$L^+ Y_\ell^\ell = 0$$

shall yield yet another differential equation

$$L^\pm = i\hbar\, e^{\pm i\varphi}\left[\frac{1}{\tan\theta}\frac{\partial}{\partial\varphi} \mp i\frac{\partial}{\partial\theta}\right]$$

$$L^\pm Y_\ell^{\pm\ell}(\theta,\varphi) = 0 \xrightarrow[\text{solution}]{} \Theta_{\ell,\pm\ell}(\theta) = C_\ell \sin^\ell\theta$$

$$Y_\ell^m(\theta,\varphi) = \frac{(-1)^\ell}{2^\ell \ell!}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}\; e^{im\varphi}\,(\sin\theta)^{-m}\left(\frac{d}{d\cos\theta}\right)^{\ell-m}(\sin\theta)^{2\ell}$$

normalized spherical harmonics

for Sakurai's choice of normalization

L02

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \quad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta, \quad Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\,e^{\pm i\varphi}\sin\theta$$

$$Y_2^0 = \sqrt{\frac{5}{64\pi}}\left(1 + 3\cos^2\theta - 3\sin^2\theta\right)$$

$$Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}}\,e^{\pm i\varphi}\sin\theta\cos\theta$$

$$Y_2^{\pm 2} = \sqrt{\frac{5}{32\pi}}\,e^{\pm i 2\varphi}\sin^2\theta$$

However, Y_ℓ^m accepts only integer values for ℓ, half-integers are forbidden. Why?

↳ $j = 1, 2, 3\ldots$ admits single valued representations
$j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ projective representation
↳ double valued

As wave functions must be single valued in all of space, we need to have single valued representations $\Rightarrow \ell = 1, 2, 3\ldots$

$R \to \pm\, \mathcal{U}(R)$

Useful Identities

$|\theta, \varphi\rangle$ → complete basis on the sphere

$$\int |\theta,\varphi\rangle\langle\theta,\varphi|\, d\Omega = \mathbb{1}$$

$$d\Omega = \sin\theta\, d\theta\, d\varphi$$

$$|\theta',\varphi'\rangle = \int |\theta,\varphi\rangle\underbrace{\langle\theta,\varphi|\theta',\varphi'\rangle}_{\frac{\delta(\varphi-\varphi')\,\delta(\theta-\theta')}{\sin\theta}} \sin\theta\, d\theta\, d\varphi$$

$\longrightarrow$ necessary if we want $\int |\theta,\varphi\rangle\langle\theta,\varphi|\, d\Omega = \mathbb{1}$ to hold

$$\sum_{l,m} Y_l^{m*}(\theta',\varphi')\, Y_l^m(\theta,\varphi) = \sum_{l,m} \langle l,m|\theta',\varphi'\rangle\langle\theta,\varphi|l,m\rangle$$

$$= \sum_{l,m} \langle\theta,\varphi|l,m\rangle\langle l,m|\theta',\varphi'\rangle$$

$$= \langle\theta,\varphi|\sum_{l,m}|l,m\rangle\langle l,m|\theta',\varphi'\rangle$$

$$= \langle\theta,\varphi|\theta',\varphi'\rangle$$

$$= \frac{\delta(\varphi-\varphi')\,\delta(\theta-\theta')}{\sin\theta}$$

$$\int Y_{l'}^{m'*}(\theta'',\varphi'')\, Y_l^m(\theta,\varphi)\, d\Omega = \int \langle l',m'|\theta'',\varphi\rangle\langle\theta,\varphi|l,m\rangle\, d\Omega$$

$$= \langle l',m'|l,m\rangle = \delta_{ll'}\,\delta_{mm'}$$

Central Potential in QM

CM $\quad V(\vec{r}) = V(r)$

QM $\quad \hat{H} = \dfrac{\hat{P}^2}{2m} + V(\hat{r})$ $\longrightarrow$ $\hat{r} = \sqrt{\hat{x}^2+\hat{y}^2+\hat{z}^2}$

$$\vec{\hat{P}}^2 \xrightarrow{\text{rotation}} \sum_i \underbrace{\mathcal{U}^\dagger(R)\hat{P}_i\,\mathcal{U}(R)}_{R_{ik}\hat{P}_k}\underbrace{\mathcal{U}^\dagger(R)\,\hat{P}_i\,\mathcal{U}(R)}_{R_{im}\hat{P}_m}$$

$$\sum_{k,m} \underbrace{\boxed{\sum_i R_{ik} R_{im}}}_{(R^T R)_{km} = \delta_{km}} \hat{P}_k \hat{P}_m = \sum_k \hat{P}_k \hat{P}_k = \vec{\hat{P}}^2$$

H is invariant under rotations

$[\mathcal{U}(R), H] = 0$

$\hookrightarrow \mathcal{U}(R) = e^{-\frac{i\vec{\alpha}\cdot\vec{J}}{\hbar}}$

$\left.\right\}$ $[\vec{J}_i, H] = 0$

$[J_3, J^2] = 0$

$[J_3, H] = 0$

$[J^2, H] = 0$

what is the $\{H, J^2, J_3\}$ common set of eigen kets ?

$\hookrightarrow |E, l, m\rangle$

$\langle r, \theta, \varphi | E, l, m\rangle = \psi_{Elm}(r, \theta, \varphi) \rightarrow$ I want to discover

Momentum

$$\vec{\hat{P}}^2 = -\hbar^2 \nabla^2 = -\hbar^2 \left[\underbrace{\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)^2}_{-\frac{\hat{P}_r^2}{\hbar^2}} - \frac{\vec{L}^2}{\hbar^2 r^2} \right]$$

Radial Momentum

$$P_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

$$P_r^2 = -\hbar^2\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial}{\partial r}\left(\frac{1}{r}\right) + \frac{1}{r^2}\right)$$

$$-\frac{1}{r^2} + \frac{1}{r}\frac{\partial}{\partial r}$$

if in doubt, recall this is a calculation with operators and throw a test function

$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)$$

$$= -\frac{\hbar^2}{r}\frac{\partial^2}{\partial r^2} r$$

Schrödinger Equation

$$\left[\frac{\hat{P}^2}{2m} + V(r)\right]\psi_{E\ell m} = E\,\psi_{E\ell m}$$

separation of variables

$$\psi_{E\ell m} = P_{E\ell m}(r)\, Y_{E\ell m}(\theta,\varphi)$$

$$= \frac{u_{E\ell m}(r)}{r}\, Y_\ell^m(\theta,\varphi)$$

$$\left[\frac{P_r^2}{2m} + \frac{L^2}{2mr^2} + V(r)\right]\psi_{E\ell m} = E\,\psi_{E\ell m}$$

$$\left[\frac{P_r^2}{2m} + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)\right]\frac{u_{E\ell m}(r)}{r} = E\,\frac{u_{E\ell m}(r)}{r}$$

no dependence on m → $u_{E\ell}(r)$

$$u_{E\ell}'' - \underbrace{\left(\frac{\ell(\ell+1)}{r^2} + \frac{2mV(r)}{\hbar^2}\right)}_{V_{eff}(r)} u_{E\ell} = -\underbrace{\frac{2mE}{\hbar^2}}_{\epsilon}\, u_{E\ell}$$

radial equation

General Properties

Suppose $\lim_{r\to 0} r^2 V(r) = 0$

$$u''_{E\ell} \approx \frac{\ell(\ell+1)}{r^2} u_{E\ell} \quad \text{for small } r$$

$\downarrow$ ansatz: r^α

$$u_{E\ell} = A r^{\ell+1} + \cancel{B r^{-\ell}} \rightarrow \text{not square integrable for small } r$$

Flux of probability

$$\vec{j} = -\frac{i\hbar}{2m}\left[\psi^* \nabla \psi - \nabla \psi^* \psi\right]$$

$\downarrow$ radial component

$$j_r = \vec{j}\cdot\hat{e}_r = \frac{\hbar}{m}\,\mathrm{Im}\left[\psi^* \frac{\partial \psi}{\partial r}\right]$$

$$= \frac{\hbar}{m}\,\frac{u_{E\ell}}{r}\,\frac{\partial}{\partial r}\left(\frac{u_{E\ell}}{r}\right)$$

$$= \frac{\hbar}{m}\left(A r^{\ell} + B r^{-\ell-1}\right)\left(A\ell r^{\ell-1} - (\ell+1) B r^{-\ell-2}\right)$$

$$= \frac{\hbar}{m}\left(A^2 \ell r^{2\ell-1} - AB(\ell+1) r^{-2} + AB\ell r^{-2} - (\ell+1) B^2 r^{-2\ell-3}\right)$$

Flux of probability exiting from a small sphere around the origin

$$4\pi r^2 j_r \approx A^2 r^{2\ell+1} - AB(\ell+1) + AB\ell - (\ell-1) B^2 r^{-2\ell-1}$$

$\hookrightarrow$ blows up for small r $\rightarrow$ B has to be zero

Suppose $\lim_{r\to\infty} V(r) = 0$ $\qquad \epsilon = \frac{2mE}{\hbar^2}$

$u''_{E\ell} \approx -\epsilon\, u_{E\ell}$ for large r

$E>0$: plane waves

$$u_{E\ell} = A e^{+i\sqrt{\epsilon}r} + B e^{-i\sqrt{\epsilon}r}$$

$E<0$: $-\epsilon = k^2$

$$u_{E\ell} = A e^{-kr} + \cancel{B e^{kr}}$$

blows up $\quad B = 0$

This suggests the new ansatz:

$$u_{E\ell}(r) = r^{\ell+1} e^{-kr} w_{E\ell}(r)$$

boring, but does work

In terms of a dimensionless variable $\rho \equiv \sqrt{\epsilon}r$, the radial equation is written as

$$\left(\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} - \frac{2m V(\rho)}{\hbar^2} + 1\right) u_{E\ell} = 0.$$

we might now either solve the differential equation, for a given potential, or explore the symmetries of the problem

Free Particle

$$\left(\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2}\right) u_{E\ell}(\rho) = - u_{E\ell}(\rho)$$

Factorization

$$\hat{D}_\ell \equiv \frac{d}{d\rho} + \frac{\ell+1}{\rho}$$

$$\hat{D}_\ell^{+} = -\frac{d}{d\rho} + \frac{\ell+1}{\rho}$$

derivative is a pure imaginary operator

Dirac chap. 04

$$\hat{D}_\ell \hat{D}_\ell^{+} = \left(\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right)\left(-\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right)$$

$$= -\frac{d^2}{d\rho^2} - \frac{\ell+1}{\rho}\frac{d}{d\rho} + \frac{d}{d\rho}\left(\frac{\ell+1}{\rho}\right) + \frac{(\ell+1)^2}{\rho^2}$$

$$= -\frac{d^2}{d\rho^2} - \frac{\ell+1}{\rho}\frac{d}{d\rho} - \frac{\ell+1}{\rho^2} + \frac{\ell+1}{\rho}\frac{d}{d\rho} + \frac{(\ell+1)^2}{\rho^2}$$

$$= -\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2}$$

Bessel operator

$$-\hat{D}_\ell \hat{D}_\ell^{+} u_{E\ell}(\rho) = - u_{E\ell}(\rho)$$

$$\hat{D}_\ell \hat{D}_\ell^{+} u_{E\ell}(\rho) = u_{E\ell}(\rho)$$

$$\hat{D}_\ell^{+} \hat{D}_\ell = -\frac{d^2}{d\rho^2} + \frac{(\ell+1)(\ell+2)}{\rho^2} = \hat{D}_{\ell+1} \hat{D}_{\ell+1}^{+}$$

With this in mind, we make

$$\hat{D}_\ell \hat{D}_\ell^+ u_{E\ell} = u_{E\ell}$$

$$\hat{D}_\ell^+ \hat{D}_\ell \hat{D}_\ell^+ u_{E\ell} = \hat{D}_\ell^+ u_{E\ell}$$

$$\hat{D}_{\ell+1} \hat{D}_{\ell+1}^+ \underbrace{\left(\hat{D}_\ell^+ u_{E\ell}\right)}_{} = \left(\hat{D}_\ell^+ u_{E\ell}\right)$$

$$u_{E,\ell+1} \equiv \hat{D}_\ell^+ u_{E\ell}$$

we might find u_{E0} and apply $\hat{D}_\ell^+$ to obtain $u_{E\ell}$

$\ell = 0$:

$$\hat{D}_0 \hat{D}_0^+ u_{E0} = u_{E0}$$

$$-\frac{d^2}{d\rho^2} u_{E0} = u_{E0}$$

historical choice

$$u_{E0}^{(A)} = \sin\rho, \qquad u_{E0}^{(B)} = -\cos\rho$$

$$\downarrow \hat{D}_0^+ \qquad\qquad \downarrow \hat{D}_0^+$$

$$u_{E1}^{(A)} = -\cos\rho + \frac{\sin\rho}{\rho} \qquad u_{E1}^{(B)} = -\sin\rho - \frac{\cos\rho}{\rho}$$

$$\downarrow \hat{D}_1^+ \qquad\qquad \downarrow \hat{D}_1^+$$

$$u_{E2}^{(A)} \qquad\qquad u_{E2}^{(B)}$$

Spherical Bessel functions

$j_\ell(\rho)$

$\sim \rho^{\ell+1}$ for small ρ

Spherical Neumann functions

$n_\ell(\rho)$

diverges for small ρ

Solution:

$$\psi_{Elm} = N \frac{j_l(\rho)}{\rho} Y_l^m(\theta, \varphi)$$ ↳ plane wave

Hydrogen-like atoms ↳ Z protons, 1 electron

Let us start by solving two-body problems

Analogy with Classical Mechanics

$$\hat{H} = \frac{\hat{\vec{P}}_{CM}^2}{2M} + \frac{\hat{\vec{P}}_{rel}^2}{2\mu} + V(\hat{r})$$

$$\hat{r} = \hat{r}_2 - \hat{r}_1$$
$$M = m_1 + m_2$$
$$\mu = \frac{m_1 m_2}{M}$$

$$= \hat{H}_{CM} + \hat{H}_{rel}$$

Factorization of the Hilbert space: $\mathcal{H} = \mathcal{H}_{cm} \otimes \mathcal{H}_{rel}$

$$\downarrow$$

$$|\psi_{cm}\rangle \otimes |\psi_{rel}\rangle$$

$$\psi(\vec{R}, \vec{r}) = \left(\left(\langle \vec{R} | \otimes \langle \vec{r} | \right) \left(|\psi_{cm}\rangle \otimes |\psi_{rel}\rangle \right) \right)$$

$$= \langle \vec{R} | \psi_{cm} \rangle \langle \vec{r} | \psi_{rel} \rangle$$

$$= \psi_{cm}(\vec{R})\, \psi_{rel}(\vec{r})$$

$$\hat{H}\psi(\vec{R}, \vec{r}) = E\,\psi(\vec{R}, \vec{r})$$

$$\left[-\frac{\hbar^2 \nabla_{\vec{R}}^2}{2M} - \frac{\hbar^2 \nabla_{\vec{r}}^2}{2\mu} + V(\hat{r}) \right] \psi_{cm}(\vec{R})\, \psi_{rel}(\vec{r}) = E\, \psi_{cm}(\vec{R})\, \psi_{rel}(\vec{r})$$

$$\left(-\frac{\hbar^2}{2M}\nabla^2_{\vec{R}}\psi_{cm}\right)\psi_{rel}+\psi_{cm}\left(-\frac{\hbar^2}{2\mu}\nabla^2_{\vec{r}}+V(\hat{r})\right)\psi_{rel}=E\,\psi_{cm}\psi_{rel}$$

$$\underbrace{-\frac{\hbar^2\nabla^2_{\vec{R}}\psi_{cm}}{2M\psi_{cm}}}_{E_{cm}}\underbrace{-\frac{\hbar^2\nabla^2_{\vec{r}}\psi_{rel}}{2\mu\psi_{rel}}+\frac{V(\hat{r})\psi_{rel}}{\psi_{rel}}}_{E_{rel}}=E$$

$$-\frac{\hbar^2}{2M}\nabla^2_{\vec{R}}\psi_{cm}=E_{cm}\psi_{cm}$$ free particle → solved!

$$-\frac{\hbar^2}{2\mu}\nabla^2_{\vec{r}}\psi_{rel}+V(r)\psi_{rel}=E_{rel}\psi_{rel}$$

For a Coulomb potential,

$$V(r)=-\frac{Ze^2}{4\pi\epsilon_0 r}=-\frac{\hat{e}^2 Z}{r}\qquad \hat{e}^2\equiv\frac{e^2}{4\pi\epsilon_0}$$

Differential equation approach: Gottfried 3.6

Path integral approach: Shulmann

Symmetry approach

Classical problem: conservation of the Laplace-Runge-Lenz vector

$$\vec{M}=\frac{\vec{P}\wedge\vec{L}}{\mu}-Z\hat{e}^2\frac{\vec{r}}{r},\qquad \dot{\vec{M}}=\vec{0}$$

QM:

$$\hat{\vec{M}} = \frac{\hat{\vec{p}} \wedge \hat{\vec{L}} - \hat{\vec{L}} \wedge \hat{\vec{p}}}{2\mu} - \frac{Z\hat{e}^2\hat{\vec{r}}}{r}$$

remark: $(\hat{\vec{p}} \wedge \hat{\vec{L}})^\dagger = -\hat{\vec{L}} \wedge \hat{\vec{p}}$

$$[\hat{\vec{M}}, \hat{H}] = 0$$

$$\hat{\vec{L}} \cdot \hat{\vec{M}} = 0 = \hat{\vec{M}} \cdot \hat{\vec{L}}$$

$$\hat{\vec{M}}^2 = \frac{2\hat{H}}{\mu}\left(\hat{\vec{L}}^2 + \hbar^2\right) + Z^2\hat{e}^4$$

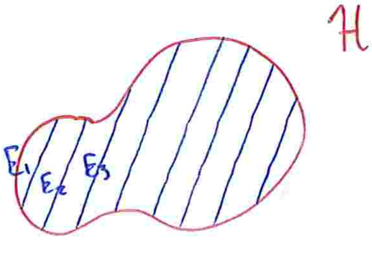
$$[\hat{L}_i, \hat{L}_j] = i\hbar\,\epsilon_{ijk}\hat{L}_k$$

$$[\hat{M}_i, \hat{L}_j] = i\hbar\,\epsilon_{ijk}\hat{M}_k$$

$$[\hat{M}_i, \hat{M}_j] = -i\hbar\,\epsilon_{ijk}\frac{2\hat{H}}{\mu}\hat{L}_k$$

the algebra is not closed

Restrict to subspaces with definite value for $\hat{H}$



the algebra is closed in this subspace

Choose subspaces with $E < 0$ (bound states)

$$\hat{\vec{N}} \equiv \left(\frac{-\mu}{2E}\right)^{1/2}\hat{\vec{M}}.$$

Now we have

$$[N_i, L_j] = i\hbar\,\epsilon_{ijk}N_k$$

$$[N_i, N_j] = i\hbar\,\epsilon_{ijk}L_k$$

and, of course, we still have

$$[L_i, L_j] = i\hbar\,\epsilon_{ijk}L_k$$

$$\vec{A} \equiv \frac{\vec{L}+\vec{N}}{2} \qquad \vec{B} \equiv \frac{\vec{L}-\vec{N}}{2}$$

$$\left.\begin{aligned} [A_i, A_j] &= i\hbar\,\epsilon_{ijk} A_k \\ [B_i, B_j] &= i\hbar\,\epsilon_{ijk} B_k \\ [A_i, B_j] &= 0 \end{aligned}\right\} \text{ algebra of } SU(2)\times SU(2) = SO(4)$$

Set of operators: $\{\vec{A}^2, A_3, \vec{B}^2, A_3\} \rightarrow |a, m_a, b, m_b\rangle$

$\hookrightarrow$ we know $a, b \in \frac{\mathbb{N}}{2}$

$$\vec{L}\cdot\vec{M} = 0 \Rightarrow \vec{L}\cdot\vec{N} = 0 = \vec{A}^2 - \vec{B}^2$$

$$\downarrow$$

$$\vec{A}^2 = \vec{B}^2$$

thus, our set of operators is actually $\{\vec{A}^2, A_3, B_3\}$

$$\downarrow$$

$$|a, m_a, m_b\rangle$$

$$\vec{A}^2 + \vec{B}^2 = \frac{\vec{L}^2 + \vec{N}^2}{2} = \frac{1}{2}\left(\vec{L}^2 - \frac{\mu}{2E}\vec{M}^2\right) = -\frac{1}{2}\left(\hbar^2 + \frac{\mu Z^2 \hat{e}^4}{2E}\right)$$

$$\underbrace{(\vec{A}^2 + \vec{B}^2)}_{-\frac{1}{2}\left(\hbar^2 + \frac{\mu Z^2 \hat{e}^4}{2E}\right)}|a, m_a, m_b\rangle = 2\hbar^2 a(a+1)|a, m_a, m_b\rangle$$

$\hookrightarrow \vec{A}^2 = \vec{B}^2$ and this is a $SO(3)$ operator

$$\therefore \quad E = -\underbrace{\frac{Z^2 \mu \hat{e}^4}{2\hbar^2}}_{\sim 13.6 \text{ eV}} \frac{1}{(2a+1)^2} \qquad n = 2a+1 \in \mathbb{N}$$

$$= -13.6 \frac{Z^2}{n^2} \text{ eV}$$

E, ℓ, m

$\uparrow$

?

$\vec{L} = \underbrace{\vec{A} + \vec{B}}_{\text{sum of angular momenta}}$ → both are angular momenta

$\ell = 0, \dots, \underbrace{a+b}_{2a}$ → or $n-1$, for fixed energy

However, electrons have spin

$$\vec{J} = \vec{L} + \vec{S}$$

Wave functions: $|E, \ell, m\rangle \otimes |s, m_s\rangle$

$$\langle r, \theta, \varphi | \left(|E, \ell, m\rangle \otimes |s, m_s\rangle \right) = \psi_{E\ell m}(r, \theta, \varphi) |s, m_s\rangle$$

Thus,

$$\psi = \sum_{\ell, m, m_s} C^{\ell}_{m, m_s} \psi_{E\ell m} |s, m_s\rangle$$

2 component object ← spinor

↳ most generic wave function

For $s = \frac{1}{2}$:

$$\psi = \begin{pmatrix} \sum_{\ell, m} C^{\ell}_{m, +\frac{1}{2}} \psi_{E,\ell,m} \\ \sum_{\ell, m} C^{\ell}_{m, -\frac{1}{2}} \psi_{E,\ell,m} \end{pmatrix}$$

for a proof, see the notes by Littlejohn ch. 19

Spherical Tensors & Wigner-Eckart Theorem

Scalar operators: S

$$|\alpha\rangle \xrightarrow{\text{rotation}} |\alpha'\rangle = \mathcal{U}(R)|\alpha\rangle$$

↳ arbitrary

$$\langle \alpha' | S | \alpha' \rangle \overset{\text{def}}{=} \langle \alpha | S | \alpha \rangle$$ → definition of a Scalar operator

$$\langle \alpha | \mathcal{U}^\dagger(R)\, S\, \mathcal{U}(R) | \alpha \rangle = \langle \alpha | S | \alpha \rangle$$

$$\mathcal{U}^\dagger(R)\, S\, \mathcal{U}(R) = S$$ → Scalar operator

Vector operators: V_i → $i = 1, 2, 3$

$$\langle \alpha' | V_i | \alpha' \rangle \overset{\text{def}}{=} R_{ik} \langle \alpha | V_k | \alpha \rangle$$

↳ rotation matrix

$$\mathcal{U}^\dagger(R)\, V_i\, \mathcal{U}(R) = R_{ik} V_k$$ → vector operator

Cartesian Tensors

Tensor operators: $T_{ijk\ldots}$

$$\mathcal{U}^\dagger(R)\, T_{m_1 m_2 \cdots m_N}\, \mathcal{U}(R) = R_{m_1 k_1} R_{m_2 k_2} \cdots R_{m_N k_N} T_{k_1 k_2 \cdots k_N}$$ → (cartesian) tensor operator

Scalar Operators and the Generators of Rotations

$$\mathcal{U}^\dagger(R)\, S\, \underbrace{\mathcal{U}(R)}_{e^{-\frac{i\vec{\alpha}\cdot\vec{J}}{\hbar}}} = S$$

expand

$$\left(\mathbb{1} + i\frac{\vec{\alpha}\cdot\vec{J}}{\hbar}\right) S \left(\mathbb{1} - i\frac{\vec{\alpha}\cdot\vec{J}}{\hbar}\right) = S$$

$$S + i\frac{\vec{\alpha}\cdot\vec{J}}{\hbar} S - i\frac{S\,\vec{\alpha}\cdot\vec{J}}{\hbar} = S$$

$$S + \frac{i\alpha_k}{\hbar}\left(J_k S - S J_k \right) = S$$

$$[J_k, S] = 0$$ scalar iff commutes with all three generators

Vecter Operators and the Generators of Rotations

$\mathbb{1} + i\alpha_m T_m$ generators of $SO(3)$ in $\mathbb{R}^3$

$$\mathcal{U}^\dagger(R) V_i \underbrace{\mathcal{U}(R)}_{\mathbb{1} - i\frac{\alpha_k J_k}{\hbar}} = R_{ik} V_k$$

$$(\alpha_m T_m)_{ij} = i\, \epsilon_{ijn}\, \alpha_n$$

$$V_i + \frac{i\alpha_k}{\hbar}[J_k, V_i] = V_i + i(\alpha_m T_m)_{ik} V_k$$

$$= V_i - \epsilon_{ikn}\alpha_n V_k$$

$$\frac{i\alpha_n}{\hbar}[J_n, V_i] = -\epsilon_{ikn}\alpha_n V_k$$ must be independent on α_n

$$\frac{i}{\hbar}[J_n, V_i] = -\epsilon_{ikn} V_k$$

$$[J_n, V_i] = i\hbar\, \epsilon_{nik} V_k$$

$$[J_i, V_j] = i\hbar\, \epsilon_{ijk} V_k$$ vector iff satisfies such a commutation relation

Cartesian tensors

$SO(3)$ representation

Example: T_{ij} → 3D, → 3D

dim: $3 \times 3 = 1 + 3 + 5$

j: $1 \times 1 = 0 + 1 + 2$

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3x3 matrix: 9-dim $\mathcal{H}$

$$\begin{bmatrix} 1\times1 & 0 & 0 \\ 0 & 3\times3 & 0 \\ 0 & 0 & 5\times5 \end{bmatrix}$$

T_{ij} transforms as a mixture of $j=0,1,2$, for the representation is reducible $\rightarrow$ not practical

Spherical Tensors $\rightarrow$ transform in an irreducible representation of SO(3)

Motivation: Spherical Harmonics

$$Y_1^0(\theta,\varphi)=\sqrt{\frac{3}{4\pi}}\,\underbrace{\cos\theta}_{\frac{z}{r}}$$

$$Y_1^{\pm1}(\theta,\varphi)=\mp\sqrt{\frac{3}{4\pi}}\,\frac{x\pm iy}{r}$$

spherical vector operator $(l=1)$

$$T_0^{(1)}\equiv\sqrt{\frac{3}{4\pi}}\,V_3$$

$$T_{\pm1}^{(1)}\equiv\mp\sqrt{\frac{3}{4\pi}}\,(V_1\pm iV_2)$$

$x_i x_j = T_{ij} \rightarrow$ tensor

$l=2$:

$$Y_2^{\pm2}=\sqrt{\frac{15}{32\pi}}\left(\frac{x\pm iy}{r}\right)^2$$

Spherical tensor: object transforms like spherical harmonics $\rightarrow$ how?

$$Y_l^m(\theta,\varphi)=\langle\theta,\varphi|l\,m\rangle$$

rotation $\rightarrow$ $Y_l^m(\theta',\varphi')=\langle\theta,\varphi|\mathcal{U}^\dagger(R)|l\,m\rangle$

$$Y_\ell^m(\theta',\varphi') = \sum_{m'} \langle \theta,\varphi | \ell m' \rangle \underbrace{\langle \ell m' | \mathcal{U}^\dagger(R) | \ell m \rangle}$$

$Y \to T$

$\mathcal{U}(R) = e^{-\frac{i\vec{\alpha}\cdot\vec{J}}{\hbar}}$

$$\left[D^{(\ell)}(R)^\dagger \right]_{mm'} = D^{(\ell)}(R)^*_{mm'}$$

expand to first order

$$Y_\ell^m(\theta',\varphi') = \sum_{m'} D^{(\ell)}(R)^*_{mm'} \, Y_\ell^{m'}(\theta,\varphi)$$

At the level of generators,

$$[J_m, T_q^{(k)}] = \sum_{q'} \langle k, q' | J_m | k, q \rangle T_{q'}^{(k)}$$

$$\downarrow$$

$$[J_3, T_q^{(k)}] = \hbar q T_q^{(k)}$$

$$[J^\pm, T_q^{(k)}] = \hbar \sqrt{k(k+1) - q(q\pm 1)}\, T_{q\pm 1}^{(k)}$$

spherical tensors transform like eigenkets $|\ell m\rangle$

Wigner-Eckart Theorem

reduced matrix element

common notation: $\langle r'j' \| T^{(k)} \| r j \rangle$

$$\langle r' j' m' | T_q^{(k)} | r j m \rangle = C^{kj'j}_{rr'} \langle j' m' | j k, m q \rangle$$

→ consequence: nonzero only when $m' = m + q$ due to the Clebsch-Gordan coefficient

→ selection rules

→ we may also analyze what happens with scalars and vectors (for they are tensors as well)

Wigner-Eckart for Scalar Operators $\rightarrow$ $k=0 \Rightarrow q=0$

$$\langle r' j' m' | S | r j m\rangle = \langle r' j' \| S \| r j\rangle \langle j' m' | j m\rangle$$

$$= \langle r' j' \| S \| r j\rangle \, \delta_{jj'} \delta_{mm'}$$

Wigner-Eckart for Vector Operators $\rightarrow$ $k=1 \Rightarrow q=-1,0,1$

$$\langle r' j' m' | \vec{V} | r j m\rangle = C^{1 j' j}_{r r'} \underbrace{\langle j' m' | j 1, m q\rangle}_{\text{nonzero when}}$$

$q=-1,0,1$

nonzero when

$j-1,\ j,\ j+1 = j'$

$m,\ m\pm1 = m'$

Electromagnetism in Quantum Mechanics

Lorentz Force

$$m\ddot{\vec{x}} = q\vec{E} + \frac{q}{c}\vec{v}\wedge\vec{B}$$

$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

$$\vec{B} = \nabla\wedge\vec{A}$$

$$\epsilon_{ikm}\epsilon_{mpn} = \delta_{in}\delta_{kp} - \delta_{ip}\delta_{nk}$$

$$m\ddot{x}_i = qE_i + \frac{q}{c}\epsilon_{ikm}\dot{x}_k B_m$$

$$= -q\,\partial_i\phi - \frac{q}{c}\partial_t A_i + \frac{q}{c}\epsilon_{ikm}\dot{x}_k \epsilon_{mnp}\partial_n A_p$$

$$= -q\,\partial_i\phi - \frac{q}{c}\partial_t A_i + \frac{q}{c}\dot{x}_k\partial_i A_k - \frac{q}{c}\dot{x}_k\partial_k A_i$$

$$L = \frac{m\dot{\vec{x}}^2}{2} + F[\dot{\vec{x}}, \vec{x}, \phi, \vec{A}]$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0$$

$$m\ddot{x}_i = -\frac{d}{dt}\frac{\partial F}{\partial \dot{x}_i} + \frac{\partial F}{\partial x_i}$$

Ansatz: $F = -q\phi + \frac{q}{c}\dot{x}_n A_n$

$$\frac{\partial F}{\partial x_i} = -q\,\partial_i \phi + \frac{q}{c}\dot{x}_n\,\partial_i A_n$$

$$\frac{\partial F}{\partial \dot{x}_i} = \frac{q}{c}A_i \longrightarrow \frac{d}{dt}\frac{\partial F}{\partial \dot{x}_i} = \frac{q}{c}\partial_t A_i + \frac{q}{c}\partial_n A_i\,\dot{x}_n$$

$$\therefore\ m\ddot{x}_i = -q\,\partial_i\phi + \frac{q}{c}\dot{x}_n\,\partial_i A_n - \frac{q}{c}\partial_t A_i - \frac{q}{c}\dot{x}_n\,\partial_n A_i$$

as desired

$$\mathcal{L} = \frac{m\dot{\vec{x}}^2}{2} - q\phi + \frac{q}{c}\dot{x}_n A_n$$

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = m\dot{x}_i + \frac{q}{c}A_i \longrightarrow \dot{x}_i = \frac{p_i - \frac{q}{c}A_i}{m}$$

$$\mathcal{H} = \vec{p}\cdot\dot{\vec{x}} - \mathcal{L} = \frac{(\vec{p} - \frac{q}{c}\vec{A})^2}{2m} + q\phi$$

Free particle $\qquad\qquad$ Charged particle in EM

$$\mathcal{H} = \frac{\vec{p}^2}{2m} \xrightarrow[\substack{\vec{p}\to\vec{p}-\frac{q}{c}\vec{A} \\ \mathcal{H}\to\mathcal{H}-q\phi}]{\text{minimum coupling}} \mathcal{H} = \frac{(\vec{p}-\frac{q}{c}\vec{A})^2}{2m} + q\phi$$

Quantum Mechanics

$\vec{A}(t,\hat{\vec{r}})$, $\phi(t,\hat{\vec{r}})$ position operator

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$$[A_i, p_k] \neq 0, \qquad [\phi, p_k] \neq 0$$

$$H = \frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2}{2m} + q\phi$$

$$= \frac{\vec{p}^{\,2}}{2m} + \frac{q^2}{2mc^2}\vec{A}^2 - \frac{q}{2mc}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + q\phi$$

Gauge Transformations

$$\begin{cases} \vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \\ \vec{B} = \nabla \wedge \vec{A} \end{cases} \xrightarrow{\text{gauge freedom}} \begin{cases} \vec{A} \to \vec{A} + \nabla\Lambda(\vec{x},t) \\ \phi \to \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}(\vec{x},t) \end{cases}$$

gauge transformation

Conjugate momentum

$$\vec{p} = m\dot{\vec{x}} + \frac{q}{c}\vec{A} \xrightarrow{\text{gauge tr}} m\dot{\vec{x}} + \frac{q\vec{A}}{c} + \frac{q}{c}\nabla\Lambda$$

gauge invariant at classical level

$$\vec{p} \to \vec{p} + \frac{q}{c}\nabla\Lambda$$

$$\vec{p} - \frac{q\vec{A}}{c} \to \vec{p} + \frac{q}{c}\nabla\Lambda - \frac{q\vec{A}}{c} - \frac{q}{c}\nabla\Lambda = \vec{p} - \frac{q\vec{A}}{c}$$

QM: what happens to states when I apply a gauge transformation?

$|\alpha\rangle$: states when I use $\vec{A}, \phi$ to computations

$|\tilde{\alpha}\rangle$: states when I use $\tilde{\vec{A}}, \tilde{\phi}$ to computations

$$\tilde{\vec{A}} = \vec{A} + \nabla\Lambda$$
$$\tilde{\phi} = \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}$$

Demand expectation values to be the same

$$\langle\alpha|\vec{r}|\alpha\rangle = \langle\tilde{\alpha}|\vec{r}|\tilde{\alpha}\rangle$$

$$\langle\alpha|\vec{p} - \frac{q}{c}\vec{A}|\alpha\rangle = \langle\tilde{\alpha}|\vec{p} - \frac{q}{c}\tilde{\vec{A}}|\tilde{\alpha}\rangle$$

$$|\tilde{\alpha}\rangle = G|\alpha\rangle$$

$$\vec{r} = G^{\dagger}\vec{r}\,G \rightarrow G^{\dagger}(\vec{r})\,\vec{r}\,G(\vec{r}) = \vec{r}\,G^{\dagger}G = \vec{r}$$

$$\vec{p} - \frac{q}{c}\vec{A} = G^{\dagger}\left(\vec{p} - \frac{q}{c}\tilde{\vec{A}}\right)G \rightarrow [p_i, G(\vec{r})] = -i\hbar\,\partial_i G$$

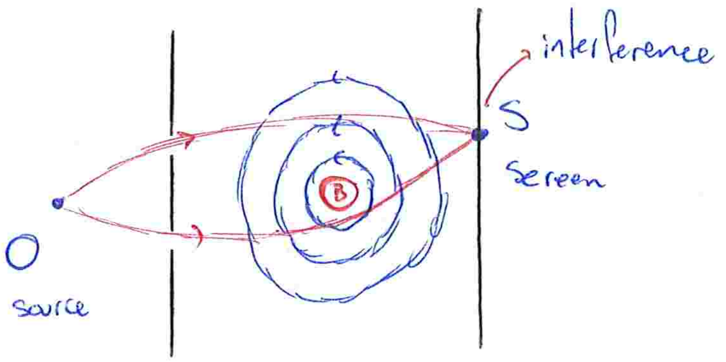
Claim: $G = e^{\frac{iq\Lambda(t,\vec{r})}{\hbar}}$

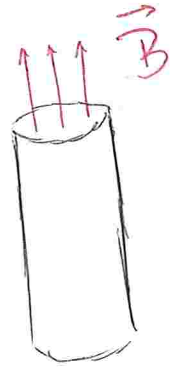
$$-i\hbar\nabla G = -i\hbar\frac{iq}{\hbar}\nabla\Lambda\, G = q\nabla\Lambda\, G$$

$c=1$

$$\begin{aligned}
G^{\dagger}\vec{p}\,G &= G^{\dagger}\left([\vec{p}, G] + G\vec{p}\right) \\
&= G^{\dagger}(q\nabla\Lambda\, G) + G^{\dagger}G\vec{p} \\
&= q\,G^{\dagger}G\,\nabla\Lambda + G^{\dagger}G\vec{p} \\
&= q\nabla\Lambda + \vec{p}
\end{aligned}$$

Aharonov - Bohm





we suppose the slits are so small only one path is possible

$$P(O\to S) = |K(S|O)|^2$$
$$= \left|K_{above}(S|O) + K_{below}(S|O)\right|^2$$

$$K_{above} = \int_{above} e^{\frac{i}{\hbar}\int \frac{m\dot{\vec{x}}^2}{2} + \frac{q}{c}\dot{\vec{x}}\cdot\vec{A}\,dt}\,\mathcal{D}x(t)$$

$$\simeq e^{\frac{i}{\hbar}\int\frac{m\dot{\vec{x}}^2}{2}dt}\; e^{\frac{i}{\hbar}\int\frac{q}{c}\dot{\vec{x}}\cdot\vec{A}\,dt}\Big|_{Above}$$

$$P = |K_{above}|^2 + |K_{below}|^2 + 2\,\mathrm{Re}\left[K^*_{Above}\, K_{below}\right]$$

1949 Eherenberg-Siday

1959 Aharonov-Bohm

1986 Tonura et al.

experimental confirmation

$$e^{-\frac{i}{\hbar}\frac{q}{c}\int \dot{\vec{x}}\cdot\vec{A}\,dt\Big|_{above}}\; e^{\frac{i}{\hbar}\frac{q}{c}\int \dot{\vec{x}}\cdot\vec{A}\,dt\Big|_{below}}$$

$$= e^{-\frac{i}{\hbar}\frac{q}{c}\left[\int_{\gamma_1}\vec{A}\cdot d\vec{x} - \int_{\gamma_2}\vec{A}\cdot d\vec{x}\right]}$$

$$= e^{\frac{-iq}{\hbar c}\oint \vec{A}\cdot d\vec{x}} = e^{\frac{-iq}{\hbar c}\Phi_B}$$

magnetic flux

We observe physical effects in a region with no physical fields

Electromagnetism of Magnetic Monopoles → the potential formulation doesn't work anymore (at least in its usual form)

$$\nabla\cdot\vec{E} = \rho_e \qquad \nabla\cdot\vec{B} = \rho_m$$

$$-\nabla\wedge\vec{E} = \frac{1}{c}\frac{\partial\vec{B}}{\partial t} + \frac{1}{c}\vec{j}^m \qquad \nabla\wedge\vec{B} = \frac{1}{c}\vec{j}^e + \frac{1}{c}\frac{\partial\vec{E}}{\partial t}$$

Point-like magnetic charge

$$\nabla\cdot\vec{B} = g_m\,\delta^3(\vec{x})$$

for we are removing the south pole of an imaginary sphere

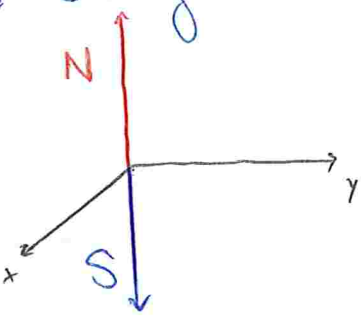
south

Dirac: $\vec{A}^s = -\frac{g\,y}{r(r+z)}\hat{e}_x + \frac{g\,x}{r(r+z)}\hat{e}_y$

$$\nabla\wedge\vec{A}^s = \underbrace{\frac{g_m\,\hat{e}_r}{r^2}}_{\text{point like magnetic field}} + \underbrace{4\pi g_m\,\delta(x)\,\delta(y)\,\theta(-z)\,\hat{e}_z}_{\text{Dirac string}}$$

north

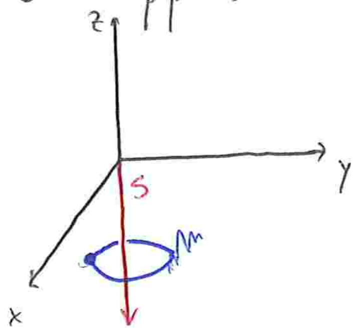
$$\vec{A}^N = \frac{g\,y}{r(r-z)}\hat{e}_x - \frac{g\,x}{r(r-z)}\hat{e}_y$$



In $\mathbb{R}^3 \setminus \{z \text{ axis}\}$, $\vec{A}^N - \vec{A}^S = \nabla \Lambda$

↳ guarantees the same $\vec{B}$ field

what happens in QM



As in the Aharonov-Bohm effect, interference depends on $\Phi_B = 4\pi g_m$

↳ cannot be physical, for Dirac strings are an expression of our insistence in using a potential formulation

Interference: $e^{\frac{i}{\hbar}\frac{q}{c}\Phi_B} = e^{i2\pi n}$

$$\frac{q}{\hbar c} 4\pi g_m = 2\pi n$$

$$q = \frac{\hbar c}{2 g_m} n$$

if there is at least one magnetic monopole in the universe, electric charge must be quantized

Atoms in a Radiation Field

↳ semiclassical $\begin{cases} \text{quantum atom} \\ \text{classical EM wave} \end{cases}$

Atoms with 1 electron

$$H = \frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2}{2m} + V_{eff}(\vec{r}) + q\phi$$

EM wave

$\nabla \cdot \vec{A} = 0 \rightarrow$ Coulomb or transverse gauge

Vacuum: $\nabla^2 \phi = 0$

$\Box^2 \vec{A} = \vec{0}$ → $\Box^2 = \nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$

$$\therefore \quad \phi = 0$$

$$\vec{A} = \vec{A}_0 \, e^{i(\vec{k}\cdot\vec{r} - \omega t)} + \underbrace{h.c.}_{\text{hermition conjugate}}$$

$$\nabla \cdot \vec{A} = 0$$

$$\vec{k} \cdot \vec{A}_0 = 0$$

transverse

QM

$$H = \underbrace{\frac{\vec{P}^2}{2m} + V_{eff}(\vec{r})}_{H_0} + \underbrace{\frac{q^2 \vec{A}^2}{2mc^2} - \frac{q}{2mc}(\vec{A}\cdot\vec{p} + \vec{p}\cdot\vec{A})}_{W}$$

Suppasing the wave is sufficiently weak to drop the $\vec{A}^2$ term, we get

$$H = H_0 - \underbrace{\frac{q}{2mc}(\vec{A}\cdot\vec{p} + \vec{p}\cdot\vec{A})}_{\text{time-dependent perturbation}}$$

$$W = -\frac{q}{2mc}(\vec{A}\cdot\vec{p} + \vec{p}\cdot\vec{A})$$

$$= -\frac{q}{2mc}\left(\vec{A}\cdot\vec{p} - i\hbar \cancelto{0}{\nabla\cdot\vec{A}} + \vec{A}\cdot\vec{p}\right)$$

$$= -\frac{q}{2mc} \cdot 2\vec{A}\cdot\vec{p} \qquad q = -e$$

$$= \frac{e}{mc}\left(e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t} \vec{A}_0\cdot\vec{p} + e^{-i\vec{k}\cdot\vec{r}} e^{i\omega t} \vec{A}_0 \cdot \vec{p}\right) \qquad \hat{\alpha}(\vec{r},\vec{p}) = e^{i\vec{k}\cdot\vec{r}} \vec{A}_0\cdot\vec{p}$$

$$= \frac{e}{mc}\left(\hat{\alpha}\, e^{-i\omega t} + \hat{\alpha}^{\dagger} e^{i\omega t}\right)$$

Time Dependent Perturbation Theory

$$\frac{E_n^\circ - E_m^\circ}{\hbar} \equiv \omega_{nm}$$

$$\begin{cases} |\psi(t)\rangle = \sum e^{-\frac{iE_n^\circ t}{\hbar}} \gamma_n(t)\,|E_n^\circ\rangle \\ \gamma_n(t) \simeq \gamma_n(0) + \frac{1}{i\hbar}\sum_m \gamma_m(0)\int_0^t \langle E_n^\circ|W|E_m^\circ\rangle\, e^{\frac{i(E_n^\circ - E_m^\circ)\tau}{\hbar}}\,d\tau \end{cases}$$

$$\gamma_n(t) \simeq \gamma_n(0) + \frac{1}{i\hbar}\sum_m \gamma_m(0)\int_0^t \frac{e}{mc}\, e^{i\omega_{nm}\tau}\left(\hat{\alpha}_{nm}e^{-i\omega\tau} + \hat{\alpha}^\dagger_{nm}e^{i\omega\tau}\right)d\tau$$

$$\simeq \gamma_n(0) + \frac{1}{i\hbar}\sum_m \gamma_m(0)\frac{e}{mc}\left(\hat{\alpha}_{nm}\int_0^t e^{i(\omega_{nm}-\omega)\tau}d\tau + \hat{\alpha}^\dagger_{nm}\int_0^t e^{i(\omega_{nm}+\omega)\tau}d\tau\right)$$

$$\simeq \gamma_n(0) + \frac{e}{i\hbar mc}\sum_m \gamma_m(0)\left(\hat{\alpha}_{nm}\frac{e^{i(\omega_{nm}-\omega)t}-1}{i(\omega_{nm}-\omega)} + \hat{\alpha}^\dagger_{nm}\frac{e^{i(\omega_{nm}+\omega)t}-1}{i(\omega_{nm}+\omega)}\right)$$

$$= \gamma_n(0) + \frac{2e}{i\hbar mc}\sum_m \gamma_m(0)\left(\frac{\hat{\alpha}_{nm}\,e^{\frac{i(\omega_{nm}-\omega)t}{2}}\sin\left(\frac{(\omega_{nm}-\omega)t}{2}\right)}{\omega_{nm}-\omega} + \frac{\hat{\alpha}^\dagger_{nm}\,e^{\frac{i(\omega_{nm}+\omega)t}{2}}\sin\left(\frac{(\omega_{nm}+\omega)t}{2}\right)}{\omega_{nm}+\omega}\right)$$

blows up for $\omega \approx \omega_{nm}$

blows up for $\omega \approx -\omega_{nm}$

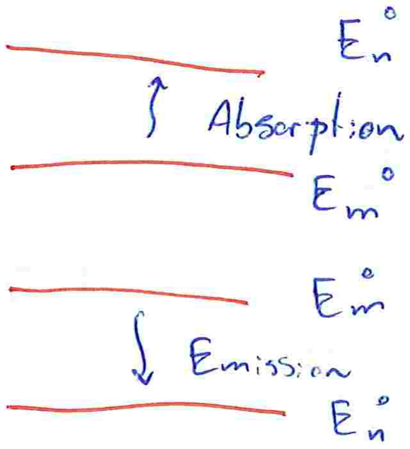
perturbation theory fails and we should use fancier ~~techniques~~ methods, but we can still obtain information

Our sistem starts at $|E_m^\circ\rangle$ and ~~we want to~~ it ends at $|E_n^\circ\rangle$

As $\omega > 0$ always, we have

If $\omega \approx \omega_{nm} = \dfrac{E_n^0 - E_m^0}{\hbar}$

If $\omega \approx -\omega_{nm} = \dfrac{E_m^0 - E_n^0}{\hbar}$



our present theory can't state that such phenomena have anything to do with photons

we are considering a classical EM wave

Suppose that $\gamma_n(0) = \delta_{ni}$. Then

$$\gamma_n(t) = \delta_{ni} + \frac{2e}{i\hbar mc}\left(\hat{\alpha}_{ni} \frac{e^{i(\omega_{ni}-\omega)t} \sin\left(\frac{(\omega_{ni}-\omega)t}{2}\right)}{\omega_{ni}-\omega} + \hat{\alpha}_{ni}^{\dagger} \frac{e^{i(\omega_{ni}+\omega)t} \sin\left(\frac{(\omega_{ni}+\omega)t}{2}\right)}{\omega_{ni}+\omega} \right)$$

Probability for the state at t to be in the state $|E_n^0\rangle$, $n \neq i$, such that there is absorption

$$\gamma_n(t) \simeq \frac{e}{i\hbar mc} \hat{\alpha}_{ni} \frac{e^{\frac{i(\omega_{ni}-\omega)t}{2}} \sin\left(\frac{(\omega_{ni}-\omega)t}{2}\right)}{\frac{\omega_{ni}-\omega}{2}}$$

$$P(t) = \frac{e^2}{\hbar^2 m^2 c^2} |\hat{\alpha}_{ni}|^2 \underbrace{\left(\frac{\sin\left(\frac{(\omega_{ni}-\omega)t}{2}\right)}{\frac{\omega_{ni}-\omega}{2}} \right)^2}_{\text{large } t:\ \pi\,\delta\left(\frac{\omega_{ni}-\omega}{2}\right) t} \longrightarrow$$

the well-defined quantity is $\dfrac{\text{probability}}{\text{time}} = \Gamma$

$$\Gamma \simeq \frac{\pi e^2}{\hbar^2 m^2 c^2} |\hat{\alpha}_{ni}|^2 \,\delta\left(\frac{\omega_{ni}-\omega}{2}\right) \rightarrow \text{Fermi Golden Rule}$$

$\hookrightarrow$ if $\hat{\alpha}_{ni} = 0$, there is no transition

$$\hat{\alpha}_{ni} = \langle E_n^0 | e^{i\vec{k}\cdot\vec{r}} \vec{p} | E_i^0 \rangle \cdot \vec{A}_0$$

$$\approx \langle E_n^0 | \vec{p} | E_i^0 \rangle \cdot \vec{A}_0$$

$\langle r \rangle \sim 10^{-10}\, m \sim a_0$ Bohr radius

$kr \sim \frac{10^{-10}\, m}{\lambda}$

If $\lambda \gg a_0$, $e^{i\vec{k}\cdot\vec{r}} \sim 1$

↳ otherwise, we must consider what happens with photons

As we do not know $|E_i^0\rangle$ and $|E_n^0\rangle$, we might write $\vec{p}$ in terms of H^0 to calculate $\langle E_n^0 | \vec{p} | E_i^0 \rangle$

$$[\vec{r}, H_0] = i\hbar \frac{\vec{p}}{m}$$

$$\hat{\alpha}_{ni} = \frac{m}{i\hbar} \langle E_n^0 | \vec{r} H_0 - H_0 \vec{r} | E_i^0 \rangle \cdot \vec{A}_0$$

$$= \frac{m}{i\hbar} (E_i^0 - E_n^0) \underbrace{\langle E_n^0 | \vec{r} | E_i^0 \rangle}_{\langle n l m | \vec{r} | i l' m' \rangle} \cdot \vec{A}_0$$

$\longrightarrow$ $\vec{r}$ is a vector operator

Wigner - Eckart

$$\boxed{\begin{aligned} m' - m &= 0, \pm 1 \\ l' - l &= 0, \pm 1 \end{aligned}}$$

By checking whether $\langle E_n^0 | \vec{r} | E_i^0 \rangle$ vanishes or not, we can know whether a transition is possible or not

selection rules

↳ in order to obtain the probability, it is necessary to calculate the integrals

Remark

$$\langle E_n^0 | \vec{r} | E_i^0 \rangle$$

$\vec{r} = \frac{\vec{d}}{e} \rightarrow$ dipole operator

This approximation is called the dipole approximation

Fine Structure Terms

H-like atoms so far

$$H = \frac{p^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$-e$

Ze

if we compute the electron's velocity classically, we obtain $v > c$

↳ makes no sense, but suggests relativity is important

Non-Relativistic Limit of the Dirac Equation → we won't study these details in this course

$$H = \frac{(\vec{p} - \frac{q}{c}\vec{A})^2}{2m} + q\phi - \frac{\vec{p}^{\,4}}{8m^3c^2} - \frac{q\hbar}{2mc}\vec{\sigma}\cdot\vec{B} - \frac{q\hbar}{4m^2c^2}\vec{\sigma}\cdot(\vec{E}\wedge\vec{p}) + \overbrace{\frac{q\hbar^2}{8m^2c^2}\nabla\cdot\vec{E}}^{\rho}$$

relativistic correction to the kinetic energy

$-\vec{\mu}\cdot\vec{B}$ magnetic dipole interaction

$$\vec{\mu} = \frac{q\hbar}{mc}\vec{S}$$

spin-orbit term

Darwin term → RQM effect

→ couples to the charge density generating $\vec{E}$

For a central potential

$$\vec{E} = -\nabla\phi = -\hat{r}\frac{\partial\phi}{\partial r}$$

the SO term becomes

$$\vec{\sigma}\cdot(\vec{r}\wedge\vec{p}) \sim \vec{S}\cdot\vec{L}$$

Terms that are proportional to $\frac{1}{c^2}$: fine-structure terms

On the abscence of external E&M fields, we have an electric field due to the nucleus and a magnetic field as well (the nucleus is moving in the electron frame) we will focus only on the fine structure terms and ignore the magnetic field

$$H = \underbrace{\frac{\vec{P}^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r}}_{H_0} \underbrace{- \frac{\vec{P}^4}{8m^3c^2} + \frac{Ze^2\hbar}{2m^2c^2}\frac{\vec{S}}{4\pi\epsilon_0 r^2}\cdot\left(\frac{\hat{r}}{r^2}\wedge\vec{p}\right) - \frac{Ze^2\hbar^2}{8m^2c^2}\delta^{(3)}(\vec{r}_N)}_{\text{perturbation}}$$

H_0 ↳ degenerate spectrum

Let's find a basis of eigenvectors in which the perturbation is diagonal

$$\begin{cases} |n\,\ell\,m_\ell\rangle \otimes |\tfrac{1}{2}\,m_s\rangle \rightarrow \{H, \vec{L}^2, L_z, \vec{S}^2, S_z\} \\ |n\,\ell\,\tfrac{1}{2}\,j\,m\rangle \longrightarrow \{H, \vec{L}^2, \vec{S}^2, \vec{J}^2, J_z\} \end{cases}$$

Kinetic energy

scalar operator ← $[\vec{p}^4, \vec{J}] = 0 \Rightarrow [\vec{p}^4, \vec{J}^2] = 0$

acting on different spaces ← $[\vec{p}^4, \vec{S}] = 0 \Rightarrow [\vec{p}^4, \vec{S}^2] = 0$

$[\vec{p}^4, \vec{L}] = 0 \Rightarrow [\vec{p}^4, \vec{L}^2] = 0$

diagonal in both angular momentum basis

Darwin term

commutes with everything → proportional to $\mathbb{1}$

Spin-Orbit

$[\vec{L}\cdot\vec{S}, \vec{L}] \neq 0$ $\xrightarrow{\text{but}}$ $[\vec{L}\cdot\vec{S}, \vec{J}] = 0$

$[\vec{L}\cdot\vec{S}, \vec{S}] \neq 0$

$$\vec{J}^2 = \vec{L}^2 + \vec{S}^2 + 2\vec{L}\cdot\vec{S}$$

$$|n\,\ell\,s\,j\,m\rangle \longleftarrow \left[\frac{\vec{J}^2 - \vec{L}^2 - \vec{S}^2}{2}, \vec{J}\right] = 0$$

Corrections to energy eigenvalues → we are skipping computations, but they are available in essentially any QM book

$\langle n\, l\, s\, j\, m | H_{FS} | n'\, l'\, s'\, j'\, m' \rangle$

Def: fine structure constant

α relates E_n to the rest mass of the electron

$$\alpha \equiv \frac{e^2}{4\pi\varepsilon_0 \hbar c}$$

$$E_n = -\frac{Z^2}{2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{m}{\hbar^2}\frac{1}{n^2} = -\frac{(Z\alpha)^2}{2}\frac{mc^2}{n^2}$$

Relativistic energy correction

$$\langle n\, l\, s\, j\, m | H_{rec} | n\, l\, s\, j'\, m' \rangle = \frac{E_n (Z\alpha)^2}{n^2}\left(\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right)$$

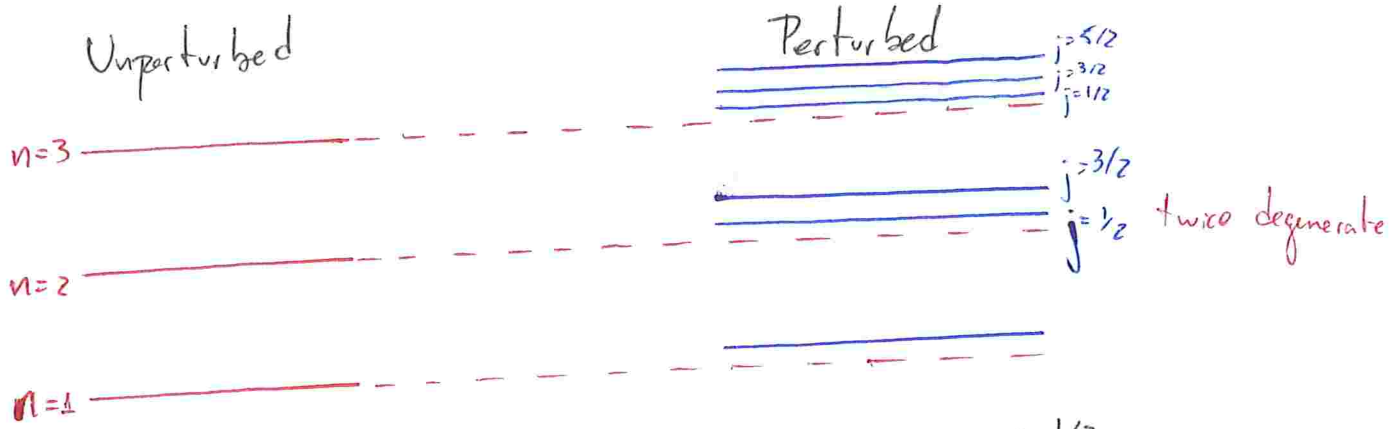
Darwin term

$$\langle\, | H_D |\, \rangle = -\frac{E_n (Z\alpha)^2}{n}\delta_{l0}$$

Spin-Orbit

$$\langle\, | H_{so} |\, \rangle = -\frac{E_n (Z\alpha)^2}{2n}\begin{cases} 0 & l = 0 \\ \frac{1}{(l+\frac{1}{2})(l+1)} & j = l + \frac{1}{2} \\ \frac{-1}{l(l+\frac{1}{2})} & j = l - \frac{1}{2} \end{cases} \quad l \neq 0$$

$$\langle n\, l\, s\, j\, m | H_{FS} | n\, l\, s\, j\, m \rangle = E_n (Z\alpha^2)\left(\frac{1}{n(j+\frac{1}{2})} - \frac{3}{4n^2}\right)$$



$n=1$: $l=0 \Rightarrow j=1/2$

$n=2$: $l=0 \Rightarrow j=1/2$
$l=1 \Rightarrow j=1/2,\ j=3/2$

$n=3$: $l=0 \Rightarrow j=1/2$
$l=1 \Rightarrow j=1/2,\ j=3/2$
$l=2 \Rightarrow j=3/2,\ j=5/2$

Remark: if we solve Dirac's Equation, the new number of energy levels is preserved

Quantization of the Electromagnetic Field

namely, for the detailed way would be way more complicated

Classic $\xrightarrow[\text{quantization}]{\text{Canonical}}$ QM

Coulomb Gauge

$$\left.\begin{aligned}\nabla\cdot\vec{A}&=0\\ \phi&=0\end{aligned}\right] \quad \Box^2\vec{A}=0$$

vacuum

$$\vec{k}\cdot\vec{A}_k=0$$

hermitian conjugate

$$\vec{A}(\vec{x},t)=\int\left(\vec{A}_k\, e^{i(\vec{k}\cdot\vec{x}-\omega t)}+h.c.\right)\frac{d^3k}{\underbrace{(2\pi)^{3/2}}_{\text{convention}}}$$

$$\vec{A}_k=\sum_{\underbrace{\lambda}_{\text{polarizations}}} A_{k\lambda}\,\hat{e}_\lambda(\vec{k})$$

$$\vec{A}_k(t) = \vec{A}_k \, e^{-i\omega t}$$

$$\dot{\vec{A}}_k(t) + i\omega \vec{A}_k(t) = 0$$

$$\ddot{\vec{A}}_k(t) + \omega^2 \vec{A}_k(t) = 0$$

$$\vec{A}(\vec{x},t) = \frac{1}{(2\pi)^{3/2}} \int \vec{A}_k(t)\, e^{i\vec{k}\cdot\vec{x}} + \underbrace{\vec{A}_k^*(t)\, e^{-i\vec{k}\cdot\vec{x}}}_{\text{split integral and make } \vec{k}\to-\vec{k}} \, d^3k$$

$$= \frac{1}{(2\pi)^{3/2}} \int \left(\vec{A}_k(t) + \vec{A}_{-k}^*(t)\right) e^{i\vec{k}\cdot\vec{x}} \, d^3k$$

Classical Hamiltonian

$$H = \int \frac{\vec{E}^2 + \vec{B}^2}{2} \, d^3x$$ Heaviside units

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}, \qquad \vec{B} = \nabla \times \vec{A}$$

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} = -\frac{1}{(2\pi)^{3/2} c} \int \left(\dot{\vec{A}}_k(t) + \dot{\vec{A}}_{-k}^*(t)\right) e^{i\vec{k}\cdot\vec{x}} \, d^3k$$

$$= \frac{-1}{(2\pi)^{3/2} c} \int \left(-i\omega \vec{A}_k(t) + i\omega \vec{A}_{-k}^*(t)\right) e^{i\vec{k}\cdot\vec{x}} \, d^3k$$

$$= \frac{1}{(2\pi)^{3/2}} \int \underbrace{\frac{i\omega}{c}}_{\|\vec{k}\|} \left(\vec{A}_k(t) - \vec{A}_{-k}^*(t)\right) e^{i\vec{k}\cdot\vec{x}} \, d^3k$$

$$\vec{B} = \nabla \times \vec{A} = \frac{1}{(2\pi)^{3/2}} \int i\vec{k} \times \left(\vec{A}_k(t) + \vec{A}^*_{-k}(t) \right) e^{i\vec{k}\cdot\vec{x}} \, d^3k$$

$$\vec{\alpha}_k \equiv \vec{A}_k(t) - \vec{A}^*_{-k}(t)$$

$$\vec{\beta}_k \equiv \vec{A}_k(t) + \vec{A}^*_{-k}(t)$$

$$\int \vec{E}^2 \, d^3x = \frac{-1}{(2\pi)^3} \int \|\vec{k}\| \cdot \|\vec{q}\| \, e^{i(\vec{k}+\vec{q})\cdot\vec{x}} \, \vec{\alpha}_k \cdot \vec{\alpha}_q \, d^3x \, d^3k \, d^3q$$

$$= -\frac{(2\pi)^3}{(2\pi)^3} \int \|\vec{k}\| \, \|\vec{q}\| \, \delta^{(3)}(\vec{k}+\vec{q}) \, \vec{\alpha}_k \cdot \vec{\alpha}_q \, d^3k \, d^3q$$

$$= -\int \vec{k}^2 \, \vec{\alpha}_k \cdot \vec{\alpha}_{-k} \, d^3k$$

$$\vec{\alpha}_{-k} = \left(\vec{A}_{-k}(t) - \vec{A}^*_k(t) \right)$$

$$= -\left(\vec{A}_k(t) - \vec{A}^*_{-k}(t) \right)^*$$

$$= -\vec{\alpha}^*_k$$

$$= \int |\vec{\alpha}_k|^2 \, \vec{k}^2 \, d^3k$$

$$\int \vec{B}^2 \, dx^3 = \int |\vec{\beta}_k|^2 \, \vec{k}^2 \, d^3k$$

→ analogous to the electric case, but the vector product must be written in components

$$H = \frac{1}{2} \int \vec{k}^2 \left(|\vec{\alpha}_k|^2 + |\vec{\beta}_k|^2 \right) d^3k$$

$$= \frac{1}{2} \int \vec{k}^2 \Big(|\vec{A}_k|^2 + |\vec{A}_{-k}|^2 + \vec{A}_k \cdot \vec{A}_{-k} - \vec{A}^*_k \cdot \vec{A}^*_{-k} + |\vec{A}_k|^2 + |\vec{A}_{-k}|^2 + \vec{A}_k \cdot \vec{A}_{-k} + \vec{A}^*_k \cdot \vec{A}^*_{-k} \Big) d^3k$$

$\vec{k} \to -\vec{k}$ once more

$$= \int \vec{k}^2 \left(|\vec{A}_k|^2 + |\vec{A}_{-k}|^2 \right) d^3k$$

$|\cdot|$ makes the time-dependent phase irrelevant

$$= 2 \int \vec{k}^2 \, |\vec{A}_k|^2 \, d^3k$$

Definition: real variables

$$\vec{Q}_k \equiv \frac{1}{c}\left[\vec{A}_k(t) + \vec{A}_k^*(t)\right]$$
$$\vec{P}_k \equiv -i\,\|\vec{k}\|\left[\vec{A}_k(t) - \vec{A}_k^*(t)\right]$$

$$\vec{A}_k = \frac{1}{2}\left(c\,\vec{Q}_k + \frac{i}{|k|}\vec{P}_k\right)$$

$$H = \int \frac{\vec{P}_k^{\,2}}{2} + \frac{\omega^2 \vec{Q}_k^{\,2}}{2}\, d^3k$$

harmonic oscillator

↓

canonical quantization

Equations of Motion

$$\begin{cases} \dot{\vec{Q}}_k = \dfrac{\partial H}{\partial \vec{P}_k} = \vec{P}_k \\ \dot{\vec{P}}_k = -\dfrac{\partial H}{\partial \vec{Q}_k} = -\omega^2 \vec{Q}_k \end{cases}$$

$$\dot{\vec{A}}_k + i\omega \vec{A}_k = 0$$

the transformation is canonical

QM

$$Q_{k\lambda},\ P_{k\lambda} \rightarrow \hat{Q}_{k\lambda},\ \hat{P}_{k\lambda}$$

$$\left[\hat{Q}_{k\lambda},\ \hat{P}_{k'\lambda'}\right] = i\hbar\, \delta^{(3)}(\vec{k}-\vec{k}')\,\delta_{\lambda\lambda'}$$

$$\hat{H} = \int \sum_\lambda \frac{\hat{P}_{k\lambda}^{2}}{2} + \frac{\omega^2 \hat{Q}_{k\lambda}^{2}}{2}\, d^3k$$

$$\hat{a}_{k\lambda} = \frac{1}{\sqrt{2\hbar\omega}}\left[\omega\,\hat{Q}_{k\lambda} + i\,\hat{P}_{k\lambda}\right]$$

$$= \int \hbar\omega \sum_\lambda \left(\hat{a}^{+}_{k\lambda}\hat{a}_{k\lambda} + \frac{1}{2}\right) d^3k$$

just like QHO

Let then $|0\rangle$ be a state such that

$$\hat{a}_{k\lambda}|0\rangle = 0$$

$$\hat{a}^{\dagger}_{k\lambda}|0\rangle = |\vec{k},\lambda\rangle \rightarrow \text{energy } \hbar\omega_k \rightarrow 1 \text{ photon}$$

$$\hat{a}^{\dagger}_{k\lambda}\hat{a}^{\dagger}_{q\lambda'}|0\rangle = |\vec{k},\lambda;\vec{q},\lambda'\rangle \rightarrow \text{energy } \hbar\omega_k + \hbar\omega_q \rightarrow 2 \text{ photons}$$

What about the $\frac{1}{2}\hbar\omega$ factor? → if ignored, everything works. Otherwise, everything fails

↳ first option: we only measure differences of energy and it is irrelevant

↳ however, if we couple gravity, every energy source is relevant, even this $\frac{1}{2}$ factor

↳ vacuum has an infinite amount of energy

↳ doesn't happen in reality ↳ $\int \frac{1}{2} d^3k$

↳ nobody knows how to solve it !!

↳ cosmological constant problem

Other possibility for quantization
Start with spin-1 massless particle (photon) and go back until you get ~~only~~ the only possible theory that describe such particles

↳ leads to Maxwell electrodynamics

↳ for the graviton, the theory obtained is General Relativity

And there was light...