path integral
Feynmann

spacetime-relativity
Einstein

imaginary unit

strong/weak/e.m. interactions
Maxwell Yang-Mills

φ - ψ interaction
Yukawa

$$\Psi = \int e^{\frac{i}{\hbar}\int\left(\frac{R}{16\pi G} - \frac{1}{4}F^2 + \overline{\psi} i \not{D} \psi - \lambda \varphi \overline{\psi} \psi + |D\varphi|^2 - V(\varphi)\right)}$$

Schrödinger
wave function

Euler
exponential

Planck
quantum

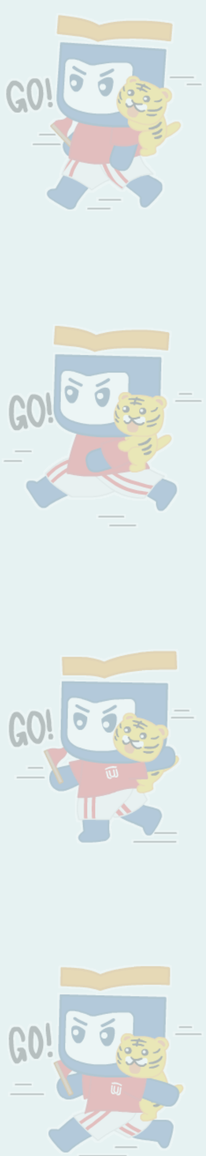
Newton
gravitation

Dirac
relativistic wave function

Kobayashi-Maskawa
CKM matrix

Higgs
Boson

Advanced Quantum Mechanics



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Contents

Chapter 0 Preparation: Quantum Mechanics is a physics *theory*

Part I. Hilbert space (Week 1 – 4)

1. Features of HS: basis, linear maps (operators / functionals)
2. Time evolution: EOM, Dyson series, three pictures
3. Perturbation theory

Part II. Path integral (Week 5 – 7)

(a) Functional integral, variational principle
(b) Wick rotation, partition function
(c) Correlation functions, Feynman diagrams

Part III. Symmerty (Week 8 – 12)

1. Continous symmetry and conservations laws
2. Symmetry group representations, degeneracies, inversion and time reversal
3. Angular momentum, Lie algebra
4. Gauge

Part IV. Entanglement (Week 13 – 16)

1. Indistinguishable particles, Fock space
2. Second quantization
3. Entanglement, Bell's inequality
4. Open quantum systems, density operator, quantum channel

References

[1] J. J. Sakurai and J. Napolitano, *Modern quantum mechanics* (Cambridge University Press, 2020).

[2] J. S. Townsend, *A modern approach to quantum mechanics* (University Science Books, 2000).

[3] R. Shankar, *Principles of quantum mechanics* (Springer Science & Business Media, 2012).

[4] P. A. M. Dirac, *The principles of quantum mechanics*, 27 (Oxford university press, 1981).

Math prerequisite: Math is Very Important!

To formulate a theory, we need MATH!
To understand a theory, we need PICTURE!

(a) Calculus (real and complex)
(b) Differential equations
(c) Linear algebra
(d) Abstract algebra (group, field, vector space, etc.)

[1] F. W. Byron and R. W. Fuller, *Mathematics of classical and quantum physics* (Courier Corporation, 2012).

[2] G. B. Arfken, H. J. Weber, and F. E. Harris, *Mathematical methods for physicists: a comprehensive guide* (Academic press, 2011).

Math Quiz

Problem 0.1. Compute

$$\int_{-\infty}^{+\infty} \mathrm{e}^{-\frac{1}{2}x^2+ax}\,\mathrm{d}x \quad (a \in \mathbb{R})$$

Solution. Handle the exponential term first

$$-\frac{1}{2}x^2 + ax = -\frac{1}{2}(x-a)^2 + \frac{1}{2}a^2 \xlongequal{u=x-a} -\frac{1}{2}u^2 + \frac{1}{2}a^2$$

then the integral is

$$\int_{-\infty}^{+\infty} \mathrm{e}^{-\frac{1}{2}u^2+\frac{1}{2}a^2}\,\mathrm{d}u = \mathrm{e}^{\frac{1}{2}a^2}\int_{-\infty}^{+\infty} \mathrm{e}^{-\frac{1}{2}u^2}\,\mathrm{d}u = \mathrm{e}^{\frac{1}{2}a^2}\cdot 2\Gamma\left(\frac{1}{2}\right) = \sqrt{2\pi}\,\mathrm{e}^{\frac{a^2}{2}}$$

Problem 0.2. Compute

$$\int_{-\infty}^{+\infty} \frac{\mathrm{e}^{\mathrm{i}kx}}{k^2+a^2}\,\mathrm{d}k \quad (a > 0)$$

Solution. The two singularities are: $k = \pm\,\mathrm{i}a$. The integrand function can be written as

$$f(k) = \frac{\mathrm{e}^{\mathrm{i}kx}}{k^2+a^2} = \frac{P(k)}{Q(k)}$$

while $Q(\pm\,\mathrm{i}a) = 0$, but $Q'(\pm\,\mathrm{i}a) = \pm 2\,\mathrm{i}a \neq 0$, so the residues of $f(k)$ are

$$\mathrm{Res}(f, \mathrm{i}a) = \frac{P(\mathrm{i}a)}{Q'(\mathrm{i}a)} = \frac{\mathrm{e}^{-ax}}{2\,\mathrm{i}a},\ \mathrm{Res}(f, -\,\mathrm{i}a) = \frac{P(-\,\mathrm{i}a)}{Q'(-\,\mathrm{i}a)} = -\frac{\mathrm{e}^{ax}}{2\,\mathrm{i}a},$$

According to the *Residue Theorem*, the result of the integration is

$$I = 2\pi\,\mathrm{i}[\mathrm{Res}(f, \mathrm{i}a) + \mathrm{Res}(f, -\,\mathrm{i}a)] = \frac{\pi}{a}(\mathrm{e}^{-ax} - \mathrm{e}^{ax})$$

Problem 0.3. Solve

$$\frac{\mathrm{d}}{\mathrm{d}x}f(x) + (x-a)f(x) = 0$$

Solution. Separate the variables

$$\frac{\mathrm{d}f(x)}{f(x)} = -(x-a)\,\mathrm{d}x$$

integrating both sides

$$\ln[f(x)] = -\frac{1}{2}(x-a)^2 + C'$$

then we get the solution

$$f(x) = \mathrm{e}^{-\frac{1}{2}(x-a)^2+C'} = C\,\mathrm{e}^{-\frac{1}{2}(x-a)^2}$$

where C is any constant.

Problem 0.4. Find the eigenvalues and the eigenvectors of the following matrix

$$\mathbf{M} = \begin{pmatrix} 0 & a \\ b & 0 \end{pmatrix}$$

Solution. Let

$$\det(\mathbf{M} - \lambda \mathbf{I}) = \begin{vmatrix} -\lambda & a \\ b & -\lambda \end{vmatrix} = \lambda^2 - ab = 0$$

Then we get the eigenvalues of matrix $\mathbf{M}$: $\lambda_1 = \sqrt{ab}$ while $\lambda_2 = -\sqrt{ab}$. Next, calculating the eigenvectors.

$$\begin{pmatrix} 0 & a \\ b & 0 \end{pmatrix} \boldsymbol{e}_{1,2} = \pm\sqrt{ab}\boldsymbol{e}_{1,2}$$

then we arrive at

$$y = \sqrt{b/a}x$$

So, the two eigenvectors can be

$$\boldsymbol{e}_1 = \left(1, \sqrt{b/a}\right)^\mathsf{T}, \ \boldsymbol{e}_2 = \left(1, -\sqrt{b/a}\right)^\mathsf{T}$$

Remark. If $b = 0$ and a is finite (or the other way around), then there's only one eigenvector.

Problem 0.5. How many configurations are there to put n indistinguishable balls into m distinguishable boxes?

Solution.

Problem 0.6. Write down one example of abelian groups and one example of non-abelian groups, respectively.

Solution.

Chapter 1 Hilbert Space

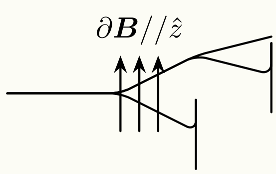
What is Hilbert space? and Why do we think it is important?

1. A $\boxed{Q}$HO (modules)
2. A Qubit (modules)
3. A piece of metal (real world objects)
4. An Atom (real world objects)

Real world objects BUILD modules
Two groups: Physics VS Math
Physics:

- Stern-Gerlach 1921, 22.

  Silver atoms -¿ electron -¿ as spin 1/2.

  * Only 2 possible outcomes to fixed measurement.

  * Always 2 outcomes by changes measurements, different intensities depend on measurements. Orthognal states:

  - Projected probability
  - Measurement (matters!)

Math:
Hierarchy of SPACES
Topological space -¿ Metric space -¿ Normed vector space -¿ Inner product space and Bonaic space -¿ Hilbert space

- Topological space: *continuity*
- Matrix: Sence of *distance*
- Normed vector space (also called linear space): *length* and distance (Linearity)
- Bonaic space: Sence of completness (limit / calcules)

- Inner product space: Projection/overlap (sence of not only length, but also *angle*)

- Hilbert space: all of the above.

Vector Space
Inner product space (sometimes called Pre-Hilbert Space)

1.1 Vector space

Vectors (u,v) & scalors (a,b)

- Vector addition "+" $\boxed{\text{Vectors form abelian group.}}$ Abelian group: 4 + 1 properties. (Closure, Identity $\mathbb{1}$, Inverse (always find another elements, add to it equals to identity), Associatity ($(a+b)+c = a+(b+c)$), Commutativity ($a+b=b+a$))

Vectors <-> Orthogonal states

- Scalar multiplication "$\times$" A: Associatity $a(bu) = (ab)u$, I: Identity, Distr $f(au+bv) = af(u)+bf(v)$.

Scalars <-> Projected probability (amplitudes)

1.2 Inner product space

by adding one more : V, F, $\langle | \rangle$ (Inner product): C(Conjugate symmerty: take two input $\langle u|v\rangle = \langle v|u\rangle^*$ for complex number), Li (Linear Reality: $\langle w|au+bv\rangle = a\langle w|u\rangle + b\langle w|v\rangle$), P (Positive definiteness: $\langle u|v\rangle > 0$ of $u \neq 0$.)

Inner Project <- orthogonal, projected, measurement

Operators:
Maps on Hilbert Space (linear): $Z : V \to V$
Two important defs:

- Operators: compute sth. like $\left|\langle u|\hat{O}|u\rangle\right|$

1.3 Features of Hilbert space

- Main basis

- Maps

Hilbert Space naturally describes quantum objects: superposition; complex probability amplitudes;

$\boxed{\text{Vector space } \boxed{\text{Inner product space}}}$ $\rightarrow |\psi\rangle = a|u\rangle + b|v\rangle$ $\rightarrow$superposition

$\boxed{\text{IPS}}$ $\rightarrow\langle u|\psi\rangle \leftrightarrow$ complex probability amplitudes.

Definition 1.3.1 (Basis ¡Mathematical definition¿).

- Linear independence For a set of vectors $A = \{v_i\}$ in a vector space: If

$$\sum_A a_i v_i = 0 \Rightarrow \forall a_i = 0$$

  then A is linearly independent.

- Linear span: $span(A) = \{\sum_A a_i v_i,\ a_i \in F\}$ (F: Field, as complex number $F \in \mathbb{C}$)

  $E = \{e_i\}$ is a basis of V. If

  - $\{e_i\}$ is linear independence
  - $span(\{e_i\}) = V$

- Dimension of Vector space: $\dim(V) = card(E)$.

- Expansion of V over E

$$V = \sum a_i e_i$$

  This expansion is unique[1].

Definition 1.3.2 (Orthonormal Basis). Use $\{|\alpha\rangle\}$ for all orthogonal states, and it satisfies

$$\langle\alpha|\alpha'\rangle = \delta_{\alpha\alpha'}$$

α is a lable, different labels means different states. If they are different, they are orthogonal.
Completness condition:

$$\sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{I}_V$$

$\mathbb{I}$ means identity in the Hilbert space. We call the operators like this the projector P_α: projector to the state $|\alpha\rangle$

Existence / construction: Gram-Schmidt orthognalization. $\mathrm{d}i = e_i - \sum_{j<i} p_j e_j$

Expension over $\{|\alpha\rangle\}$.

$$|\psi\rangle = \sum_\alpha \psi_\alpha |\alpha\rangle$$

$$\langle\alpha|\psi\rangle = \sum_{\alpha'} \psi'_{\alpha'} \langle\alpha|\alpha'\rangle,\ \psi_\alpha \in \mathbb{C}$$

Example 1.3.1. $\alpha \to x$, $\psi_\alpha \to \psi(x)$ wavefunction

$\alpha \to k$, $\psi(k) = \int \mathrm{d}x\, \mathrm{e}^{\mathrm{i}kx}\psi(x)$

$\{\alpha\} \to \{0, 1\}$, $\psi_\alpha \to (\psi_0, \psi_1)^\mathsf{T}$

$|0\rangle, |1\rangle$.

$\alpha \to \{(k, \sigma)\}$, $\psi_\alpha \to \psi_\sigma(k)$

[1]

1.3.1 Change of Basis

$\{|\alpha\rangle\} \to \{|\beta\rangle\}$

$$|\psi\rangle = \sum_\alpha \psi_\alpha |\alpha\rangle = \sum_\beta \psi_\beta |\beta\rangle$$

$$\psi_\beta = \langle\beta|\psi\rangle = \sum_\alpha \langle\beta|\alpha\rangle\langle\alpha|\psi\rangle = \sum_\alpha U_{\beta\alpha}\psi_\alpha.$$

$\beta \to k$, $\alpha \to x$

$$U_{\beta\alpha} \to \langle k|x\rangle = \mathrm{e}^{-\mathrm{i}kx}$$

1.4 Maps

Maps: just the arrow.

For vector space (V, F) (sth we call vectors and scalors).

From V to F: linear function

From V to V: linear operator

Linear:

$f : V \to W$

$f(au + bv) = af(u) + bf(v)$

$$\{f(\text{linear}) : V \to W\} = \mathrm{Hom}_F(V, W)\text{is V.S.}$$

$\boxed{\text{Scalor is just the one Dimension of V.S..}}$

$f, g \in \mathcal{V}$. $\forall v \in V$, $(f + g) = f(v) + g(v) \in W$.

For commutativity‘’, $f \cdot g = g \cdot f \in W$.

Basis	ON. Basis	Components
$\{f_i, f_i(e_j) = \delta_{ij}\}$	$\{\langle\alpha|\cdot\rangle\}$	
$\{f_{ij} : f_{ij}(l_n) = e_i\delta_{jk}\}$	$\{\langle\alpha|\}$	
$\{f_{ij} : f_{ij}(e_k) = e'_i\delta_{jk}\}$		

$\langle\hat{F}|\hat{G}\rangle = \sum_\alpha \langle\hat{F}_\alpha|\hat{G}_\alpha\rangle$ and $\hat{F}|G\rangle = \sum_n \langle\alpha|\alpha\rangle\langle G|$

$$\langle F\beta| = \sum_\alpha \langle\beta|\alpha\rangle\langle\hat{F}_\alpha|,\ F|\beta\rangle = \sum_\alpha \hat{F}|\alpha\rangle\langle\alpha|\beta\rangle$$

with $\sum_\beta |\beta\rangle\langle\beta| = \mathbb{1}$

$$\sum_\beta \langle\hat{F}\beta|\hat{G}\beta\rangle = \sum_{\beta\alpha\alpha'} \langle\beta|\alpha\rangle\langle F\alpha|G\alpha'\rangle\langle\alpha'|\beta\rangle$$

Then, we have

$$\langle\hat{F}|\hat{G}\rangle = \mathrm{Tr}(F^{-1}G) = \sum_\alpha \langle F\alpha|G\alpha\rangle = \sum_\alpha \langle\alpha|F^\dagger G|\alpha\rangle$$

$$\mathrm{Tr}[(|\alpha'\rangle\langle\alpha|)^\dagger(|\beta\rangle\langle\beta'|)] = \delta_{\alpha\beta}\delta_{\alpha'\beta'}$$

$$\hat{O} = \sum_{\alpha\beta}|\alpha\rangle\langle\alpha|\hat{O}|\beta\rangle\langle\beta| = \sum_{\alpha\beta}O_{\alpha\beta}|\alpha\rangle\langle\beta|$$

How about $V \times V$? — Inner product, a set of all pairs. It has to BILINEAR.

$$f(au + bv, w) = a^* f(u, w) + *b^f(v, w)$$

$V \times V \to V \otimes V$ ($\otimes$: $V \times V \to V \otimes V$, a map)

$$w = \sum_{ij} W_{ij}(e_i \otimes e_j) = u \otimes v$$

Given u and v, what the Components of $u \otimes v$?
Suppose u is written as $u = \sum_i u_i e_i$ and v is written as $v = \sum_j v_j e_j$. Then,

$$u \otimes v = \left(\sum_i u_i e_i\right) \otimes \left(\sum_j v_j e_j\right) = \sum_i u_i(e_i \otimes \sum_j v_j e_j) = \sum_{ij} u_i v_j (e_i \otimes e_j)$$

We start from something like

$$w = w_i e_1 \otimes e_1 + w_2 e_2 \otimes e_2$$

which w_1 and w_2 are both finite. Suppose $w = u \otimes v$ is true, then

$$w = \sum_{ij} u_i v_j (e_i \otimes e_j)$$

but we have chosen a specific w, it means that

$$w = u_1 v_1(e_1 \otimes e_2) + u_1 v_2(e_1 \otimes e_2) + u_2 v_1(e_2 \otimes e_1) + u_2 v_2(e_2 \otimes e_2)$$

Comparing with $w = w_i e_1 \otimes e_1 + w_2 e_2 \otimes e_2$, we have

$$w_1 = u_1 v_2,\ 0 = u_1 v_2,\ 0 = u_2 v_1,\ w_2 = u_2 v_2$$

1.4.1 Case study: (Re)discover Fourier Transform

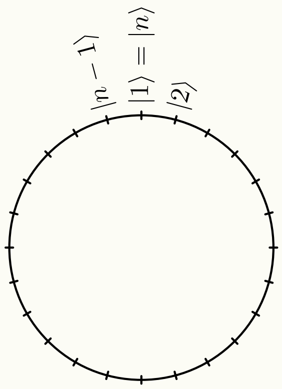
We've always talk about $\{|\alpha\rangle\}$, but now, consider a Hilbert space, label basis $\{|l\rangle\}$ with order number index:

$$\{|l\rangle,\ l = 1,\ 2,\ \ldots.\ N\}$$

and also we may want to $N + 1 \equiv 1$, something like a circle with all the states $|1\rangle, |2\rangle, \ldots, |n\rangle$ in the right figure.
In this basis, we define translation (operator $\hat{T}_L$)

$$\hat{T}_L|l\rangle = |l+1\rangle,$$

and we may also write it differently like



$$\hat{T}_L = \sum_l |l+1\rangle\langle l|, \tag{1.1}$$

The eigenvalue

$$\hat{T}_L|\psi\rangle = \lambda|\psi\rangle$$

while $|\psi\rangle = \sum_l \psi_l |l\rangle$, that is

$$\hat{T}_L|\psi\rangle = \sum_l \psi_{l-1}|l\rangle$$
$$\lambda|\psi\rangle = \sum_l \lambda\psi_l|l\rangle$$

Then we have

$$\psi_l = \lambda\psi_l,\ \psi_l = \lambda^{1-l}\psi_l,\ \psi_1 = \psi_{N+1} = \lambda^{-N}\psi_1$$

then we have $\lambda^{-N} = 1$. So, we can specify λ

$$\lambda = \lambda_m \equiv \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}m} \tag{1.2}$$

Concering the eigenstates of $\hat{T}_L$, which are $|m\rangle$. Since

$$\psi_{1,m} = \lambda_m^{-1},\ \psi_{l,m} = \lambda_m^{1-l}\psi_{1,m} = \lambda_m^{-l}$$

So,

$$|m\rangle = \sum_l \psi_{l,m}|l\rangle = \frac{1}{\sqrt{N}}\sum \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}ml}|l\rangle$$

Now, consider the new basis ($m = 1, 2, \ldots, N$), the relation between it and the old basis is

$$\{|l\rangle\} \xleftrightarrow{\text{Fourier Transform}} \{|m\rangle\}$$

In this basis, the definition of the operator is

$$\hat{T}_L = \sum_m \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}m}|m\rangle\langle m|. \tag{1.3}$$

with $N+1 \equiv 1$. and the inner product

$$\langle l|m\rangle = \frac{1}{\sqrt{N}}\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}lm} \tag{1.4}$$

To make the problem more interesting: the translation of the m-basis, express $\hat{T}_M$ in terms of l

$$\hat{T}_M = \sum_m |m+1\rangle\langle m| = \sum_{mll'} |l\rangle\langle l|m+1\rangle\langle m|l'\rangle\langle l| \tag{1.5}$$

If we put $m+1$ instead of m

$$\langle l|m+1\rangle = \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}l}\langle l|m\rangle$$

subsitute it into $\hat{T}_M$

$$\hat{T}_M = \sum_l \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}l}|l\rangle\langle l|$$

To summarize

$$\hat{T}_L = \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}\hat{M}},\ \hat{M} = \sum_m m|m\rangle\langle m| \tag{1.6}$$

$$\hat{T}_M = \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}\hat{L}},\ \hat{M} = \sum_m m|l\rangle\langle l| \tag{1.7}$$

This is only a start. How about the translation over m:

$$\hat{T}_L\hat{T}_M = \underline{?}\hat{T}_M\hat{T}_L,$$

means we can measure M first, then measure L; or reverse. They will differ by something like

$$\hat{T}_M\hat{T}_L = \hat{T}_L\hat{T}_M\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}}$$

Comparing with $[\hat{q},\hat{p}] = \mathrm{i}$. Just consider in the l basis, expand $\hat{T}_L$ and $\hat{T}_M$

$$\begin{aligned}\hat{T}_L\hat{T}_M &= \sum_{ll'}|l+1\rangle\langle l|\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}l'}|l'\rangle\langle l'| = \sum_l \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}l}|l+1\rangle\langle l| \\ \hat{T}_M\hat{T}_L &= \sum_{ll'}\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}l'}|l'\rangle\langle l'|l+1\rangle\langle l| = \sum_l \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}(l+1)}|l+1\rangle\langle l|\end{aligned}$$

That is

$$\hat{T}_M\hat{T}_L = \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}}\hat{T}_L\hat{T}_M \tag{1.8}$$

When $N=2$: we reach *Ultra Quantum*; When $l = 0, 1$: $\hat{T}_M \to \sigma_z$, and $\hat{T}_L \to \sigma_x$. We get the anti-commute relation

$$\sigma_z\sigma_x = -\sigma_x\sigma_z \tag{1.9}$$

When $N\to\infty$, $q = la$ while $a \to 0$, similarly, $p = mb = m\frac{2\pi}{Na}$. Eventually, $b\to 0$, $N\to\infty$. Let $\hat{Q} = \hat{L}a$, $\hat{P} = \hat{M}b$, now

$$\hat{T}_M \to \hat{T}_Q = \mathrm{e}^{\mathrm{i}b\hat{Q}}, \quad \text{and} \quad \hat{T}_L \to \hat{T}_P = \mathrm{e}^{-\mathrm{i}a\hat{P}}$$

Next, what we need to do is to expand the exponential to linear order: from (1.8), we have

$$(\mathbb{1} + \mathrm{i}b\hat{Q})(\mathbb{1} - \mathrm{i}a\hat{P}) = (\mathbb{1} + \mathrm{i}ab)(\mathbb{1} - \mathrm{i}a\hat{P})(\mathbb{1} + \mathrm{i}b\hat{Q})$$

Omit the high order terms, then we have

$$\hat{Q}\hat{P} = \mathrm{i} + \hat{P}\hat{Q}, \quad \text{or} \quad [\hat{Q},\hat{P}] = \mathrm{i} \tag{1.10}$$

Q and P are Hermitian Operators.

$$\hat{O}\ (V\to V)\begin{cases}\text{Invertible:} & \text{Symmetry Operators (e.g. projection: } |\alpha\rangle\langle\alpha| \text{ or } \sum_{\{\alpha\}\in\text{H.S.}}|\alpha\rangle\langle\alpha|) \\ & \text{Transformation, time evolution: Unitary } U^\dagger U = \mathbb{1} \\ \text{Non-Invertible:} & \text{Generators <-> Observables} \\ & \text{Hamiltonian, position <-> momentum: Hermitian } O^{-1} = O\end{cases}$$

For any $\Psi X \Psi$, the unitary operation should satisfy the following relation

$$\langle \hat{U} X | \hat{O} \Psi \rangle = \langle X | \Psi \rangle \tag{1.11}$$

while the Hermitian operator should satisfy

$$\langle \hat{O} X | \Psi \rangle = \langle X | \hat{O} \Psi \rangle \tag{1.12}$$

Another kind of unitary: Anti-Unitary <- Anti-Linear

1.5 Time Evolution

$$|\Psi(t)\rangle = \hat{U}(t, t_0) |\Psi(t_0)\rangle$$

$$\langle \hat{O} \Psi(t_0) | \hat{O} \Psi(t_0) \rangle = \langle \Psi(t_0) | \Psi(t_0) \rangle$$

The two statements: Operator $\hat{O}$ satisfies

- $\forall \psi$, $\langle \hat{O}\psi | \hat{O}\psi \rangle = \langle \psi | \psi \rangle$ (Preserve norm)
- $\forall X, \psi$, $\langle \hat{O} X | \hat{O}\psi \rangle = \langle X | \psi \rangle$ (Preserve inner product)

Prove that they are equivalent.

Proof. Obviously, 2 to 1 is trivial. Let $u = X + \Psi$, $V = X + \mathrm{i}\Psi$, then subsitute them in to the above formulas. □

1.5.1 Equation of Motion

$\hat{U}$: linear, continous with time.
We need to consider ϵ time difference, that is somethint like

$$|\Psi(t+\epsilon)\rangle = \hat{U}(t+\epsilon, t) |\Psi(t)\rangle$$

$$\lim_{\epsilon \to 0} \frac{|\Psi(t+\epsilon)\rangle - |\Psi(t)\rangle}{\epsilon} = \lim_{\epsilon \to 0} \frac{\hat{U}(t+\epsilon, t) - \hat{U}(t, t)}{\epsilon} |\Psi(t)\rangle$$

$$\text{LHS} = \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle, \; \lim_{\epsilon \to 0} \frac{\hat{U}(t+\epsilon, t) - \hat{U}(t, t)}{\epsilon} = \frac{\mathrm{d}}{\mathrm{d}t} \hat{U}(t', t) \Big|_{t'=t} \equiv \frac{1}{\mathrm{i}\hbar} \hat{H}(t)$$

Finally, we approach the Schrödinger Equation

$$\frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle = \frac{1}{\mathrm{i}\hbar} \hat{H}(t) |\Psi(t)\rangle \tag{1.13}$$

Prove: $\hat{g}$ is Hermitian

$$\frac{\mathrm{d}}{\mathrm{d}\theta} \hat{U}(\theta) \Big|_{\theta=0} = \mathrm{i}\hat{g} \tag{1.14}$$

while $\hat{U}(0) = \mathbb{1}$.

Proof. We know that

$$\hat{U}(\epsilon) = \mathbb{1} + \mathrm{i}\hat{g}\epsilon$$

Since the definition of Hermitian is

$$\langle \hat{O}X|\Psi\rangle = \langle X|\hat{O}\Psi\rangle,$$

Then plug $\hat{U}(\epsilon)$ into the definition

$$\langle \hat{U}(\epsilon)X|\hat{U}(\epsilon)\Psi\rangle = \langle X|\psi\rangle + (-\mathrm{i}\epsilon)\langle \hat{g}X|\Psi\rangle + (\mathrm{i}\epsilon)\langle X|\hat{g}\Psi\rangle = \langle X|\Psi\rangle$$

then we have

$$\langle \hat{g}X|\Psi\rangle = \langle X|\hat{g}\Psi\rangle$$

means that $\hat{g}$ is Hermitian. □

$\hat{g}$ is called the generator; *ℏ / Hamiltonian is the generator of time evolution.*

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle \tag{1.15}$$

$\hat{H}$ is canonical quantization. Replace $|\psi(t)\rangle$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0) \tag{1.16}$$

Given $\hat{H}(t)$, find $\hat{U}(t_f,t_i)$. For t-independent $\hat{H}$, do small steps from t_i to t_f by $\delta t = (t_f - t_i)/N$

$$\hat{U}(t_f,t_i) = \hat{U}(t_f,t_f-\delta t)\hat{U}(t_f-\delta t,t_f-2\delta t)\ldots\hat{U}(t_i+\delta t,t_i) \tag{1.17}$$

When $N\to\infty$, $\delta t\to 0$, that become

$$\hat{U}(t_f,t_i) = \lim_{N\to\infty}(\mathbb{1}-\mathrm{i}\hat{H}\delta t)^N = \lim_{N\to\infty}\left(\mathbb{1}-\mathrm{i}\hat{H}\frac{t_f-t_i}{N}\right)^N = \mathrm{e}^{-\mathrm{i}\hat{H}(t_f-t_i)} = \mathbb{1} + ()\hat{H} + ()\hat{H}^2 + \cdots$$

1.5.2 Dyson series

When it's time-independent, the order doesn't matter. Now, consider the t-dependent case of $\hat{H}(t)$

$$\hat{U}(t_f,t_i) = \lim_{\delta t\to 0}(\mathbb{1}-\mathrm{i}\hat{H}(t_f)\delta t)(\mathbb{1}-\mathrm{i}\hat{H}(t_f-\delta t)\delta t)\cdots(\mathbb{1}-\mathrm{i}\hat{H}(t_i+\delta t)\delta t)$$

and convert every term into exponential $\mathrm{e}^{-\mathrm{i}\hat{H}(t_i+\delta)\delta t}$, the first term gets $\mathrm{e}^{-\mathrm{i}\hat{H}(t_f)\delta t}$. Multiply all the exponential function, $\mathrm{e}^{-\mathrm{i}\int_{t_i}^{t_f}\mathrm{d}t\hat{H}(t)}$.

Since $\mathrm{e}^A\,\mathrm{e}^B \sim \mathrm{e}^C$, but $C = A + B + ()[A,B] + \cdots$. And a time ordering operator $\mathcal{T}$ is applied before the exponential.

Now, rewrite the S.E

$$\int_{t_i}^{t_f}\mathrm{d}\hat{U}(t,t_i) = \int_{t_i}^{t_f}[-\mathrm{i}\hat{H}(t)]\hat{U}(t,t_i)\,\mathrm{d}t \tag{1.18}$$

since the lower limit of the integral t_i and the second time variable of $\hat{U}$: t_i conduct an identity, that is

$$\text{LHS} = \hat{U}(t_f, t_i) - \hat{U}(t_i, t_i) = \hat{U}(t_f, t_i) - \mathbb{1}$$

so

$$\begin{aligned}
\hat{U}(t_f, t_i) &= \mathbb{1} + \int_{t_1}^{t_f} \mathrm{d}t_1[-\mathrm{i}\hat{H}(t)]\hat{U}(t_1, t_i) \\
&= \mathbb{1} + \int_{t_1}^{t_f} \mathrm{d}f_1(-\mathrm{i}\hat{H}(t_1)) + \int_{t_i}^{t_f} \mathrm{d}t_1(-\mathrm{i}\hat{H}(t_1)) \int_{t_i}^{t_1} \mathrm{d}t_2(-\mathrm{i}\hat{H}(t_2)) \\
&+ \cdots + \int_{t_i}^{t_f} \mathrm{d}t_1 + \int_{t_i}^{t_1} \mathrm{d}t_2 \cdots + \int_{t_i}^{t_{n-1}} \mathrm{d}t_n(-\mathrm{i}\hat{H}(t_1)) \cdots (-\mathrm{i}\hat{H}(t_N)) + \cdots
\end{aligned}$$

That's what we called the *Dyson's Series.* Now, let's take a look at N's order term

$$\begin{aligned}
\int_{t_i}^{t_f} \mathrm{d}t_1 \int_{t_i}^{t_1} \mathrm{d}t_2 \cdots \int_{t_i}^{t_{n-1}} \mathrm{d}t_n \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n) = \int_{t_i}^{t_f} \mathrm{d}t_1 \int_{t_i}^{t_f} \mathrm{d}t_2 \int_{t_i}^{t_f} \mathrm{d}t_n \\
\theta(t_1 - t_2)\cdots\theta(t_{n-1} - t_n)\hat{H}\cdots\hat{H}
\end{aligned} \tag{1.19}$$

while

$$\theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \tag{1.20}$$

is the Heaviside Stage Function. It could

$$\int_{x_0}^{x_1} \mathrm{d}x = \int_{x_0}^{\infty} \mathrm{d}x\theta(x_0 - x) \tag{1.21}$$

x_0 x_1 ∞

t_1, t_2, ..., are Dummy variables. Then, sum over all of the permutations

$$\begin{aligned}
&\int_{t_i}^{t_f} \mathrm{d}t_1 \int_{t_i}^{t_f} \mathrm{d}t_2 \int_{t_i}^{t_f} \mathrm{d}t_n \theta(t_1 - t_2)\cdots\theta(t_{n-1} - t_n)\hat{H}\cdots\hat{H} \\
=&\frac{1}{n!}\sum_{\sigma} \int_{t_i}^{t_f} \mathrm{d}t_{\sigma_1} \int_{t_i}^{t_f} \mathrm{d}t_{\sigma_2} \cdots \int_{t_i}^{t_f} \mathrm{d}t_{\sigma_n} \theta(t_{\sigma_1} - t_{\sigma_2})\cdots\theta(t_{\sigma_{n-1}} - t_{\sigma_n})\hat{H}(t_{\sigma_1})\cdots\hat{H}(t_{\sigma_n}) \\
=&\frac{1}{n!}\int_{t_i}^{t_f} \mathrm{d}t_1 \int_{t_i}^{t_f} \mathrm{d}t_2 \cdots \int_{t_i}^{t_f} \mathrm{d}t_{\sigma_n} \sum_{\sigma}[\theta(t_{\sigma_1} - t_{\sigma_2})\cdots\theta(t_{\sigma_{n-1}} - t_{\sigma_n})\hat{H}(t_{\sigma_1})\cdots\hat{H}(t_{\sigma_n})] \\
\equiv&\mathcal{T}[\hat{H}(t_1)\cdots\hat{H}(t_n)] = \frac{1}{n!}\mathcal{T}\left[\int_{t_i}^{t_f} \mathrm{d}t\hat{H}(t)\right]^n
\end{aligned}$$

while $\sigma : \{1, 2, \ldots, n\} \to \{1, 2, \ldots, n\}$ is called permutation: E.g., σ_2: 1, 2, 3 $\to$ 3, 1, 2. And we introduced the time ordering operator $\mathcal{T}$ to prevent a Hamiltonian operator with an latter time $\hat{H}(t_j)$ "knocked" on $|\Psi(t)\rangle$ earlier that a Hamiltonian operator with an earlier time $\hat{H}(t_i)$ will "knock on": that is $\hat{H}(t_i)\hat{H}(t_j)|\Psi(t)\rangle$.

Review: Time Evolution

The Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \tag{1.22}$$

and we can rewrite it in terms of time-evolution operator

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0) \tag{1.23}$$

and initially, we can write

$$\hat{H}(t) = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t',t)\bigg|_{t'=t} = \mathrm{i}\left[\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t,t_0)\right]\hat{U}^{-1}(t,t_0)$$

the bracket can be generalize something like

$$\hat{g}_\theta = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\theta}\hat{U}(\theta)\bigg|_{\theta=0} \tag{1.24}$$

and we can have the identity

$$\hat{U}(0) = \mathbb{1} \tag{1.25}$$

In general, the expression of the time-evolution operator is something like

$$\hat{U}(t,t_0) = \mathcal{T}\,\mathrm{e}^{-\mathrm{i}\int_{t_0}^{t}\mathrm{d}t'\hat{H}(t)}$$

The time-ordering operator is inserted since

$$\mathrm{e}^{A}\,\mathrm{e}^{B} = \mathrm{e}^{C} \neq \mathrm{e}^{A+B}$$

BCH formula will tell how to write C:

$$C = A + B + \frac{1}{2}[A,B] + \cdots$$

The time-ordering operator can be also separate into two cases

$$\begin{cases} \hat{U}(t,t_0) = \mathrm{e}^{-\mathrm{i}(t-t_0)\hat{H}}, & \text{time-independent} \\ \hat{U}(t,t_0) = \mathbb{1} + (-\mathrm{i})\int_{t_0}^{t}\mathrm{d}t_1\hat{H}(t_1) + (-\mathrm{i})\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\hat{H}(t_1)\hat{H}(t_2) + \cdots, & \text{time-dependent} \end{cases}$$

1.5.3 Three Pictures

Considering representation, the basis $\{|\alpha\rangle\}$. and in state and operator

$$|\psi\rangle = \sum_\alpha \psi_\alpha|\alpha\rangle \tag{1.26}$$

$$\hat{O} = \sum_{\alpha\beta}\hat{O}_{\alpha\beta}|\alpha\rangle\langle\beta| \tag{1.27}$$

where $\psi_\alpha = \langle\alpha|\psi\rangle$ and $O_{\alpha\beta} = \langle\alpha|\hat{O}|\beta\rangle$.

- Schrödinger: $\{|\alpha\rangle^S = |\alpha\rangle\}$, where $|\alpha\rangle$ is const in time.

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_\alpha^s(t) = \frac{\mathrm{d}}{\mathrm{d}t}^s\langle\alpha|\psi(t)\rangle = (-\mathrm{i})^s\langle\alpha|\hat{H}(t)|\psi(t)\rangle = \sum_\beta(-\mathrm{i})H_\alpha(t)\psi_\beta^s(t)$$

when $\alpha \to x$, $\psi_\alpha(t) = \psi(x,t)$

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = \int \mathrm{d}x' H(x,x',t)\psi(x',t) \to H(x,-\mathrm{i}\,\partial_x,t)\psi(x,t)$$

the propotion $H(x,x',t)$ is something like $\delta(x-x')$.

- Heisenberg

$$\{|\alpha(t)\rangle^H = \hat{U}(t,t_0)|\alpha(t_0)\rangle\}$$

for the state,

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_\alpha^H(t) = \frac{\mathrm{d}}{\mathrm{d}t}^H\langle\alpha(t)|\psi(t)\rangle = 0 \tag{1.28}$$

means the state is not moving at all. Assume $\alpha(t_0) = \alpha$, $\hat{U}(t,t_0) = \hat{U}(t)$, and $\psi(t_0) = \psi$.

$$\frac{\mathrm{d}}{\mathrm{d}t}O_{\alpha\beta}^H(t) = \frac{\mathrm{d}}{\mathrm{d}t}^H\langle\alpha(t)|\hat{O}|\beta(t)\rangle^H = \frac{\mathrm{d}}{\mathrm{d}t}\langle\alpha|\hat{U}^{-1}(t)\hat{O}\hat{U}(t)|\beta\rangle$$

where $\hat{U}^{-1}(t)\hat{O}\hat{U}(t) = \hat{O}^H(t)$. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}^H(t) = \frac{\mathrm{d}}{\mathrm{d}t}(O^{-1}(t)\hat{O}\hat{U}(t))$$

where $\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}^{-1}(t) = \mathrm{i}\hat{U}^{-1}(t)\hat{H}(t)$. Finally, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}^H(t) = \mathrm{i}[\hat{H}^H(t),\hat{O}^H(t)] \tag{1.29}$$

which is so called the Heisenberg equation (EOM), where

$$\hat{H}^H(t) = \hat{U}^(t)^{-1}\hat{H}(t)\hat{U}(t)$$

- Interaction

We have two part of Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}$$

what is important is that $\hat{H}_0$ is the easy part, we can easily compute the time evolution $\hat{U}_0(t)$. Then, the basis will be chosen as

$$\{|\alpha(t)\rangle^I = \hat{U}_0(t)|\alpha\rangle\}$$

then

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_\alpha^I(t) = \frac{\mathrm{d}}{\mathrm{d}t}^I\langle\alpha(t)|\psi(t)\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle\alpha|\hat{O}^{-1}\hat{U}(t)|\psi\rangle. \tag{1.30}$$

and we consider $\hat{O}^{-1}\hat{U}(t)|\psi\rangle = |\psi(t)\rangle^I$. Similarly,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\psi_\alpha(t)\rangle^I &= \mathrm{i}\hat{U}_0^{-1}(\hat{H}_0(t)-\hat{H}(t))\hat{U}(t)|\psi\rangle = \frac{\mathrm{d}}{\mathrm{d}t}(\hat{U}_0^{-1}\hat{U}(t)|\psi\rangle)(?)\\ &= -\mathrm{i}\hat{U}_0^{-1}(t)\hat{V}(t)\hat{U}_0(t)\hat{U}_0^{-1}(t)\hat{V}(t)|\psi\rangle = -\mathrm{i}\hat{V}^I(t)|\psi(t)\rangle^I\end{aligned}$$

where $\hat{U}_0^{-1}(t)\hat{V}(t)\hat{U}_0(t) = \hat{V}^I(t)$ and $\hat{U}_0^{-1}(t)\hat{V}(t)|\psi\rangle = |\psi(t)\rangle^I$, and $\hat{O}(t) = \hat{U}_0^{-1}(t)\hat{O}\hat{U}_0(t)$.

$$\frac{\mathrm{d}\hat{O}^I(t)}{\mathrm{d}t} = \mathrm{i}[\hat{H}_0^I(t), \hat{O}^I(t)] = \frac{\mathrm{d}}{\mathrm{d}t}(\hat{U}_0^{-1}(t)\hat{O}\hat{U}_0(t))$$

Quiz 4

Problem 0.7. Given

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}_0(t,t_0) = -\mathrm{i}\hat{H}_0(t)\hat{U}_0(t,t_0),$$

show that

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}_0^{-1}(t,t_0) = \mathrm{i}\hat{U}_0^{-1}(t,t_0)\hat{H}_0(t).$$

Solution.

Problem 0.8. Given

$$f(z) = \mathrm{e}^{-\frac{1}{2}(x-z)^2}, \quad (x\in\mathbb{R},\ z\in\mathbb{C})$$

compute

$$\int_{-\infty}^{+\infty} |f(x)|^2\,\mathrm{d}x.$$

1.5.4 Case study

<u>Case 1</u> Quantum Harmonic Oscillator

Certainly, this is a time-independent problem, the Hamiltonian is given as

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{X}^2.$$

For simplifaction, we define $l_0 = \sqrt{\frac{\hbar}{m\omega}}$, then

$$\hat{X} = \frac{\hat{x}}{l_0}, \quad \text{and} \quad \hat{k} = \frac{\hat{p}l_0}{\hbar}.$$

So, the original commutation relation becomes

$$[\hat{x},\hat{p}] = \mathrm{i}\hbar \longrightarrow [\hat{x},\hat{k}] = \mathrm{i}.$$

Certaily, we need

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{x}+\mathrm{i}\hat{k}), \quad \text{and} \quad [\hat{a},\hat{a}^\dagger] = 1$$

and let $\hbar = 1$. Then

$$\hat{H} = \omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$$

where $\hat{a}^\dagger\hat{a} = \hat{N}$, the number operator.

i. The eigenstates $|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle$, and $\hat{a}|0\rangle = 0$. Consider

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

Then

$$\langle n(t)|\hat{x}|n(t)\rangle = 0, \quad \text{and} \quad \langle n(t)|\hat{k}|n(t)\rangle = 0$$

where

$$\hat{x} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger), \hat{k} = \frac{1}{\sqrt{2}\,\mathrm{i}}(\hat{a} - \hat{a}^\dagger)$$

In Heisenberg picture

$$\dot{\hat{x}}(t) = \mathrm{i}[\hat{H}(t), \hat{x}(t)] = \omega\hat{k}(t), \quad \text{and} \quad \dot{\hat{k}}(t) = \mathrm{i}[\hat{H}, \hat{k}(t)] = -\omega\hat{x}(t)$$

and we have

$$\dot{\hat{a}}(t) = -\,\mathrm{i}\omega\hat{a}(t) \Rightarrow \hat{a}(t) = \mathrm{e}^{-\mathrm{i}\omega t}\hat{a}$$

$$\hat{x}(t) = \cos\omega t\hat{x} + \sin\omega t\hat{k}, \hat{k}(t) = -\sin\omega t\hat{x} + \cos\omega t\hat{k}.$$

ii. Coherent States $\{|\alpha\rangle\}$

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle,\ \alpha \in \mathbb{C}$$
$$|\psi\rangle \sim \sum_\alpha \psi_\alpha|\alpha\rangle,\ |\psi(t)\rangle = \sum_\alpha \psi_\alpha|\alpha(t)\rangle$$
$$\hat{a}(-t)|\alpha(t)\rangle = \alpha|\alpha(t)\rangle,\ \hat{U}^{-1}\hat{a}\hat{I}^{-1}(-t)\hat{U}(t)|\alpha\rangle$$
$$\mathrm{e}^{\mathrm{i}\omega t}\hat{a}|\alpha(t)\rangle = \alpha|\alpha(t)\rangle \Rightarrow \alpha(t) = \mathrm{e}^{-\mathrm{i}\omega t}\alpha$$

What if $|x(t)\rangle$, or in other words $|\psi\rangle$ is $|x_0\rangle$

$$\langle\alpha|x_0\rangle = \int_{x_0}(\alpha)$$

$$|\alpha\rangle = \sum_n^\infty f_{\alpha,n}|n\rangle$$

while

$$\hat{a}|\alpha\rangle = \sum_n f_{\alpha,n}\sqrt{n}|n-1\rangle = \sum_n f_{\alpha,n+1}|n\rangle$$

where

$$f_{\alpha,n+1} = \frac{\alpha}{\sqrt{n+1}}f_{\alpha,n}, \quad f_{\alpha.n} = \frac{\alpha^n}{\sqrt{n!}}f_{\alpha,0}$$

and

$$|\alpha\rangle = N\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle = N\,\mathrm{e}^{\alpha}a^{n-1}|0\rangle, \quad |n\rangle = \ldots$$

Concering $\langle x|\alpha\rangle$: since

$$\alpha f_\alpha(x) = \langle x|\hat{a}|\alpha\rangle = \int \mathrm{d}x'\langle x|\hat{a}|x'\rangle\langle x'|\alpha\rangle$$

substitute $\hat{a} = \frac{1}{\sqrt{2}}(\hat{x} + \hat{k})$

$$\alpha f_\alpha(x) = \frac{1}{\sqrt{2}}(x + \partial_x) f_\alpha(x)$$

and

$$f_\alpha(x) = N\, \mathrm{e}^{-\frac{1}{2}(x-\sqrt{2}a)^{\frac{\alpha}{2}}}$$

where $|f_\alpha(x)|^2 = \frac{1}{\sqrt{\pi}}\, \mathrm{e}^{-(x-\sqrt{2}\alpha_x)^2}$

Case 2 Rabi Problem
The Hamiltonian

$$\hat{H}(t) = \begin{pmatrix} \frac{\Omega}{2} & \gamma\, \mathrm{e}^{-\mathrm{i}\omega t} \\ \gamma\, \mathrm{e}^{\mathrm{i}\omega t} & -\frac{\Omega}{2} \end{pmatrix}$$

bascially time-dependent. $\frac{\Omega}{2}$ and $-\frac{\Omega}{2}$ means the gap between $|0\rangle$ and $|1\rangle$ is Ω; and driver frenquency ω, intensity γ.

$$U(t) = \begin{pmatrix} |0\rangle \to |0\rangle & |1\rangle \to |0\rangle \\ |0\rangle \to |1\rangle & |1\rangle \to |1\rangle \end{pmatrix}$$

Compute $H_0 = \begin{pmatrix} \frac{\omega}{2} & 0 \\ 0 & -\frac{\omega}{2} \end{pmatrix}$.

Firstly, the definiton of $U_0(t)$. Normally, $U_0(t) = \mathrm{e}^{-\mathrm{i}tH_0}$; In this case

$$U_0(t) = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\frac{\omega}{2}t} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\frac{\omega}{2}t} \end{pmatrix}$$

and

$$U_0^{-1}(t) H(t) U_0(t) = \begin{pmatrix} \frac{\Omega}{2} & \gamma \\ \gamma & -\frac{\Omega}{2} \end{pmatrix}, \; V = \begin{pmatrix} \frac{\Omega-\omega}{2} & \gamma \\ \gamma & -\frac{\Omega-\omega}{2} \end{pmatrix}$$

We get a matrix equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} U(t) = V U(t)$$

the solution is

$$U(t) = \cos Delta_\omega t - \mathrm{i} \sin \Delta_\omega t (\cos\theta_\omega \sigma_z + \sin\theta_\omega \sigma_x)$$

where

$$\Delta_\omega = \sqrt{\left(\frac{\Omega-\omega}{2}\right)^2 + r^2}, \quad \tan\theta_\omega = \frac{2\gamma}{\Omega-\omega}$$

and

$$P_{0\to 1}(t) = \frac{\gamma^2}{\left(\frac{\Omega-\omega}{2}\right)^2 + \gamma^2} \sin^2(\Delta_\omega t)$$

probability: Center: Ω, and γ (coupling strength), giving a width. It's very small, means the peek is sharp; If γ is large, ...

Chapter 2 Path Integral

* What is a path? $-\ x(t)$. $\phi : I \equiv [0,1] \to R^d, t \in I, t_i = 0, t_f = 1$.

  $I \to R^d$, $I \to M$, $R^{d+1} \to M$: $\phi \in$ Function space. ($d+1$: dimension and time)

* What to integrate? $\sum_\phi G[\phi]$. $G : V \to \mathbb{C}$.

  E.g.: $F[x(t)] \to f(x_1, x_2, \cdots x_N) \leftarrow f(x) = ax^m$

* Quantization Schemes: Canonical Quantization $\Leftrightarrow$ Path Integral

  States & Operators.

  In qm, $\langle O_1, O_2 \rangle \to$ trasition amplitudes, propagate.

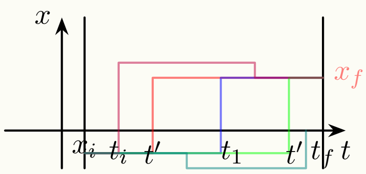
  Something like $\int \mathcal{D}\phi G[\phi]$ will eventually produce something like $\langle O_1, O_2 \rangle$.

2.1 Compare Quantum with Classical Limit

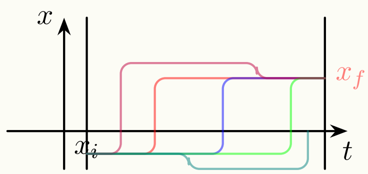
(a) Quantum

$$\hat{U}(t_f, t_i) = \mathbb{1} + \left(-\frac{\mathrm{i}}{\hbar}\right)\int_{t_i}^{t_f} \mathrm{d}t_1 \hat{H}(t_1) + \left(-\frac{\mathrm{i}}{\hbar}\right)^2 \int_{t_i}^{t_f} \mathrm{d}t_1 \int_{t_i}^{t_1} \mathrm{d}t_2 \hat{H}(t_1)\hat{H}(t_2) + \cdots$$

Problem: Discontinuous! The Hamiltonian actually shall be "local". One of H act on state, it could not jump.



It should be



U can be decompose like

$$\hat{U}(t_f, t_i) = \hat{U}(t_f, t_{N-1}) \cdots \hat{U}(t_N, t_{N-1}) \cdots \hat{U}(t_i,)$$

(b) Path Integral

$$\begin{aligned} &U(x_f, t_f; x_i, t_i) \equiv \langle x_f | \hat{U}(t_f, t_i) | x_i \rangle \\ =& \int \mathrm{d}x_i \cdots \mathrm{d}x_{N-1} \langle x_f | \hat{U}(t_f, t_{N-1}) | x_{N-1} \rangle \langle x_{N-1} | \hat{U}(t_{N-1}, t_{N-2}) | x_{N-2} \rangle \cdots \\ &\langle x_n | \hat{U}(t_n, t_{n-1}) | x_{n-1} \rangle \cdots \langle x_1 | \hat{U}(t_1, t_i) | x_i \rangle \end{aligned}$$

Basically, we can write the time evolution

$$U(x_n, t_n; x_{n-1}, t_{n-1}) = \langle x_n | \hat{U}(t_n, t_{n-1}) | x_{n-1} \rangle \approxeq \langle x_n | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t_n)\delta t} | x_{n_1} \rangle$$

it's vavid when δt is very small. Insert a complete basis

$$
\begin{aligned}
U(x_n,t_n;x_{n-1},t_{n-1}) &\approxeq \int \mathrm{d}p_n \langle x_n|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t_n)\delta t}|p_n\rangle\langle p_n|x_{n_1}\rangle \\
&= \frac{1}{2\pi\hbar}\int \mathrm{d}p_n\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}}[p_n(x_n-x_{n-1}) - H(x_n,p_n,t_n)\delta t]
\end{aligned}
$$

Consider

$$
\int \prod_{n=1}^{N-1} \mathrm{d}x_n \int \prod_{n=1}^{N} \mathrm{d}p_n
$$

which is so called "path": in phase space path integral. (Consider the time is divided in many pieces). Then $U(x_n,t_n;x_{n-1},t_{n-1})$ can be

$$
U(x_n,t_n;x_{n-1},t_{n-1}) = \int \mathrm{d}p_n\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[p_n\dot{x}_n - \frac{p_n^2}{2m} - V(x_n,t_n)]\delta t} = \left(\frac{m}{2\pi\,\mathrm{i}\hbar\delta t}\right)^{1/2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\frac{1}{2}m\dot{x}_n^2 - V(x_n,t_n)]\delta t}
$$

where $\dot{x}_n = \frac{x_n - x_{n-1}}{\delta t}\big|_{\delta t\to 0}$, and $\frac{1}{2}m\dot{x}_n^2 - V(x_n,t_n)$ is the Lagrangian $\mathcal{L}(x_n,\dot{x}_n,t_n)$. Eventually,

$$
U(x_f,t_f;t_i,t_i) = \left(\frac{m}{2\pi\,\mathrm{i}\hbar\delta t}\right)^{N/2} \int \prod_{n=1}^{N-1} \mathrm{d}x_n\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sum_{n=1}^{N-1}\mathcal{L}(x_n,\dot{x}_n,t_n)\delta t} = \int \mathcal{D}x(t)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{S}[x]}
$$

where $\mathcal{D} = \int\prod_{n=1}^{N-1}\mathrm{d}x_n$, and $\mathcal{S}[x] \equiv \int_{t_i}^{t_f}\mathrm{d}t\mathcal{L}(x,\dot{x},t)$ ($N\to\infty$). In summary, we obtain

$$
U(x_f,t_f;x_i,t_i) \equiv \int \mathcal{D}x(t)\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathcal{S}[x(t)]} \tag{2.1}
$$

where $x(t_i) = x_i$ and $x(t_f) = x_f$.

(c) Classical

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

Using $\mathrm{e}^{-\mathrm{i}\hat{H}\delta t} \approxeq 1 - \mathrm{i}\hat{H}\delta t$. Then, we can simply evalute $\langle x_n|\hat{H}|p_n\rangle$.

$$
\langle x_n|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t_n)\delta t}|p_n\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(x_n,p_n,t_n)\delta t}\langle x_n|p_n\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(x_n,p_n,t_n)\delta t + \frac{\mathrm{i}}{\hbar}p_n x_n}
$$

where $H(x_n,p_n,t_n) = \frac{p_n^2}{2m} + V(x_n,t_n)$.

Principle of Least Action, EOM determines $x_c(t)$. The equation can be derived by

$$\delta\mathcal{S} = 0, \quad \text{or} \quad (\delta_x\mathcal{S})[\eta] = 0, \forall\eta \tag{2.2}$$

we fix the initial (x_i, t_i) and the final (x_f, t_f). Consider the other path $x'(t)$, the different is $\eta(t)$. Starting from the action

$$\mathcal{S}[x(t)] = \int_{t_i}^{t_f} \mathrm{d}t\mathcal{L}(x(t), \dot{x}(t), t) \tag{2.3}$$

On another path, the action is

$$\mathcal{S}[x_c + \eta_c] = \int_{t_i}^{t_f} \mathrm{d}t\mathcal{L}(x_t + \eta_t, \dot{x}_t + \dot{\eta}_t, t) = \int_{t_i}^{t_f} \mathrm{d}t\Big[\mathcal{L}(x_t, \dot{x}_t, t) + \frac{\partial\mathcal{L}}{\partial x_t}\eta t + \frac{\partial\mathcal{L}}{\partial\dot{x}_t}\dot{\eta}_t + \mathcal{O}(\eta^2)\Big]$$

where

$$\int_{t_i}^{t_f} \mathrm{d}t\Big(\frac{\partial\mathcal{L}}{\partial x_t}\eta t + \frac{\partial\mathcal{L}}{\partial\dot{x}_t}\dot{\eta}_t\Big)$$

is so-called *functional derivative*[1]: $(\delta_x\mathcal{S})[\eta]$. Apply the partition integration

$$(\delta_x\mathcal{S})[\eta] = \frac{\partial L}{\partial\dot{x}_t}\eta_t\Big|_{t_i}^{t_f} + \int_{t_i}^{t_f} \mathrm{d}t\Big(\frac{\partial\mathcal{L}}{\partial x_t} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}_t}\Big)\eta_t$$

since $\eta(t_i) = \eta(t_f) = 0$, so

$$(\delta_x\mathcal{S})[\eta] = \int_{t_i}^{t_f} \mathrm{d}t\Big(\frac{\partial\mathcal{L}}{\partial x_t} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}_t}\Big)\eta_t$$

the integral kernel can be converted to

$$\Big(\frac{\partial\mathcal{L}}{\partial x_t} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}_t}\Big)\eta_t = \langle\frac{\partial\mathcal{S}}{\partial x_i}|\eta\rangle$$

For $\forall\eta$, the integral kernel should be zero

$$\frac{\partial\mathcal{L}}{\partial x_t} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}_t} = 0 \tag{2.4}$$

it's so-called the *Euler-Lagrangian Equation*.

Let's talk more about functional derivative.

$$(\delta_x^{(n)}\mathcal{S})[\eta] = \frac{\mathrm{d}^n\mathcal{S}[x(t) + \epsilon\eta(t)]}{\mathrm{d}\epsilon^n}\Big|_{\epsilon=0}$$

the x is supposed to "where we take the derivative". $\mathcal{S}[x(t) + \epsilon\eta(t)]$ gives a number, but the number is depend on ϵ. So we can define

$$\frac{\mathrm{d}^n f_{x,\eta}(\epsilon)}{\mathrm{d}\epsilon^n} = \mathcal{S}[x(t) + \epsilon\eta(t)]$$

Quiz. Let's try an example.

$$\mathcal{L}(x(t), \dot{x}(t)) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2$$

[1] From functional space to functional space: $V^* \to V^*$.

Try to find $\delta_x^{(0)}\mathcal{S}[\eta]$, $\delta_x^{(1)}\mathcal{S}[\eta]$, $\delta_x^{(2)}\mathcal{S}[\eta]$, $\delta_x^{(3)}\mathcal{S}[\eta]$ using the definition. (Solution: $\delta_x^{(0)}\mathcal{S}[\eta] = \mathcal{S}[x]$, $\delta_x^{(1)}\mathcal{S}[\eta]$: $\ddot{x} = -\omega^2 t$, $\delta_x^{(2)}\mathcal{S}[\eta] = 2\mathcal{S}[\eta]$, $\delta_x^{(>2)}\mathcal{S}[\eta] = 0$.)
Let's try to write the Taylor expression of $\mathcal{S}[x+\eta]$

$$\mathcal{S}[x+\eta] = \mathcal{S}[x+\eta]\big|_{\epsilon=1} = f(\epsilon)_{x,\eta}, \tag{2.5}$$

then, just expand $f(\epsilon)_{x,\eta}$

$$\mathcal{S}[x+\eta] = f(0) + f'(0)\epsilon + \cdots + \frac{1}{n!}f^{(n)}(0)\epsilon^n + \cdots$$

Concering $f_{x,\eta}^{(n)} = (\delta_x^{(n)}\mathcal{S})[\eta]$, then

$$\mathcal{S}[x+\eta] = (\delta^{(0)}\mathcal{S})[\eta] + (\delta^{(1)}\mathcal{S})[\eta] + \cdots + \frac{1}{n!}(\delta^{(n)}\mathcal{S})[\eta] = \left(\mathrm{e}^{\delta_x}\mathcal{S}\right)[\eta] \tag{2.6}$$

$\boxed{\text{ELE} \to x_i(t)}$

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{S}[x+\eta]} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\mathcal{S}[x] + (\delta_x^{(0)}\mathcal{S})[\eta] + \frac{1}{2}(\delta_x^{(1)}\mathcal{S})[\eta] + \cdots)} \tag{2.7}$$

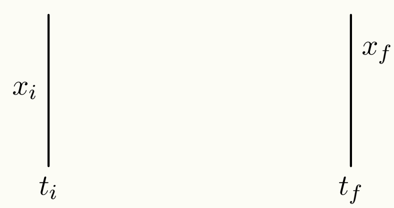
Since $\int \mathcal{D}\eta(t)$ taken the first order, then the other terms should vanish. Since classical limit require $\hbar$ to be small.

2.2 PI & Sta. Mech.

Review Starting from propagator

$$\langle x_f|\hat{U}(t_f,t_i)|x_i\rangle = \sum_{x(t)} \mathrm{e}^{\mathrm{i}S[x(t)]}$$

Summing over all the functions (paths). This is precisely the quantum interference



We can use a fancier symbol

$$\langle x_f|\hat{U}(t_f,t_i)|x_i\rangle = \int_{x(t_{i,f})=x_{i,f}} \mathcal{D}x(t)\, \mathrm{e}^{\mathrm{i}S[x(t)]}$$

Statistics Mechanics Starting from the partition function

$$Z = \sum_n \mathrm{e}^{-\beta E_n} = \sum_{\boxed{?}} \boxed{?} \tag{2.8}$$

n means we sum over the *microstates*: they are configuration.

Example 2.2.1. A general picture about what are microstates and configurations.

1. Two configurations: $\{\uparrow, \downarrow\}$.
2. Four configurations: $\{\uparrow, \uparrow, \downarrow, \downarrow\}$
3. It can also a continous set, a circle, spin point to all possible orientation in a plane, the configuration space of the case.

$$\{\ ,\ ,\ , \cdots\}$$

4. We can also have two objects, two circles cross to each others

$$\{\} \approxeq S^1 \times S^1$$

5. About (Quantum) H.O.: $\{\ ,\ \}$ Something like a string, can be stationary. The shapes for the string can be also configurations.
6. Oscillator: energy levels.

Recall the P.I. $\phi = x(t)$, Generalize it

$$\begin{array}{c} \mathbb{I}(\ \overset{t_i \quad t_f}{\overline{}}\ ) \longrightarrow \mathbb{R}(\{x\}) \\ \downarrow \\ \mathbb{R}^{d+1}(\mathbb{Z}^{d+1}) \longrightarrow M \end{array}$$

We can say we sum over the states, i.e., sum over different configurations

$$Z = \sum_{\phi} \mathrm{e}^{-\beta E(\phi)}$$

The configurations can be how these levels are occupied. Concering the βE term: Energy depends on the configuration, a kind of map, then it contribute to a Boltzman function.

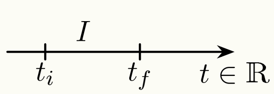
(a) How the P.I. can be the P.F.

(b) How the P.F. can be something of P.I.

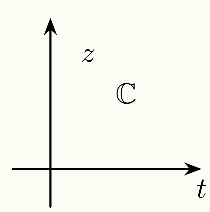
$$Z = \operatorname{Tr} \mathrm{e}^{-\beta \hat{H}}$$

2.2.1 Analytic Continuation

This somehow we go from P.I. to P.F. We have a targest space M. From the I, between t_i and t_f, mapping to the space M, where $t \in \mathbb{R}$. And a complex plane $\mathbb{C}$.



$\rightarrow$The space M $\leftarrow$



$$\phi(t) \mapsto \phi(z)\phi(\tau)$$

Map from a real axix to the target space, map from the imaginary axis in the complex plane to the target space. The property of the two maps really colse link together.

In summary: First, from t to z, $t \mapsto z$, then choose Z to be part of the imaginary axis or numbers, i.e., $z = -\mathrm{i}\tau$. As the following examples

Example 2.2.2. $t \mapsto z = -\mathrm{i}\tau$ **Example 2.2.4.** $\frac{\partial}{\partial t} \mapsto \mathrm{i}\frac{\partial}{\partial \tau}$ **Example 2.2.6.** $\dot{\phi}^2 \mapsto -\dot{\phi}_\tau^2$

Example 2.2.3. $\mathrm{d}t \mapsto -\mathrm{i}\,\mathrm{d}\tau$ **Example 2.2.5.** $\frac{\partial}{\partial t}\phi \equiv \dot{\phi} \mapsto \mathrm{i}\dot{\phi}_\tau$

Example 2.2.7 (The Lagrangian).

$$\mathcal{L}(\phi, \dot{\phi}) = \frac{1}{2}m\dot{\phi}^2 - V(\phi) \mapsto -\frac{1}{2}m\dot{\phi}_\tau^2 - V(\phi_\tau) = -\mathcal{L}_E(\phi_\tau, \dot{\phi}_\tau)$$

where E stands for Euclidean, contrast with Minkovsky, the distance in space-time

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + (\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2) = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2 + \mathrm{d}\tau^2$$

By going from t on the real axis to τ on the imaginary axis, which is so-called the Wick Rotation.

Example 2.2.8 (The Action).

$$\mathrm{i}S[\phi] \equiv (\mathrm{i})\int_{t_1}^{t_f} \mathrm{d}t\mathcal{L} \mapsto -S_E[\phi_\tau]$$

where

$$S_E[\phi_\tau] = \int_{\tau_i}^{\tau_f} \mathrm{d}\tau\mathcal{L}_E$$

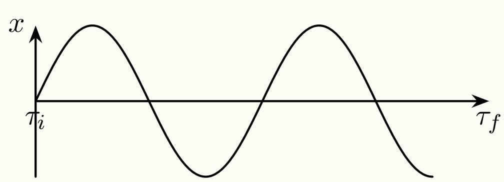
So, after the integral, the propagator should be

$$\int_{x(t_{i,f})=x_{i,f}} \mathcal{D}x(t)\,\mathrm{e}^{\mathrm{i}S[x(t)]} \mapsto \int \mathcal{D}x(\tau)\,\mathrm{e}^{-S_E[x(\tau)]}, \quad \text{where} \quad \mathcal{D} \sim \sum_{x(\tau)}$$

In **Example 2.2.7**, if we use x as the new variable, i.e., $\phi \to x_i$

$$\mathcal{L}(\phi, \dot{\phi}) = \frac{1}{2}m\dot{x}^2 - V(x) \longrightarrow \mathcal{L}_E(x_\tau, \dot{x}_\tau) = \frac{1}{2}m\dot{x}_\tau^2 + V(x_\tau)$$

The string can be displace in one direction. On the top of the string of each τ, we change from $\dot{x}_t^2 \sim [x(\tau_n) - x(\tau_{n-1})]^2$



We can interrupt it with tension $x(\tau)$ and potention $V(x(\tau))$, completely a classical problem. So, in the end, $\mathcal{L}_E$ is the energy density respects to the τ-axis after the translation. Concerning S_E

$$S_E[x(\tau)] = \int \mathrm{d}\tau\mathcal{L}_E(x(t), \dot{x}(t))$$

it is of course the total energy after the translation. In other words, t is replaced by τ. i.e., in $\mathbb{R}^{d+1}$, d is supposed to the space dimension, and one for time.

2.2.2 Quantum P.F.

The partition function is

$$Z = \mathrm{Tr}\,\mathrm{e}^{-\beta\hat{H}}, \quad \text{where} \quad \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{2.9}$$

where trace can be identity, i.e.,

$$Z_n = \int \mathrm{d}x_n \langle x_0|\mathrm{e}^{-\beta\hat{H}}|x_0\rangle$$

by inserting the identity $\int \mathrm{d}x_0|x_0\rangle\langle x_0| = \mathbb{1}$. What we need to do is to compare

$$\langle x_0|\mathrm{e}^{-\beta\hat{H}}|x_0\rangle \quad \text{with} \quad \langle x_f|\hat{U}(t_f,t_i)|x_i\rangle$$

by slicing $\beta \sim t_f - t_i$ into N pieces, each segment has a length of $\delta\tau = \beta/N$. Then

$$Z = \int \mathrm{d}x_0\,\mathrm{d}x_1\cdots\mathrm{d}x_{N-1}\langle x_0|\mathrm{e}^{-\delta\tau\hat{H}}|x_{N-1}\rangle\cdots\langle x_n|\mathrm{e}^{-\delta\tau\hat{H}}|x_{n-1}\rangle\cdots\langle x_1|\mathrm{e}^{-\delta\tau\hat{H}}|x_0\rangle$$

What we have derived is

$$\langle x_n|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\delta t\hat{H}}|x_{n-1}\rangle = \left(\frac{m}{2\pi\,\mathrm{i}\hbar\delta t}\right)^{1/2}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathcal{L}(x_n,\dot{x}_n)\delta t}$$

simply replace $\frac{\mathrm{i}}{\hbar}\delta t \to \delta\tau$, then

$$\langle x_n|\mathrm{e}^{-\delta\tau\hat{H}}|x_{n-1}\rangle = \left(\frac{m}{2\pi\hbar\delta\tau}\right)^{1/2}\mathrm{e}^{-\mathcal{L}_E(x(\tau_n),\dot{x}(\tau_n))\delta\tau}$$

with the periodic boundary condition $x_N \equiv x_0$, substitute it back, the partition function becomes

$$Z = \left(\frac{m}{2\pi\,\mathrm{i}\hbar\delta t}\right)^{N/2}\int\prod_{n=0}^{N-1}\mathrm{d}x_n\,\mathrm{e}^{-\sum_{n=0}^{N-1}\delta\tau\mathcal{L}_E(x(\tau_n),\dot{x}(\tau_n))} \xlongequal{N\to\infty} \int_{x(0)=x(f)}\mathcal{D}x(\tau)\,\mathrm{e}^{-S_E[x(\tau)]} \tag{2.10}$$

then the action

$$S_E[x_\tau] = \int_0^\beta \mathrm{d}\tau\mathcal{L}_E(x(\tau),\dot{x}(\tau)) \tag{2.11}$$

Quiz

Problem 0.9. Gaussian Integral

$$\int \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{e}^{-(x_1,x_2)\begin{pmatrix}1 & 1/2\\ 1/2 & 1\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}}$$

Change the variable x to a vector $\boldsymbol{x} = (x_1, x_2)$, i.e.

$$\int \mathrm{d}\boldsymbol{x}\,\mathrm{e}^{-\boldsymbol{x}\cdot\mathbf{A}\cdot\boldsymbol{x}} = \det\left(\frac{\mathbf{A}}{\pi}\right)^{-1/2}$$

Problem 0.10.

$$F[\pi] = \frac{1}{2}\int_{t_i}^{t_f}\mathrm{d}t_1\,\mathrm{d}t_2\phi(t_1)A(t_1,t_2)\phi(t_2)$$

then compute the second derivative $(\delta_\phi^2 F)[\eta]$.

$$(\delta_\phi^2 F)[\eta] = 2F[\eta]$$

Problem 0.11. The Lagrangian

$$L(\phi_t, \dot{\phi}_t) = a\phi_t^2 + b\dot{\phi}_t^2 + c\phi_t\dot{\phi}_t$$

show that $S[\phi] = S[\phi_c] + S[\phi - \phi_c]$, where ϕ_c is a classical path: $(\delta_\phi S)\big|_{\phi=\phi_c} = 0$.

Taylo expansion to $S[x+\eta]$

$$S[x_c + \eta] = S[x] + (\delta_{x_c} S[\eta]) + \frac{1}{2}(\delta_{x_c}^2 S)[\eta] = S[x_c] + 0 + S[\eta]$$

Case study We start from a Lagrangian

$$\mathcal{L}(x(t), \dot{x}(t)) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 \tag{2.12}$$

and we want to compute the propagator $\int_{x(t_{i,f})=x_{i,f}} \mathcal{D}(x)\, \mathrm{e}^{\mathrm{i}S[x(t)]}$. This computation would be purely quantum. We choose the staring point: $x(t_{i,f}) = x_{i,f}$. We separate

$$x(t) = x_c(t) + \eta(t)$$

Since x_i and x_f are fixed, so we get the boundary condition $\eta(t_i) = \eta(t_f) = 0$. Then the action

$$S[x_c + \eta] = \mathrm{e}^{\mathrm{i}S[x_c]} \cdot \int_{\eta(t_i)=\eta(t_f)=0} \mathcal{D}\eta(t)\, \mathrm{e}^{\mathrm{i}S[\eta(t)]}$$

where $S[x(t)] = S[x_c] + S[\eta_c]$.

(a) Comput $S[x_c]$

$$S[x_c] = \int_{t_i}^{t_f} \mathrm{d}t \mathcal{L}(x_c(t), \dot{x}_c(t)) = \int_{t_i}^{t_f} \mathcal{L}(t)$$

Concering $x_c(t)$, using the E-L eq. (EOM)

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} = 0, \quad \text{or} \quad (\partial_t^2 + \omega^2)x(t) = 0$$

Before getting the solution, applying the boundary condition

$$x(t_i) = x_i, \quad \text{and} \quad x(t_f) = x_f$$

The solution would be generally

$$x_c(t) = x_0 \sin(\omega t + \phi_0)$$

where x_0 and ϕ_0 will be fixed by the boundary condition. Substitute it into the Lagrangian

$$\mathcal{L}_{x_c}(t) = \frac{1}{2}m\omega^2 x0^2 \cos[2(\omega t + \phi_0)]$$

and the actioin

$$S[x_c] = \frac{m\omega}{2\sin(\omega\Delta t)}[(x_i^2 + x_f^2)\cos(\omega\Delta t) - 2x_i x_f]$$

Now, we shall handle

$$\int \mathcal{D}\eta\, \mathrm{e}^{\mathrm{i}S[\eta]}, \quad \text{where} \quad S[\eta] = \int_{t_i}^{t_f} \mathrm{d}t\Big(\frac{1}{2}m\dot{\eta}^2 - \frac{1}{2}m\omega^2\eta^2\Big)$$

Referring **Quiz 0.9**, $\int \mathrm{d}\boldsymbol{x}\, \mathrm{e}^{-\boldsymbol{x}\cdot\mathbf{A}\boldsymbol{x}}$, we can convert the integral kernel to

$$-\frac{1}{2}m\eta(\partial_t^2+\omega^2)\eta$$

where $(\partial_t^2+\omega^2)$ is the "sandwich" term $\mathbf{A}$. Since

$$\int \mathrm{d}t\dot{\eta}^2 = \cancel{(\eta\dot{\eta})\big|_{t_i}^{t_f}} - \int \mathrm{d}t\ddot{\eta}$$

Then the expression of the action is

$$\int \mathcal{D}\eta\, \mathrm{e}^{\mathrm{i}S[\eta]} = \det\left(\frac{\mathbf{A}}{\pi}\right)^{-1/2} = \det\left[\frac{\mathrm{i}m}{2\pi}(\partial_t^2+\omega^2)\right]^{-1/2}$$

Given a matrix M, its determent $\det(\mathbf{M}) = \prod_i \lambda_i$, where λ_i is the eigenvalue of $\mathbf{M}$. That is how we interrupt the determine of $\mathbf{A}$

$$(\partial_t^2+\omega^2)\psi_n = \lambda_n\psi_n$$

We just define X

$$X = \det(\partial_t^2+\omega^2) = \prod_n \lambda_n$$

we need to solve the ODE by applying the boundary condition $\eta(t_i) = \eta(t_f) = 0$, i.e., $\psi_n(t_i) = \psi_n(t_f) = 0$. The eigenvalue

$$\lambda_n = \omega^2 - (n\pi/\Delta t)^2 = \omega^2 - (n\Omega)^2, \quad n = 1, 2, \ldots, \infty$$

and substitute it into X

$$X = \prod_n \left(\omega^2 - n^2\Omega^2\right)$$

Take the log

$$\ln X = \sum_n \ln(\omega^2 - n^2\Omega^2)$$

then take the derivative of ω

$$\frac{\partial \ln X}{\partial\omega} = \sum_{n=1}^{\infty}\frac{2\omega}{\omega^2-n^2\Omega^2} = \frac{\pi}{\Omega}\operatorname{ctg}\left(\frac{\pi\omega}{\Omega}\right) - \frac{1}{\omega}$$

integral to both sides

$$\ln X = \ln\left(\frac{\sin\omega\Delta t}{\omega} + \text{Const}\right)$$

Directly jump to the determine

$$\det(\quad)^{-1/2} = C\left(\frac{\omega}{\sim(\omega\Delta t)}\right)^{1/2}$$

When $\omega \to 0$, the Lagrangian

$$\mathcal{L} = \frac{1}{2}m\dot{x}^2$$

which is the free particle, and the determine $\det(\quad)^{-1/2} \sim \Delta t^{-1/2}$. For the boundaty condition of the free particle

$$\langle x=0|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0\Delta t}|x=0\rangle = \int \mathrm{d}x \langle x=0|k\rangle\, \mathrm{e}^{-\mathrm{i}\frac{\hat{k}^2}{2m}\Delta t}\langle k|x=0\rangle = \frac{1}{2\pi}\int \mathrm{d}k\, \mathrm{e}^{-\mathrm{i}\frac{k^2}{2m}\Delta t} = \left(\frac{m}{2\pi\,\mathrm{i}\Delta t}\right)^{1/2}$$

where $H_0 = \frac{\hat{p}^2}{2m} = \frac{\hat{k}^2}{2m}$, set $\hbar = 1$, and $\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}kx}$. To infer C, comparing the result with the determine

$$\left(\frac{m}{2\pi\,\mathrm{i}\Delta t}\right)^{1/2} = (\Delta)^{-1/2}, \quad \text{and} \quad C = \left(\frac{m}{2\pi\,\mathrm{i}}\right)^{1/2}$$

Then we get X.

$$\psi_n(t) \sim \sin\left[\frac{n\pi}{\Delta t}(t-t_i)\right]$$

Then substitute it into the ODE to obtain the normalization constant.

2.3 PI & Correlation functions

Review what we get in the last section

$$\begin{aligned} Z &= \int \mathrm{d}x_0\, \mathrm{e}^{\overset{\mathrm{i}S[x_c]}{x_i=x_f=x_0}}\left[\frac{m\omega}{2\pi\,\mathrm{i}\sin(\omega t)}\right]^{1/2} \\ &= \left[\frac{\pi}{im\omega\tan(\omega\Delta t/2)}\cdot\frac{m\omega}{2\pi\,\mathrm{i}\sin(\Omega\Delta t)}\right]^{1/2} \xlongequal{\Delta\mapsto-\mathrm{i}\beta} \left[2\,\mathrm{sh}\left(\frac{\beta\omega}{2}\right)\right]^{-1} \end{aligned} \tag{2.13}$$

where the action

$$S[x_c] = \frac{m\omega}{2\sin\omega\Delta t}[(x_i^2+x_f^2)\cos(\omega\Delta t) - 2x_ix_f] \xlongequal{x_i=x_f=x_0} -\left(m\omega\tan\frac{\omega\Delta t}{2}\right)x_0^2 \tag{2.14}$$

Two key points we need to keep in mind

- The time interval $\Delta t \equiv t_f - t_i$, from the dictionary (Wick rotation) $t \mapsto -\mathrm{i}\tau$, then $\Delta t \mapsto -\mathrm{i}\beta$.
- The periodic boundary condition $x_i = x_f = x_0$.

The partition function should be like

$$Z = \mathrm{Tr}\left[\mathrm{e}^{-\beta\omega\left(\hat{n}+\frac{1}{2}\right)}\right] = \sum_{n=0}^{\infty}\mathrm{e}^{-\beta\omega\left(n+\frac{1}{2}\right)} = \frac{\mathrm{e}^{-\beta\omega/2}}{1-\mathrm{e}^{-\beta\omega}} \equiv \left[2\,\mathrm{sh}\left(\frac{\beta\omega}{2}\right)\right]^{-1} \tag{2.15}$$

where we have two context

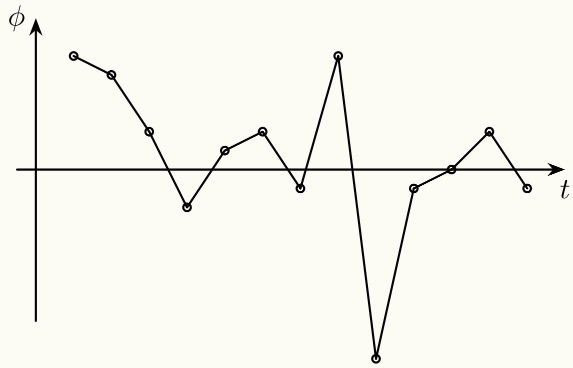
(a) Quantum mechaincs context $\langle x_f|\hat{U}(t_f,t_i)|x_i\rangle$

(b) Statistics mechanics context

The path integration

$$\frac{Z}{Z} = \sum_{\substack{\phi \\ \text{configuration}}} \frac{\rho[\phi]}{Z}$$

where ρ is so-called the raw probability, and $\rho[\phi]/Z$ is the actual probability. Distinguish $\mathrm{e}^{\mathrm{i}S}$, e^{-S_E}, $\mathrm{e}^{\beta H}$.



If one measure for many tims, he may get something like a curve.

$$\frac{1}{N}\sum_i \phi_i \xlongequal{N\to\infty} \langle\phi\rangle = \int \mathrm{d}\phi(\phi)\phi$$

and

$$\frac{1}{N}\sum_i \phi_i = \langle\phi^2\rangle = \int \mathrm{d}\phi p(\phi)\phi^2 z\phi^2$$

and we call $\langle\hat{\phi}\rangle$, n-th moments. The variance

$$(\phi - \langle\phi\rangle)^2 = \langle\phi\rangle^2 - \langle\phi^2\rangle$$

Caldular ϕ

$$\langle\phi^2\rangle^d = \langle\phi-\phi\rangle^3, \quad \text{cumulants} \quad \langle\phi\rangle^3 = \langle\phi^3\rangle - \langle\phi\rangle^3 \tag{2.16}$$

Computing $\langle\phi_i, \phi_j\rangle$, where i and j can be treated as different time. We define

$$\frac{1}{N_\phi}\sum_{\phi(t)} \phi_i\phi_j = \langle\phi_i\phi_j\rangle = \int \mathcal{D}\phi p[\phi]\cdot\phi_i\phi_j \tag{2.17}$$

N_ϕ means how many times we take the sequence. Means integrating with all the configurations. This is the correlation function we are talking about.
What we care about more is $\frac{1}{N}\sum_i \phi_i\phi_{i+\delta}$ instead the specific i and j.
We can also expand to

$$\langle\phi_i\phi_j\cdots\phi_n\rangle = \langle\phi_i\phi_j\cdots\phi_n\rangle - (a\langle\phi_i\rangle\langle\phi_i\phi_j\cdots\phi_n\rangle + b\langle\phi_i\phi_j\rangle\langle\phi_i\phi_j\cdots\phi_n\rangle + \cdots + c\langle\phi_i\rangle\langle\phi_j\rangle\cdots\langle\phi_n\rangle)$$

2.3.1 Generating Function(al) SI Partition Function

Generating Function The set

$$\{m_0, m_1, m_2, m_3, \cdots\}$$

We introduce a function of auxiliary variable a

$$f(a) = m_0 + m_1 a + \frac{1}{2}m_2 a^2 + \frac{1}{3!}m_3 a^3 + \cdots = \sum_{n=0}^{\infty}\frac{1}{n!}m_n a^n \tag{2.18}$$

We just let the set of numbers as the series coefficients. In the end, we have

$$C_n = \left.\frac{\mathrm{d}^n f}{\mathrm{d}a^n}\right|_{a=0}$$

and we treat m_n as

$$m_n = \langle \phi^n \rangle = \int \mathrm{d}\phi p(\phi)\phi^n \tag{2.19}$$

Then, $f(a)$ becomes

$$f_m(a) = \sum_n \frac{1}{n!}a^n \int \mathrm{d}\phi p(\phi)\phi^n = \int \mathrm{d}\phi p(\phi)\,\mathrm{e}^{a\phi} = \langle \mathrm{e}^{a\phi}\rangle, \quad f_c(a) = \ln f_m(a) \tag{2.20}$$

where $m_0 = 1$.

$$\begin{aligned}
K_0 &= f_c(0) = \ln f_m(0) = \ln m_0 = 0, \\
K_1 &= \left.\frac{\mathrm{d}f_C(a)}{\mathrm{d}a}\right|_{a=0} = \frac{1}{f_m(0)}\left.\frac{\mathrm{d}f_m(a)}{\mathrm{d}a}\right|_{a=0} = m_1, \\
K_2 &= \left.\frac{\mathrm{d}^2 f_C(a)}{\mathrm{d}a^2}\right|_{a=0} = \left.\frac{f_m''(a)f_m(a) - f_m'(a)f_m'(a)}{f_m^2(a)}\right|_{a=0} = m_2 - m_1^2 = \langle\phi^2\rangle - \langle\phi\rangle^2 \\
K_3 &= \frac{\mathrm{d}}{\mathrm{d}a}\left(\frac{f_m'}{f_m} - \left(\frac{f_m'}{f_m}\right)^2\right) = \left.\frac{f_m^{(3)}f_m - f_m''f_m'}{f_m^2} - 2\frac{f_m'}{f_m}\frac{f_m''f_m - f_m'f_m'}{f_m^2}\right|_{a=0} \\
&= m_3 - 3m_2m_1 + 2m_1^3 = \langle\phi^3\rangle - 3\langle\phi^2\rangle\langle\phi\rangle + 2\langle\phi\rangle^3
\end{aligned}$$

Generating Functional

Function	$f(\phi)$	single variable	ϕ
Functional	$F[\phi(t)]$	multiple variable / vector	$\{\phi_i\}$
		continous variables	$\phi(t)$ (function)

Now the coefficients set becomes

$$\{C_0,\ C_1(x),\ C_2(x_1,x_2),\ \dots,\ C_n(x_1,\ x_2,\ \dots,\ x_n),\ \dots\}$$

Then the auxiliary function is $a(x)$

$$\begin{aligned}
F[a(x)] = C_0 + \int \mathrm{d}x_1 C_1(x_1)a(x_1) + \frac{1}{2!}\int \mathrm{d}x_1\,\mathrm{d}x_2 C_2(x_1x_2)a(x_1)a(x_2) + \cdots \\
+ \frac{1}{n!}\int \mathrm{d}x_1\cdots\mathrm{d}x_n C_n(x_1,\ x_2,\ \dots,\ x_n)a(x_1)a(x_2)\cdots a(x_n)
\end{aligned} \tag{2.21}$$

Each term here to the n-th order is we used to call the functional derivative $(\delta^n F)[a]$. Considering C_n

$$C_n(x_1,\ x_2,\ \dots,\ x_n) \sim \langle\phi(x_1)\phi(x_2)\cdots\phi(x_n)\rangle = \left.\frac{\delta F^n[a]}{\delta a(x_1), a(x_2), \cdots, a(x_n)}\right|_{a=0}$$

Someone hasn't understand functional (derivative) NOW!!!

$a = (a_1, a_2)$, $\phi = (\phi_1, \phi_1)$.

$$F[a] = a_1\phi_1 + a_2\phi_2 = \sum_{i=1}^{2} a_i\phi_i = a^\mathsf{T}\phi$$

$$C^{(1)}_{i=1,2} = \frac{\delta F}{\delta a_{1,2}} = \phi_{1,2}, \quad C^{(2)}_{ij} = \frac{\delta^2 F}{\delta a_i, a_j^2},$$

or more complex

$$F[a] = (a_1, a_2)\mathbf{A}_{2\times 2}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a^\mathsf{T}\mathbf{A}a$$

Quiz

Example 2.3.1.

$$C_n(x_1,\ x_2,\ \ldots,\ x_n) = \langle \phi(x_1)\phi(x_2)\cdots\phi(x_n)\rangle = \int \mathcal{D}\phi p[\phi]\phi(x_1)\phi(x_2)\cdots\phi(x_n)$$

Calculate the generating function $F[a(x)]$ first.

$$F[a(x)] = \int \mathcal{D}\phi p[\phi]\, \mathrm{e}^{\int \mathrm{d}x a(x)p(x)} = \langle \mathrm{e}^{a^\mathsf{T}\phi}\rangle$$

Consider $p[\phi]/Z$, $Z = \int \mathcal{D}\phi p[\phi]$, where $p[\phi] = \mathrm{e}^{-S_E[p]}$. Write $F[a(x)]$ explicitly

$$F[a(x)] \xlongequal{p[\phi]=\mathrm{e}^{-S[\phi]}/Z} \frac{1}{Z}\underbrace{\int \mathcal{D}\phi\, \mathrm{e}^{-\overbrace{S[\phi]-a^\mathsf{T}\phi}^{}_{S_a[\phi]}}}_{Z_a} = \frac{Z_a}{Z_0}$$

where a is the *control variable*, and ϕ is the *system variable*. Z_a can be $Z_a(\mathbf{H}, \mathbf{m})$ or $Z_a(\mathbf{A}, \mathbf{j})$.

$$\left.\frac{\partial\langle m(x_1)\rangle}{\partial h(x_2)}\right|_{h=0} = \frac{\delta}{\delta h(x_2)}\left(\frac{\delta F[h]}{\delta h(x_1)}\right) = \langle m(x_1)m(x_2)\rangle|_{h=0}$$

In contrast, h is a, m is ϕ. It's what we called the *susceptibility*, or *linear response function.*

Example 2.3.2. Action function $S[\phi] = \frac{1}{2}\phi^\mathsf{T}A\phi$. Calculate $\langle \phi_i, \phi_j\rangle$.

$$Z_a = \int \mathcal{D}\phi\, \mathrm{e}^{-S[\phi]+a^\mathsf{T}\phi} = \int \mathcal{D}\phi\, \mathrm{e}^{-\frac{1}{2}\phi^\mathsf{T}A\phi+a^\mathsf{T}\phi} = \det\left(2\pi\mathbf{A}^{-1}\right)^{1/2}\mathrm{e}^{a^\mathsf{T}\mathbf{A}^{-1}a/2}, \quad Z_0 = Z_a\big|_{a=0}.$$

and Z_0 is just the Gaussian term.

$$F[a] = \frac{Z_a}{Z_0} = \mathrm{e}^{a^\mathsf{T}\mathbf{A}^{-1}a/2}$$

Define $\mathbf{A}^{-1} = G$, matsubara Green function.

$$\langle\phi_i\phi_j\rangle = \left.\frac{\partial^2 F}{\partial a_i\,\partial a_j}\right|_{a=0} = G_{ij}$$

Quiz 8 Make a sentense with the following phrases:
Path Integral Partition Function (is) **Generating Functional** (of) **Correlation Functions**
and combine them with "is", "are", "of", "at", "on", "in", "below", "above", etc.
DeepSeek: The Path Integral formulation of quantum mechanics reveals that the Partition Function is a specific type of Generating Functional, from which all Correlation Functions can be derived by taking functional derivatives."

Explanation The partition function

$$Z = \sum_n \mathrm{e}^{-\beta E_n}$$

is a kind of generating function, i.e., we want the average and the fluctuation of energy

$$\langle E \rangle, \quad \text{and} \quad \langle E^2 \rangle - \langle E \rangle^2$$

So, the Generating function for energy is, for momentum, we try to evalute

$$f_m(a) = \langle \mathrm{e}^{aE} \rangle = \frac{1}{Z_0} \underbrace{\sum_n \mathrm{e}^{(a-\beta)E_n}}_{Z_a} = \frac{Z_a}{Z_0}$$

Then, the critical generating function

$$f_c = \ln f_m(a) = \ln Z_a - \ln Z_0$$

Since $\langle E^2 \rangle^c = \langle E^2 \rangle - \langle E \rangle^2$, then the cumulent

$$\langle E \rangle^c = \langle E \rangle = \frac{\mathrm{d}}{\mathrm{d}a} f_c(a) \Big|_{a=0} = \frac{\mathrm{d} \ln Z}{\mathrm{d}a} \Big|_{a=0} = -\frac{\mathrm{d} \ln Z}{\mathrm{d}\beta}$$

By construction, the cumulent

$$\langle E^2 \rangle^c = \langle E^2 \rangle - \langle E \rangle^2 = \frac{\mathrm{d}^2 f_C(a)}{\mathrm{d}a^2} \Big|_{a=0} = \frac{\mathrm{d}^2 \ln Z}{\mathrm{d}\beta^2} \equiv \frac{\beta^2}{k_B} C_v$$

In the new context, upgrade to "functional": consider the general form of the partition function

$$\mathcal{Z} = \int \mathcal{D}\phi(\tau)\, \mathrm{e}^{-\mathcal{S}_E[\phi]}$$

we integrate over all the configuration, since they are very complicated, so we use the "fancy" expression. Starting from the n-point correlation function

$$\langle \phi(\tau_1)\phi(\tau_2)\cdots\phi(\tau_n) \rangle \xlongequal{\text{variables are continous}} \langle \phi_i \phi_j \cdots \phi_l \rangle^{(c)} = \frac{\partial^n F_{m,c}[a]}{\partial a_i^{n-3}\, \partial a_j\, \partial \cdots \partial a_l} \Big|_{a=0}$$

and the definition of $F_m[a]$ is

$$F_m[a] = \langle e^{a^\intercal \phi} \rangle = \frac{1}{Z} \int \mathcal{D}\phi\, \mathrm{e}^{-S_E + \underbrace{a^\intercal \phi}_{\text{'source' term}}} = \frac{Z_a}{Z_0}$$

where we take $Z_a = \mathrm{e}^{-S_a}$ and $S_a = S_E - a^\mathsf{T}\phi$. The term $a^\mathsf{T}\phi = \phi^\mathsf{T} a$ is symmetric, can be expressed as

$$a^\mathsf{T}\phi = \int \mathrm{d}\tau a(\tau)\phi(\tau) \sim \sum_i a_i\phi_i$$

and critical one is $F_c[a] \sim \ln Z_a$.
Then the fluctuation

$$\langle\phi_i\phi_j\rangle^c = \langle\phi_i\phi_j\rangle - \langle\phi_i\rangle\langle\phi_j\rangle.$$

Define

$$(\chi_\phi)_{ij} = \frac{\partial\langle\phi_i\rangle_a}{\partial a_j}\bigg|_{a=0} = \frac{\partial}{\partial a_j}\frac{\partial F_c[a]}{\partial a_i}\bigg|_{a=0} = \frac{\partial \ln Z_a}{\partial a_i a_j}\bigg|_{a=0} \equiv \langle\phi_i\phi_j\rangle^c$$

This relation, is so-called the *Fluctuation-Dissipation Theorem.*

2.4 Green's Function

Consider

$$S_{E,\mathrm{ora}}[\phi] = \frac{1}{2}\phi^\mathsf{T} A\phi - a^\mathsf{T}\phi$$

which is the same format of $S_a = S_0 - a^\mathsf{T}\phi$, and A is symmetric, $A = A^\mathsf{T}$. Here,

$$\phi^\mathsf{T} A\phi = \sum_{ij} A_{ij}\phi_i\phi_j = \int \mathrm{d}\tau\,\mathrm{d}\tau' A(\tau,\tau')\phi(\tau)\phi(\tau')$$

A is symmetric. Then,

$$F_m[a] = \frac{Z_a}{Z_0} = \frac{\int \mathcal{D}\phi\,\mathrm{e}^{-S_a}}{\int \mathcal{D}\phi\,\mathrm{e}^{-S_0}} = \mathrm{e}^{\frac{1}{2}a^\mathsf{T} A^{-1} a}$$

we define the Green's function is the inverse

$$G \equiv A^{-1}, \quad \text{or} \quad AG = \mathbb{1} \tag{2.22}$$

Rewrite it

$$\sum_j A_{ij}G_{jl} = \delta_{il}$$

make it continuous

$$\int \mathrm{d}\tau A(\tau_1,\tau)G(\tau,\tau_2) = \delta(\tau_1 - \tau_2)$$

The propagator $\langle x_f|\hat{U}(t_f,t_i)|x_i\rangle$ can be just what Green's function is. The EOM here can be

$$\delta\phi S_a = 0$$

(a) then we have

$$\delta\phi S_a[\eta] = \frac{\mathrm{d}S[\phi+\epsilon\eta]}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} = \frac{1}{2}(\eta^\mathsf{T} A\phi + \phi^\mathsf{T} A\eta) - a^\mathsf{T}\eta \xlongequal[a^\mathsf{T}\eta=\eta^\mathsf{T} a]{\phi^\mathsf{T} A\eta=\eta^\mathsf{T} A\phi} \eta^\mathsf{T}(A\phi - a)$$

The solution is

$$A\phi = a, \quad \text{exist} \quad A\phi_0, \quad \text{then} \quad \phi_c = A^{-1}a + \phi_0 \xlongequal{G\equiv A^{-1}} Ga + \phi_0$$

where G can be a matrix, a can be a vector. Now, $\phi_c(\tau)$ can be

$$\phi_c(\tau) = \int \mathrm{d}\tau' \underbrace{G(\tau, \tau')}_{\text{propagator}} \underbrace{a(\tau')}_{\text{source}} + \phi_0(\tau)$$

the source $a(\tau)$ can be charge distribution, ϕ can be the field propagated by the charge.

(b) The functional derivative

$$\frac{\delta S_a[\phi]}{\delta \phi_i} = \sum_j A_{ij}\phi_j - a_i = 0$$

since $\sum_{jl} A_{jl}\phi_j\phi_l = \phi^\mathsf{T} A \phi$ and $a^\mathsf{T}\phi = \sum_j a_j \phi_j$.

Case study: Quantum Harmonic Oscillator The Hamiltonian ($\hbar = 0$)

$$\hat{H} = \frac{\hat{k}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

which is basically the Canonical Quantization. Then, we can write down the Path Integral form. We need the Lagrangian

$$\mathcal{L}(x(t), \dot{x}(t)) = \frac{1}{2}m(\dot{x}^2 - \omega^2 x^2)$$

The action is a functional of

$$\mathcal{S}[x(t)] = \int_{t_i}^{t_f} \mathrm{d}t \mathcal{L}(x, \dot{x}) = -\int_{t_i}^{t_f} \mathrm{d}t \frac{1}{2}mx(t)(\partial_t^2 + \omega^2)x(t) + S_{\text{boundary term}}$$

The $S_{\text{boundary term}}$ is due to "integral by part". Therefore

$$\mathcal{Z} = \int \mathcal{D}x\, \mathrm{e}^{\mathrm{i}\mathcal{S}[x]}$$

one can let $\mathrm{i}t \leftrightarrow \tau$. The Wick rotation version can be $\mathrm{i}\mathcal{S} \leftrightarrow -S_E$, and the Euclidian version can be $S \leftrightarrow S_E = \int_0^\beta \mathrm{d}\tau \mathcal{L}_E(x(\tau), \dot{x}(\tau))$, and the boundary term does not appear here.

$$S_E = \int_0^\beta \mathrm{d}\tau \mathcal{L}_E(x(\tau), \dot{x}(\tau)) = \int_0^\beta \mathrm{d}\tau \frac{1}{2}mx(\tau)(\omega^2 - \partial_\tau^2)x(\tau)$$

$\phi(\tau)$ is now replaced by $x(\tau)$, i.e.,

$$\frac{1}{2}x^\mathsf{T} A x = \frac{1}{2}\int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau' x(\tau)A(\tau, \tau')x(\tau')$$

If we insert the identity $\int_0^\beta \mathrm{d}\tau' \delta(\tau - \tau')$, then, we will have a prime for the first x, i.e.,

$$S_E = \int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau' \delta(\tau - \tau')\frac{1}{2}mx(\tau)(\omega^2 - \partial_\tau^2)x(\tau)$$

Therefore, A will be

$$A(\tau', \tau) = m\delta(\tau' - \tau)(\omega^2 - \partial_\tau^2)$$

So, finally, we can use

$$\int \mathrm{d}\tau A(\tau_1, \tau)G(\tau, \tau_2) = \delta(\tau_1 - \tau_2) \tag{2.23}$$

to generate the Green's funciton.

$$\text{LHS} = \int \mathrm{d}\tau \delta(\tau_1 - \tau)[m(\omega^2 - \partial_\tau^2)]G(\tau, \tau_2) = m(\omega^2 - \partial_{\tau_1}^2)G(\tau_1 - \tau_2) = \delta(\tau_1 - \tau_2) = \text{RHS}$$

Denote $\Delta\tau = \tau_1 - \tau_2$, then

$$\text{LHS} = m(\omega^2 - \partial_{\Delta_\tau}^2)G(\Delta\tau) = \delta(\Delta\tau) = \text{RHS}$$

and G satisfies the periodic boundary condition

$$G(\Delta\tau) = G(\Delta\tau + \beta).$$

means that if we have a range, $\tau \in [0, \beta]$, and the fourier transform

$$\left\{ f_l(\tau) = \frac{1}{\sqrt{\beta}} \mathrm{e}^{\mathrm{i}\frac{2\pi}{\beta} l\tau} \right\}$$

where $l \in \mathbb{Z}$ is a label. Such that $G(\Delta\tau)$ can be expanded over this space

$$G(\Delta\tau) = \sum_l g_l \left(\frac{1}{\sqrt{\beta}} \mathrm{e}^{\mathrm{i}\omega_l \Delta\tau} \right) \tag{2.24}$$

where we denote $\omega_l \equiv \frac{2\pi}{\beta} l$. Then, the left hand side

$$\text{LHS} = \sum_l g_l m(\omega^2 + \omega_l^2) \left(\frac{1}{\sqrt{\beta}} \mathrm{e}^{\mathrm{i}\omega_l \Delta\tau} \right)$$

Since the δ-function, the right hand side

$$\text{RHS} = \delta(\Delta\tau) = \sum_l \left(\frac{1}{\sqrt{\beta}} \mathrm{e}^{\mathrm{i}\omega_l \Delta\tau} \right) \frac{1}{\sqrt{\beta}}$$

which satisfies the orthogonality

$$\sum_l \left(\frac{1}{\sqrt{\beta}} \mathrm{e}^{\mathrm{i}\omega_l \tau_2} \right)^* \left(\frac{1}{\sqrt{\beta}} \mathrm{e}^{\mathrm{i}\omega_l \tau_1} \right) = \sum_l \frac{1}{\beta} \mathrm{e}^{\mathrm{i}\omega_l \Delta\tau} = \delta(\Delta\tau)$$

then, we will derive the coefficient

$$g_l = \frac{1}{\sqrt{\beta}} \frac{1}{m(\omega^2 + \omega_C^2)}$$

Therefore, the Green's function, or the correlation function, is

$$\langle x(\tau_1) x(\tau_2) \rangle = G(\Delta\tau) = \sum_l \frac{1}{\beta} \frac{\mathrm{e}^{\mathrm{i}\omega_l \Delta\tau}}{m(\omega^2 + \omega_l^2)} = \frac{1}{2\pi m} \int_{-\infty}^{\infty} \mathrm{d}\Omega \frac{\mathrm{e}^{\mathrm{i}\Omega\Delta t}}{\omega^2 + \Omega^2} = \frac{\mathrm{e}^{-\omega|\Delta\tau|}}{2\pi m}. \tag{2.25}$$

where we denote $\omega \to \Omega$ when ground state $T \to 0$, $\beta \to \infty$. In order to obtain the compact form, consider when $\Delta\tau$ is larger/less than zero, we need to use the Heavisine step function

$$\langle x(\tau_1) x(\tau_2) \rangle = G(\Delta\tau) = \theta(+\Delta\tau) \frac{\mathrm{e}^{-\omega\Delta\tau}}{2m\omega} + \theta(-\Delta\tau) \frac{\mathrm{e}^{\omega\Delta\tau}}{2m\omega} \tag{2.26}$$

To do the Wick rotation, let $\Delta\tau \leftrightarrow \mathrm{i}\Delta t$. Then, $\theta(\Delta\tau) \leftrightarrow \theta(\Delta t)$, $\mathrm{i}G(\Delta\tau) \leftrightarrow G(\mathrm{i}\Delta t)$, i.e., the *time-ordered Green's function* (in real time)

$$G(\Delta t) = \theta(+\Delta t)\frac{\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\omega\Delta t}}{2m\omega} + \theta(-\Delta t)\frac{\mathrm{i}\,\mathrm{e}^{+\mathrm{i}\omega\Delta t}}{2m\omega} = G^{\mathrm{ret}}(\Delta t) + G^{\mathrm{adv}}(\Delta t) \tag{2.27}$$

and $\langle x(\tau_1)x(\tau_2)\rangle = \langle x(\tau_2)x(\tau_1)\rangle$. To make it symmetric,

$$\langle \mathcal{T}\hat{x}(t_1)\hat{x}(t_2)\rangle = \underbrace{\theta(t_1-t_2)\langle\hat{x}(t_1)\hat{x}(t_2)\rangle}_{\text{operator definition of the Retarded Green functioin}} + \underbrace{\theta(t_2-t_1)\langle\hat{x}(t_2)\hat{x}(t_1)\rangle}_{\text{operator definition of the Advanced Green functioin}} \tag{2.28}$$

where $\hat{x}(t) = \mathrm{e}^{\mathrm{i}\hat{H}t}\hat{x}\,\mathrm{e}^{-\mathrm{i}\hat{H}t}$. To accurate it, consider the first term with respect to the ground state

$$\begin{aligned}\mathrm{i}\langle 0|\hat{x}(t_1)\hat{x}(t_2)|0\rangle_{t_1>t_2} &= \mathrm{i}\langle 0|\mathrm{e}^{\mathrm{i}\hat{H}t_1}\hat{x}\,\mathrm{e}^{-\mathrm{i}\hat{H}(t_1-t_2)}\hat{x}\,\mathrm{e}^{-\mathrm{i}\hat{H}t_2}|0\rangle = \mathrm{i}\,\mathrm{e}^{\mathrm{i}(\frac{1}{2}\omega)\Delta t}\langle 0|\hat{x}\,\mathrm{e}^{-\mathrm{i}\hat{H}\Delta t}\hat{x}|0\rangle \\ &= \frac{\mathrm{i}}{2m\omega}\,\mathrm{e}^{\mathrm{i}(\frac{1}{2}\omega)\Delta t}\langle 1|\mathrm{e}^{-\mathrm{i}\hat{H}\Delta t}|1\rangle = \frac{\mathrm{i}}{2m\omega}\,\mathrm{e}^{+\mathrm{i}(\frac{1}{2}\omega)\Delta t}\,\mathrm{e}^{-\mathrm{i}(\frac{3}{2}\omega)\Delta t}\end{aligned}$$

where $\hat{H}|0\rangle = \left(\frac{1}{2}\omega\right)|0\rangle$, $\Delta t \equiv t_1 - t_2$, and $\hat{x} = \frac{1}{\sqrt{2m\omega}}(\hat{a}+\hat{a}^\dagger)$. Now, go back to the Formalism.

Wick Theorem Consider

$$\mathcal{S}[\phi] = \frac{1}{2}\phi^{\mathsf{T}}A\phi$$

and

$$\langle\phi_i\phi_j\cdots\phi_l\rangle = \left.\frac{\delta^{n-3}\left(Z_a/Z_0\right)}{\delta a_i, a_j, \ldots, a_l^{n-3}}\right|_{a=0}$$

apply Taylor-expansion to the factor

$$Z_a/Z_0 = \mathrm{e}^{\frac{1}{2}a^{\mathsf{T}}Ga} = 1 + \left(\frac{1}{2}a^{\mathsf{T}}Ga\right) + \frac{1}{2!}\left(\frac{1}{2}a^{\mathsf{T}}Ga\right)^2 + \cdots + \frac{1}{n!}\left(\frac{1}{2}a^{\mathsf{T}}Ga\right)^n + \cdots$$

we denote n: $\underbrace{\langle\phi_i\phi_j\cdots\phi_l\rangle}_{n}$.

(a) If n is odd, then $\langle\phi_i\phi_j\cdots\phi_l\rangle = 0$.

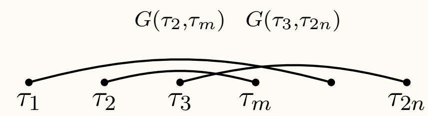
(b) If n is even, or let $n = 2n$, for any term contains the order of a larger than the order of derivative, then this term will vanish since we take $a = 0$. Expand the secoond term

$$(a^{\mathsf{T}}Ga)(a^{\mathsf{T}}Ga) = \left(\sum_{i_1j_1}a_{i_1}G_{i_1j_1}a_{j_1}\right)\left(\sum_{i_2j_2}a_{i_2}G_{i_2j_2}a_{j_2}\right)$$

then

$$\underbrace{\langle\phi_i\phi_j\cdots\phi_l\rangle}_{2n} = \sum_{(\quad)}(\quad)\underbrace{\overbrace{G_{i_1j_1}G_{i_2j_2}}^{\langle\phi_{i_1}\phi_{j_1}\rangle}\cdots G_{i_nj_n}}_{n}$$

Let the labels $i \to \tau_1$, $j \to \tau_2$, …, $l \to \tau_{2n}$. The map can be visualization as



The accumulant version is

$$\underbrace{\langle\phi_i\cdots\phi_l\rangle}_{n}^c = \frac{\delta^n}{\delta a_i, ..., a_l^n}\left(\frac{1}{2}a^\mathsf{T} G a\right)$$

Add the interaction term, i.e.,

$$\mathcal{S}[\phi] = \frac{1}{2}\phi^\mathsf{T} A\phi + \frac{\lambda}{4!}\phi^4$$

S_{int} is a functional of ϕ

$$S_{\text{int}} = \frac{\lambda}{4!}\phi^4 \sim \int \mathrm{d}\tau\phi^4(\tau)$$

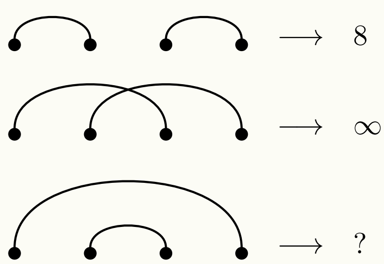
compare this guy maybe more general

$$\int \mathrm{d}\tau_1\,\mathrm{d}\tau_2\,\mathrm{d}\tau_3\,\mathrm{d}\tau_4 A(\tau_1\tau_2\tau_3\tau_4)\phi(\tau_1)\phi(\tau_2)\phi(\tau_3)\phi(\tau_4)$$

By Taylor expansion

$$\mathrm{e}^{-\sin t} = 1 + \frac{\lambda}{4!}\langle\phi^4\rangle + \frac{1}{2!}\left(\frac{\lambda}{4!}\langle\phi^4\rangle\right)^2 + \cdots$$

Since $Z \to \int \mathcal{D}\phi\,\mathrm{e}^{-S\Delta\tau}(\quad)$ and $Z_{\text{int}} \sim \langle\mathrm{e}^{-\sin t}\rangle_0$, all the four point becomes



i.e., the core of Feynmann diagram.

Chapter 3 Symmetry

What is symmetry?

(a) Leibniz: Symmetry is *indiscernability of ~~differences~~ changes →transformations.*

(b) Physical: invariance (under) transformations.

Action part. V is the Hilbert space, and we have a map $V \mapsto V$, which is the operator. The map is invertible. Transformation stands for something like $X \mapsto \Omega(X)$, i.e., map something to something else, but "something else" is in the same space, such as mapping a vector to a vector. For example,

$$\begin{cases} |\psi\rangle \mapsto \hat{\Omega}|\psi\rangle, & \text{Transformation of state} \\ \hat{O} \mapsto \hat{\Omega}\hat{O}\hat{\Omega}^{-1}, & \text{Transformation of Operator} \\ \phi(x) \mapsto (\Omega\phi)(x), & \text{Path Integral} \end{cases}$$

Invariance part. When $X \sim Y$, i.e., X is equivalent to Y, then it calles the invariance. After the map, we get something equivalent to X: $\Omega(x) \sim X$. The invariance in the context can be, for example

$$\text{equations / constraints } \Omega(x) \sim X \longrightarrow \begin{cases} \Omega|\psi\rangle = |\psi\rangle\, \mathrm{e}^{\mathrm{i}\varphi} & \text{Transformation of state} \\ \hat{\Omega}\hat{H}\hat{\Omega}^{-1} = \hat{H} & \text{Transformation of Operator} \\ \mathcal{S}[\phi] = \mathcal{S}[\Omega\phi] & \text{Path Integral} \end{cases}$$

To symmetry, $\Omega(x) \sim X$ is just equations/constraints: Each equation is a kind of constraint on the object.

Symmary For symmetry constraints, what constraints do is a limited possibility: it is simplicity, or what understandability comes from. How this happens is related to *Symmetry & Group Theory.*
The group is a set: we consider a set of transformation Ω_i

$$G = \{\Omega_i\}, \quad \text{and the operation} \quad \Omega_1 \circ \Omega_2$$

The operation says that $\circ:\ G \times G \to G$. Concerning the basic properties of Group

(a) Closure: If $\Omega_{1,2}(X) \sim X$, then the combination $\Omega_1(\Omega_2(X)) \sim \Omega_i(X) \sim X$ is also in this set.

(b) Identity: Also okay, to do nothing.

(c) Inverse: We can have $\Omega(X) \sim X$ then do the inverse Ω^{-1} on both side

$$X \sim \Omega^{-1}(X)$$

By equivalent, this is so-called the inflective.

(d) Associativity: Such as by Hamiltonian, etc.

Referring to the Group theory, we shall talk about the

3.1 Group Representation Theory

(a) Group: Introduce the space; elementary "particles"

(b) Representation: We can "lable" (name) all the representations

  i. Different labels, which is closely related to conserved quantities (quantum numbers);

  ii. Dimension: closely related to degeneracy.

3.1.1 Translation

A trivial example is just to move the entire function $\phi(x)$ towards one direction by a, we get

$$\phi(x) \mapsto \phi(x-a) \equiv \tilde{\phi}(x)$$

where $x \in \mathbb{R}$. And we can define the translation operator $\hat{T}_a$

$$\phi(x-a) = \tilde{\phi}(x) = (\hat{T}_a\phi)(x)$$

where $\phi(x)$ is the wavefunction, and we can get the new state

$$\phi(x) = \langle x|\phi\rangle \mapsto \phi(x-a) = \langle x|\hat{T}_a\phi\rangle$$

Try to write it in the way of expansion

$$\hat{T}_a|\phi\rangle = \int \mathrm{d}x|x\rangle\langle x|\hat{T}_a\phi\rangle = \int \mathrm{d}x|x\rangle\phi(x-a) \xlongequal{\tilde{x}=x-a} \int \mathrm{d}x|x-a\rangle\phi(x)$$

So, this transformation operator is a linear operator. Insert the identity

$$|\phi\rangle = \int \mathrm{d}x|x\rangle\langle x|\phi\rangle, \quad \text{then,} \quad \hat{T}_a|\phi\rangle = \int \mathrm{d}x\hat{T}_a|x\rangle\phi(x)$$

In short, we have

$$\hat{T}_a|x\rangle = |x+a\rangle$$

If $|x\rangle$ refers to a delta function $\delta(x)$, then the transformation just move it to $\delta(x+a)$. To write T_a in basis

$$\hat{T}_a = \int \mathrm{d}x|x+a\rangle\langle x|$$

Quiz. Try to compute $\hat{T}_a\hat{T}_b$.

$$\hat{T}_a\hat{T}_b = \hat{T}_{a+b=b_a} = \hat{T}_b\hat{T}_a$$

3.1.2 Reflection

$$\phi(x) \mapsto \phi(2a-x)$$

We call the operation ρ_a. The same logic.

$$\hat{\rho}_a|\phi\rangle = \int \mathrm{d}x|x\rangle\langle x|\hat{\rho}_a\phi\rangle = \int \mathrm{d}x|x\rangle\phi(2a-x) = \int \mathrm{d}x|2a-x\rangle\phi(x)$$

Remember no minus sign here: the integration range also reversed. So, we obtain

$$\hat{\rho}_a|x\rangle = |2a-x\rangle$$

Quiz Compute $\hat{\rho}_a\hat{\rho}_b$.

$$\hat{\rho}_a\hat{\rho}_b = \hat{T}_{2a-ab}$$

Quiz Compute $\hat{\rho}_a\hat{\rho}_b\hat{\rho}_c$.

$$\hat{\rho}_a\hat{\rho}_b\hat{\rho}_c = \hat{\rho}_{a-b+c}$$

There are some identities

$$\hat{\rho}_a^2 = \mathbb{1}, \tag{3.1}$$

$$\hat{\rho}_a\hat{\rho}_b \neq \hat{\rho}_b\hat{\rho}_a, \quad \text{where } a \neq b \tag{3.2}$$

Quiz Prove if $\hat{T}_a\hat{\rho}_b \stackrel{?}{=} \hat{\rho}_b\hat{T}_a$.

$$\hat{T}_a = \rho_{a/2}\rho_0$$

So, $\hat{T}_a\hat{\rho}_b = \rho_{a/2+b}$, and $\hat{\rho}_b\hat{T}_a = \rho_{b-a/2}$. They are not equal.

3.1.3 Invariance

With translation If we compose

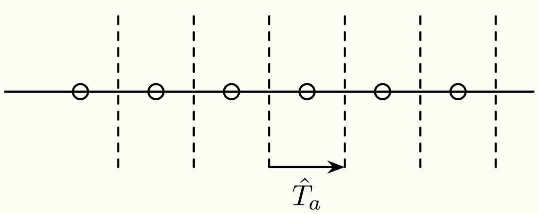
$$\hat{T}_a|\phi\rangle = \mathrm{e}^{\mathrm{i}\phi}|\phi\rangle$$

then, the wavefunction $\langle x|\phi\rangle$ must be periodic. *The formula above becomes the eigen equation.* We can consider it as a complex plane wave $\mathrm{e}^{\mathrm{i}kx}$, i.e., a series loop, perpendicular to x. Then, the wavelength is proportional to the period.

With Reflection Consider the eigen value equation

$$\hat{\rho}_a|\psi\rangle = \mathrm{e}^{\mathrm{i}\varphi}|\psi\rangle$$

and we have the identity $\hat{\rho}_a^2 = \mathbb{1}$, then, the eigenvalue $\lambda^2 = 1$, $\lambda = \pm 1$.
Let $a \in \mathbb{R}$, which is continuous, then we can have $\hat{T}_a \xrightarrow{a\to 0} \mathbb{1}$.
Consider a seires of atoms and the mirror planes,



the two mirror planes is related to $\hat{T}_a$. It is not possible to have a a to make $\hat{\rho}_a \to \mathbb{1}$.
With the two examples above, we can generalize

General Transformation $\hat{\Omega}$ The operator $\hat{\Omega}$ is unitary, and sometimes it can be anti-unitary, and it is time-reversal. The operator acts on states (vectors in Hilbert Space)

$$|\psi\rangle \mapsto \hat{\Omega}|\psi\rangle = \sum_{\alpha} \hat{\Omega}|\alpha\rangle\psi(\alpha)$$

always induce an action $\hat{\Omega}$ on operators

$$\hat{O} = \sum_{\alpha\beta} O_{\alpha\beta}|\alpha\rangle\langle\beta|$$

Then, the action $\hat{\Omega}$ on operators always induce

$$\hat{O} \mapsto \sum_{\alpha\beta} O_{\alpha\beta}|\Omega\alpha\rangle\langle\Omega\beta|$$

It is trivial that $|\Omega\alpha\rangle = \Omega|\alpha\rangle$, but $\langle\Omega\beta| = \langle\beta|\Omega^{-1}$. Ω is unitary, means that whatever v,

$$\langle\Omega u|v\rangle = \langle\Omega^{-1}\Omega u|\Omega^{-1}v\rangle = \langle u|\Omega^{-1}|v\rangle.$$

So, we have

$$\sum_{\alpha\beta} O_{\alpha\beta}|\Omega\alpha\rangle\langle\Omega\beta| = \hat{\Omega}\hat{O}\hat{\Omega}^{-1}$$

3.2 Continuous symmetry and conservation laws

3.2.1 Continuous symmetry

<u>Continuous is connected to $\mathbb{1}$</u>

$$\begin{array}{ccc} \hat{\Omega}_\theta & \xleftrightarrow[\hat{\Omega}_\epsilon = \mathbb{1} - \mathrm{i}\epsilon\hat{g}]{\text{infinitesimal}} & \hat{g} \\ \downarrow & & \downarrow \\ \text{Unitary} & & \text{Hermition} \end{array}$$

We can give the

Theorem 3.2.1 (Stone's theorem). $\forall u$, v, the inner product

$$\langle u|v\rangle = \langle\Omega_\epsilon u|\Omega_\epsilon v\rangle$$

Proof.

$$\cancel{\langle u|v\rangle} = \cancel{\langle u|v\rangle} + \mathrm{i}\epsilon(\langle\hat{g}u|v\rangle - \langle u|\hat{g}v\rangle)$$

then, we obtain

$$\langle\hat{g}u|v\rangle = \langle u|\hat{g}v\rangle$$

and the adjoint

$$\langle\hat{O}u|v\rangle = \langle u|\hat{O}'v\rangle$$

If this is illegal $\forall u$, v, then we have

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

□

So, the generator $\hat{g}$ in this sense can be expressed as

$$\hat{g} = \mathrm{i}\frac{\hat{\Omega}_\epsilon - \mathbb{1}}{\epsilon}\bigg|_{\epsilon\to 0} = \mathrm{i}\frac{\mathrm{d}\hat{\Omega}_\theta}{\mathrm{d}\theta}\bigg|_{\theta=0}$$

With translation Given the definition

$$\hat{T}_a|x\rangle = |x+a\rangle$$

then, consider $\hat{T}_a\hat{x}\hat{T}_a^{-1}$. SInce $\hat{x} = \int \mathrm{d}x|x\rangle x\langle x|$

$$\hat{T}_a\hat{x}\hat{T}_a^{-1} = \int \mathrm{d}x|x-a\rangle x\langle x+a| = \hat{x} - a$$

Assume $a \to \epsilon$, then, we have

$$\hat{T}_\epsilon\hat{x}\hat{T}_\epsilon^{-1} = \hat{x} - \epsilon$$

Substitute $\hat{T}_\epsilon = \mathbb{1} - \mathrm{i}\epsilon\hat{g}_T$, we have

$$(\mathbb{1} - \mathrm{i}\epsilon\hat{g}_T)\hat{x}(\mathbb{1} + \mathrm{i}\epsilon\hat{g}_1) - \mathrm{i}\epsilon(\hat{g}_T\hat{x} - \hat{x}\hat{g}_T) = -\epsilon$$

which means

$$[\hat{x}, \hat{g}_T] = \mathrm{i}, \quad \text{obviously,} \quad \hat{g}_T = \hat{k}$$

With rotation Consider the action (in 3D)

$$\hat{R}_{(\boldsymbol{e}_a,\epsilon)}|\boldsymbol{r}\rangle = |?\rangle$$

Firstly, $\delta\boldsymbol{r} = \epsilon\boldsymbol{e}_a \times \boldsymbol{r}$, then,

$$\hat{R}_{(\boldsymbol{e}_a,\epsilon)}|\boldsymbol{r}\rangle = |\boldsymbol{r} + \epsilon\hat{e}_a \times \boldsymbol{r}\rangle$$

So, we have

$$\hat{R}_{(\boldsymbol{e}_a,\epsilon)}\hat{\boldsymbol{r}}\hat{R}^{-1}_{(\boldsymbol{e}_a,\epsilon)} = \hat{\boldsymbol{r}} + \epsilon\boldsymbol{e}_a \times \hat{\boldsymbol{r}}$$

The generator $\hat{R}_{(\boldsymbol{e}_a,\epsilon)} = \mathbb{1} - \mathrm{i}\epsilon\hat{g}_{\boldsymbol{a}}$, we can simply replace ϵ with the whole term

$$[\hat{\boldsymbol{r}}, \hat{g}_{\boldsymbol{e}_a}] = \mathrm{i}\boldsymbol{e}_a \times \hat{\boldsymbol{r}}$$

The key difference is that the equation is the vector equation, for the scalar,

$$[\hat{x}, \hat{g}_{\boldsymbol{e}_a}] = \mathrm{i}(\boldsymbol{e}_a \times \hat{\boldsymbol{r}})_x$$

To expand it,

$$[\hat{x}, \hat{g}_{\boldsymbol{e}_a}] = \mathrm{i}[(e_a)_y\hat{z} - (e_a)_z\hat{y}]$$

Similarly, for $\hat{y}$ and $\hat{z}$, the single equation corresponds to 3 sub-equations in total. Eventually, we will find

$$\hat{g}_{\boldsymbol{e}_a} = \boldsymbol{e}_a \cdot (\hat{\boldsymbol{r}} \times \hat{\boldsymbol{k}}) = \boldsymbol{e}_a \cdot \hat{\boldsymbol{L}}$$

where $\hat{\boldsymbol{L}} \equiv \hat{\boldsymbol{r}} \times \hat{\boldsymbol{k}}$. If the rotation is actually the symmetry, then, the projection $\boldsymbol{e}_a$ can be removed.

If a is no more infinitesimal, i.e., to the exponential $U(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t}$, we can divide a into n-steps, then take the multiplication into power N of small steps of translations

$$\hat{T}_a = \mathbb{1} - \mathrm{i}\epsilon\hat{g}_T \Rightarrow \hat{T}_a = (\hat{T}_{a/N}) \xlongequal{N\to\infty} \left(1 - \mathrm{i}\frac{a}{N}\hat{g}_T\right)^N = \mathrm{e}^{-\mathrm{i}a\cancel{\hat{g}_T}\,k}$$

Similarly for the rotation, we have

$$\hat{R}_{(\boldsymbol{e}_a,\epsilon)} = \mathbb{1} - \mathrm{i}\epsilon\hat{g}_{\boldsymbol{a}} \Rightarrow \hat{R}_{(\boldsymbol{e}_a,\epsilon)} = \mathrm{e}^{-\mathrm{i}\theta\boldsymbol{e}_a\cdot\hat{\boldsymbol{L}}} = \mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}\cdot\hat{\boldsymbol{L}}}$$

Usually, we say $\boldsymbol{e}_a$ is fixed, then we have only one parameter θ. Now, we can rewrite this trivially

$$\hat{R}_{\boldsymbol{\theta}} = \mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}\hat{\boldsymbol{L}}}$$

It means we have 3 free parameters, which allows us to do the exponential mapping. Functions themselves make the Hilbert space: $\{f(\boldsymbol{r})\}$

$$f(\boldsymbol{r}) = (\hat{R}f)(\boldsymbol{r})$$

TL;DR $\hat{g}_\Omega$ is the transformation generator of the rotation symmetry $\hat{\Omega}_\epsilon$

$$\hat{\Omega}_\epsilon = \mathbb{1} - \mathrm{i}\epsilon\hat{g}_\Omega \tag{3.3}$$

The equation of the rotation operator

$$\hat{R}_{(\underset{\text{axis}}{\boldsymbol{e}_a},\ \underset{\text{angle}}{\epsilon})} = |\boldsymbol{r} + \epsilon\boldsymbol{e}_a \times \boldsymbol{r}\rangle. \tag{3.4}$$

It change the eigenstate from $|\boldsymbol{r}\rangle$ to $|\boldsymbol{r} + \epsilon\boldsymbol{e}_a \times \boldsymbol{r}\rangle$. The equation of the generator of the operator is

$$[\hat{\boldsymbol{r}}, \hat{g}_{\boldsymbol{e}_a}] = \mathrm{i}\boldsymbol{e}_a \times \boldsymbol{r}. \tag{3.5}$$

Consider each component of the vector $\hat{\boldsymbol{r}}$ ($\boldsymbol{r} = (r_1, r_2, r_3) = (x, y, z)$)

$$[\hat{r}_i, \hat{g}_{\boldsymbol{e}_a}] = \mathrm{i}[(e_a)_2\hat{r}_3 - (e_a)_3\hat{r}_2] = \mathrm{i}[(e_a)_2\hat{r}_3 - (e_a)_3\hat{r}_2]\hat{k}_1 + (312) + (123) = (\boldsymbol{e}_a \times \hat{\boldsymbol{r}}) \times \hat{\boldsymbol{k}} = \boldsymbol{e}_a \cdot \hat{\boldsymbol{L}}$$

where $\hat{g}_{\boldsymbol{e}_a} = \boldsymbol{e}_a \cdot \hat{\boldsymbol{r}}$, $\hat{L} \equiv \hat{\boldsymbol{r}} \times \hat{\boldsymbol{k}}$.
Then, we take the Infinitesimal (single-parameter)

$$\hat{R}_{(\boldsymbol{e}_a,\theta)} = \hat{R}^N_{(\boldsymbol{e}_i,\frac{\theta}{N})} = \left(1 - \mathrm{i}\frac{a}{N}\hat{g}_T\right)^N = \mathrm{e}^{-\mathrm{i}\theta\boldsymbol{e}_a\cdot\hat{\boldsymbol{L}}} \xlongequal{\theta\boldsymbol{e}_a \equiv \boldsymbol{\theta}} \mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}\cdot\hat{\boldsymbol{L}} = \sum_{j=1,2,3}\theta_j\hat{L}_j}$$

Translation Symmetry The operator $\hat{T}_{\boldsymbol{a}}|\boldsymbol{r}\rangle = |\boldsymbol{r} + \boldsymbol{a}\rangle$. When act on a state $|\psi\rangle$ in the basis of real state

$$\langle\boldsymbol{r}|(\hat{T}_a|\psi\rangle) = \langle\boldsymbol{r} - \boldsymbol{a}|\psi\rangle = \psi(\boldsymbol{r} - \boldsymbol{a}) \tag{3.6}$$

where consider it is unitary transformation operator

$$\langle\boldsymbol{r}|\hat{T}_a = \langle\hat{T}_{-a}|\boldsymbol{r} = \langle\boldsymbol{r} - \boldsymbol{a}|$$

and $\psi(\boldsymbol{r}) = \langle \boldsymbol{r}|\psi\rangle$. We can have the map

$$\hat{T}_{\boldsymbol{a}}:\ \psi(\boldsymbol{r}) \longmapsto (\hat{T}_a\psi)(\boldsymbol{r}) \equiv \psi(\boldsymbol{r}-\boldsymbol{a}) \tag{3.7}$$

Similarly, for the rotation

$$\hat{R}_{\boldsymbol{\theta}=\boldsymbol{e}_a\theta}|\boldsymbol{r}\rangle = |R_{\boldsymbol{\theta}}\boldsymbol{r}\rangle \tag{3.8}$$

i.e., in the vector form

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \hat{R}_{\boldsymbol{g}} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

where $\boldsymbol{r} = (x,y,z)^\mathsf{T}$ $\boldsymbol{r}' = (x',y',z')^\mathsf{T}$. Since the norm of the vectors are conserved, i.e.,

$$\boldsymbol{r}'^\mathsf{T}\boldsymbol{r}' = \boldsymbol{r}^\mathsf{T}\boldsymbol{r} = \boldsymbol{r}^\mathsf{T}\hat{R}_{\boldsymbol{\theta}}^\mathsf{T}\hat{R}_{\boldsymbol{\theta}}^\mathsf{T}\boldsymbol{r} \tag{3.9}$$

Then, we can derive

$$\hat{R}_{\boldsymbol{\theta}} = \mathrm{e}^{\boldsymbol{\theta}\cdot\hat{\boldsymbol{L}}} \tag{3.10}$$

from which

$$\begin{cases} \hat{R}_{\boldsymbol{\theta}}^\mathsf{T}\hat{R}_{\boldsymbol{\theta}} = \mathbb{1}, \\ \det(\hat{R}_{\boldsymbol{\theta}}) = +1. \end{cases}$$

We can have the anti-symmetric real matrix $\hat{\boldsymbol{L}}$

$$L_i^\mathsf{T} = -L_i \tag{3.11}$$

where can be expanded as

$$\begin{pmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{pmatrix} = a\begin{pmatrix} & 1 & \\ -1 & & \\ & & 0 \end{pmatrix} + b\begin{pmatrix} & & 1 \\ & 0 & \\ -1 & & \end{pmatrix} + c\begin{pmatrix} 0 & & \\ & & 1 \\ & -1 & \end{pmatrix} = a\hat{L}_3 + b\hat{L}_2 + c\hat{L}_1 \tag{3.12}$$

where thet label 1, 2, 3 means that the naught 0 on the third / second / first row. We can have the expooniential form, e.g.,

$$\mathrm{e}^{a\hat{L}_3} = \begin{pmatrix} \cos a & -\sin a & 0 \\ \sin a & \cos a & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where we use the identity

$$\begin{pmatrix} A & \\ & 0 \end{pmatrix}^n = \begin{pmatrix} A^a & \\ & 0 \end{pmatrix}$$

Then, theeuqation for the opeartor becomes

$$\langle \boldsymbol{r}|\hat{R}_\theta|\psi\rangle = \langle \hat{R}_{-\boldsymbol{\theta}}\boldsymbol{r}|\psi\rangle \tag{3.13}$$

and we have the map

$$\hat{R}_{\boldsymbol{\theta}}:\ \psi(\boldsymbol{r}) \longmapsto (\hat{R}_{\boldsymbol{\theta}}\psi)(\boldsymbol{r}) \equiv \psi(R_{-\boldsymbol{\theta}}\boldsymbol{r}) \tag{3.14}$$

The transfromation in coordinate space induces the transformation in Hilbert space. The generator

$$\hat{\boldsymbol{g}}_{\hat{R}_{\boldsymbol{\theta}}} = \hat{\boldsymbol{L}} = (\hat{L}_1, \hat{L}_2, \hat{L}_3)$$

and the commutators

$$\hat{T}_{a_y}\hat{T}_{a_x}|\boldsymbol{r}\rangle = |\boldsymbol{r} + a_x\hat{x} + a_y\hat{y}\rangle, \tag{3.15}$$

$$\hat{R}_{\theta_y}\hat{R}_{\theta_x}|\boldsymbol{r}\rangle = |\hat{R}_{\theta_y}\hat{R}_{\theta_x}\boldsymbol{r}\rangle \neq |\hat{R}_{\theta_x}\hat{R}_{\theta_y}\boldsymbol{r}\rangle \tag{3.16}$$

Quiz Calculate $[\hat{L}_1, \hat{L}_2]$.
Back to the commutator

$$[\hat{L}_1, \hat{L}_2] = [\hat{y}\hat{k}_z, \hat{z}\hat{k}_x] + [\hat{z}\hat{k}_y, \hat{x}\hat{k}_z] = [\hat{y}\hat{k}_z, \hat{z}]\hat{k}_x + \hat{x}[\hat{z}\hat{k}_y, \hat{k}_z] = \hat{y}[\hat{k}_z, \hat{z}]\hat{k}_x + \hat{x}[\hat{z}, \hat{k}_z]\hat{k}_y = \mathrm{i}(\hat{x}\hat{k}_y - \hat{y}\hat{k}_x) = \mathrm{i}\hat{L}_3$$

So, there are three equations.

3.2.2 Conservation Laws

Remark (BCH). The commutator

$$[A, \cdot](BC) \equiv [A, BC] = [A, B]C + B[A, C], \quad \text{and} \quad \partial_A(BC) = (\partial_A B)C + B(\partial_A)C$$

also for $BC \to BCD$. Consider the BCH identity

$$\mathrm{e}^A B\,\mathrm{e}^{-A} = B + [A, B] + \frac{1}{2!}[A, B]_2 + \cdots + \frac{1}{n!}[A, B]_n$$

where $[A, B]_n = \underbrace{[A, [A, \cdots [A, B]]]}_{n} \mapsto \partial_A^n B$

The transformation

$$\hat{\Omega}_\theta \hat{H} \hat{\Omega}_\theta^{-1} = \hat{H}$$

where $\hat{H}$ is time-independent. We take the infinitesimal $\theta \to \epsilon$, $\hat{\Omega}_\theta = \mathbb{1} - \mathrm{i}\epsilon\hat{g}_\Omega$. It is trivial that

$$[\hat{g}_\Omega, \hat{H}] = 0$$

Take the time-evolution operator

$$\hat{U}(t, 0) = \mathrm{e}^{-\mathrm{i}t\hat{H}}, \quad \hat{U}(\epsilon, 0) = \mathbb{1} - \mathrm{i}\epsilon\hat{H}$$

then, we have the sandwitch

$$\hat{U}(t, 0)\hat{g}_\Omega\hat{U}(t, 0)^{-1} = \hat{g}_\Omega$$

The evolution

$$\langle\psi(0)|\hat{g}_\Omega|\chi(0)\rangle = \langle\psi(t)|\hat{U}(t, 0)\hat{g}_\Omega\hat{U}(t, 0)^{-1}|\chi(t)\rangle = \langle\psi(t)|\underbrace{\hat{g}_\Omega}_{\text{conserved quality}}|\chi(t)\rangle$$

Then, the Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = -\,\mathrm{i}\hat{H}(t)|\psi(t)\rangle$$

and the time derivative

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(0)|\hat{g}_\Omega|\chi(0)\rangle = \mathrm{i}\langle\psi(t)|[\hat{H}(t), \hat{g}_\Omega]|\chi(t)\rangle = 0$$

It vanishes because the symmetry.

Energy conservation We certainly have one trival contribution that goint to give us the commutator between $\hat{H}(t)$ and $\hat{(}t)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(0)|\hat{g}_\Omega|\chi(0)\rangle = \mathrm{i}\langle\psi(t)|[\hat{H}(t),\hat{H}(t)|\chi(t)]\rangle + \langle\psi(t)|\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}}_{=0}\hat{H}(t)|\chi(t)\rangle$$

We can have $\hat{H}(t) = t\hat{H}_0$.

Theorem 3.2.2 (Noether's Theorem)**.** We need to change out language to $\mathcal{S}[q(t)] \mapsto \mathcal{S}[(\Omega_\alpha q)(t)]$. The continuous transformation of "Path"

$$\Omega_\theta : \ q(t) \longmapsto (\Omega_\theta q)(t) \equiv q_\theta(t)$$

In the examples, we can generally write

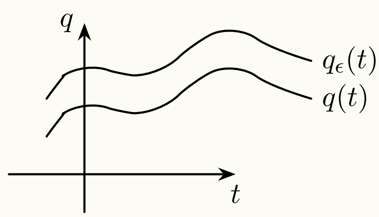
$$f(\epsilon) = f(0) + \epsilon f'(0), \quad \text{where} \quad f(t) = \frac{\mathrm{d}q_\theta}{\mathrm{d}\theta}$$

q is still a function of time. Then,

$$q_\epsilon = q(t) + \epsilon f(t)$$

Example 3.2.1 (Translation)**.**

$$q_\epsilon(t) = q(t) + \epsilon, \quad f(t) = 1$$



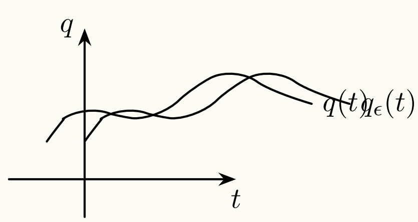
Example 3.2.2 (rotation)**.**

$$\boldsymbol{q}_\epsilon(t) = \boldsymbol{q}(t) + \epsilon\boldsymbol{e}_a \times q(t), \quad \boldsymbol{f}(t) = \boldsymbol{e}_a \times \boldsymbol{q}(t)$$

The rotation of the world line. Figure: the world line rotate a angle between two time point real surface.

Example 3.2.3 (time-translation)**.**

$$q_\epsilon(t) = q(t-\epsilon), \quad f(t) = -\dot{q}(t)$$



For t-independent Ω_θ, the functional derivative

$$\begin{aligned}0 &= \frac{\mathrm{d}\mathcal{S}[\Omega_\theta q]}{\mathrm{d}\theta}\bigg|_{\theta=0} = \frac{1}{\epsilon}(\mathcal{S}[\Omega_\epsilon q] - \mathcal{S}[q])\bigg|_{\epsilon\to 0} = \int_{t_i}^{t_f} \mathrm{d}t\left(\frac{\partial\mathcal{L}}{\partial q}\frac{\partial q_\theta}{\partial\theta} + \frac{\partial\mathcal{L}}{\partial\dot{q}}\frac{\partial\dot{q}_\theta}{\partial\theta}\right) \\ &= \int_{t_i}^{t_f} \mathrm{d}t\,\underbrace{\left(\frac{\partial\mathcal{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{q}}\right)f}_{\text{E-L Equation}} + \left(\frac{\partial\mathcal{L}}{\partial\dot{q}}f\right)\bigg|_{t_i}^{t_f}\end{aligned}$$

where we integral on shell, and

$$\mathcal{S}[q_\theta(t)] = \int_{t_i}^{t_f} \mathrm{d}t\mathcal{L}(q_\theta(t), \dot{q}_\theta(t), t)$$

Since the E-L equation, we have

$$\left(\frac{\partial\mathcal{L}}{\partial\dot{q}}f\right)\bigg|_{t_i}^{t_f} = 0$$

But t_i and t_f are arbitrary, so we can derive that

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{q}}f = 0$$

means that it is independent from time, we get the conserved quantity.

So, in the first example p is conserved; In the second one,

$$\mathcal{S}[q_\theta(t)] = \int_{t_i}^{t_f} \mathrm{d}t\mathcal{L}(\boldsymbol{q}_\theta(t), \dot{\boldsymbol{q}}_\theta(t), t)$$

and

$$\left(\sum_i \frac{\partial\mathcal{L}}{\partial\dot{q}_i}f\right)\bigg|_{t_i}^{t_f} = 0$$

so, $\boldsymbol{e}_a \cdot L = \boldsymbol{p}\cdot(\boldsymbol{e}_a \times \boldsymbol{q}(t))$ in the second example.

In the time-translation,

$$\mathcal{S}[q_\epsilon(t)] = \int_{t_i+\epsilon}^{t_f+\epsilon} \mathrm{d}t\mathcal{L}(q_\epsilon(t-\epsilon), \dot{q}_\epsilon(t-\epsilon), t) \xlongequal{\tilde{t}=t-\epsilon} \int_{t_i}^{t_f} \mathrm{d}\tilde{t}\mathcal{L}(q(\tilde{t}), \dot{q}(\tilde{t}), \tilde{+}\epsilon)$$

The derivative

$$0 = \frac{\mathrm{d}\mathcal{S}[\Omega_\theta q]}{\mathrm{d}\theta}\bigg|_{\theta=0} = \frac{1}{\epsilon}(\mathcal{S}[\Omega_\epsilon q] - \mathcal{S}[q]) = \int_{t_i}^{t_f} \mathrm{d}t\frac{\partial\mathcal{L}}{\partial t} \Rightarrow \frac{\partial\mathcal{L}}{\partial t} = 0$$

To interrupt it, we consider the total derivative

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{L} = \frac{\partial}{\partial q}\mathcal{L}\dot{q} + \frac{\partial}{\partial t}\mathcal{L}\left(\frac{\mathrm{d}}{\mathrm{d}t}\dot{q}\right) + \frac{\partial}{\partial t}\mathcal{L}$$

The second term

$$\frac{\partial}{\partial t}\mathcal{L}\left(\frac{\mathrm{d}}{\mathrm{d}t}\dot{q}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial q}\dot{q}\right) - \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{q}}\right)\dot{q}$$

Substitute it and rearrange

$$0 = \frac{\partial\mathcal{L}}{\partial t} = \frac{\mathrm{d}}{\mathrm{d}t}\underbrace{\left(\mathcal{L} - \frac{\partial\mathcal{L}}{\partial\dot{q}}\dot{q}\right)}_{\text{Hamiltonian}} - \underbrace{\left(\frac{\partial\mathcal{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial q}\right)}_{\text{E-L equation}}\dot{q}$$

Then, we have the on-shell

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = 0$$

i.e., the energy is conserved.

From (good) quantum numbers to group irrepresentation The statement is if

$$[\hat{A}, \hat{B}] = 0, \Rightarrow \exists \text{basis}\{|\lambda\rangle\}$$

The basis vector is the eigenvector of both $\hat{A}$ and $\hat{B}$

$$\hat{A}|\lambda\rangle = \lambda_A|\lambda\rangle, \quad \text{and} \quad \hat{B}|\lambda\rangle = \lambda_B|\lambda\rangle.$$

Proof. Consider $\hat{A}$ and $\hat{B}$ are Hermition. Take the ground state

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

In the case of degeneracy,

$$\hat{A}|\alpha_i\rangle = \alpha|\alpha_i\rangle, \quad i = 1, \ldots, d_\alpha$$

Then, consider

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

means that

$$\begin{cases} \hat{B}|\alpha\rangle = b^{(\alpha)}|\alpha\rangle, & \text{no-degeneracy} \\ \hat{B}|\alpha_i\rangle = \sum_j |\alpha_j\rangle b_{ji}^{(\alpha)}, & \text{degeneracy} \end{cases}$$

where $b_{ji}^{(\alpha)} = \langle\alpha_j|\hat{B}|\alpha_i\rangle$. We can always diagonalize

$$b^{(\alpha_i)} = VDV^{-1}, \quad b^{(\alpha_i)}V = VD$$

D being a diagonal matrix $D_{ml} = \beta_l^{(\alpha)}\delta_{ml}$. Then,

$$\sum_i b_{ji}^{(\alpha)} V_{il} = \sum_m V_{jm} D_{ml} = V_{jl}\beta_l^{(\alpha)}$$

By take one superposition of the orginal α

$$|\tilde{\alpha}_l\rangle = \sum_i |\alpha_i\rangle V_{il}$$

It is easy to know

$$\hat{B}|\tilde{\alpha}_\lambda\rangle = \sum_i \hat{B}|\alpha_i\rangle V_{il} = \sum_{ij} |\alpha_j\rangle b_{ji}^{(\alpha)} V_{il} = |\tilde{\alpha}_l\rangle \beta_l^{(\alpha)}$$

Then, the site

$$\{|\tilde{\alpha}_l\rangle\} = \{|\lambda\rangle\}$$

if there is no degeneracy, then $|\tilde{\alpha}\rangle = |\alpha\rangle$. □

3.3 Symmetry group representations, degeneracies, inversion and time reversal

3.3.1 Group representations

Starting from

$$\hat{\Omega}_\theta |\boldsymbol{r}\rangle = |h_\theta(\boldsymbol{r})\rangle$$

Example 3.3.1.

(a) Translation $h_{\boldsymbol{a}}(\boldsymbol{r}) = \boldsymbol{r} + \boldsymbol{r}$

(b) Reflection $h_{\boldsymbol{e}}(\boldsymbol{r}) = \boldsymbol{r} - 2\boldsymbol{r}_{\parallel}$ (Figure required).

(c) Rotation $h_{\boldsymbol{\theta}=(\boldsymbol{e}_a,\theta)}(\boldsymbol{r}) = \boldsymbol{r}_{\parallel} + \cos\theta \boldsymbol{r}_{\perp} + \sin\theta(\boldsymbol{e}_a \times \boldsymbol{r}_{\perp})$.

For an arbitary state $|\psi\rangle$, how the operator act on the arbitary state

$$(\hat{\Omega}_\theta\psi)(\boldsymbol{r}) = \langle \boldsymbol{r}|\hat{\Omega}_\theta|\psi\rangle = \langle h_\theta^{-1}(\boldsymbol{r})|\psi\rangle = \psi(h_\theta^{-1}(\boldsymbol{r}))$$

Then, consider a general

$$(\hat{\Omega}_2\hat{\Omega}_1\psi)(\boldsymbol{r}) = \langle \boldsymbol{r}|\hat{\Omega}_2\hat{\Omega}_1|\psi\rangle = \langle h_2^{-1}(\boldsymbol{r})|\Omega_1\psi\rangle = \langle (h^{-1}h_2^{-1})(\boldsymbol{r})\rangle|\psi\rangle$$

where we can treat $\hat{\Omega}_2\hat{\Omega}_1 = \hat{\Omega}_3$. The transformation converses the distance $\boldsymbol{r}_1 - \boldsymbol{r}_2$, then, all the h

$$h(\boldsymbol{r}_1 - \boldsymbol{r}_1) = |h(\boldsymbol{r}_1) - h(\boldsymbol{r}_1)| = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$$

form the Euclidian space (Group)

$$E(d): \ \{h||h(\boldsymbol{r}_1 - \boldsymbol{r}_2) = |\boldsymbol{r}_1 - \boldsymbol{r}_2|\} \tag{3.17}$$

(a) All the translation form $T(d)$

(b) All the reflection form $O \in$ reflection place

(c) All the rotationform $O(d)$, orthogonal group.

But, in Euclidian space, it will become a semi-direct product

$$T_d \rtimes O(d)$$

where $O(d) = \mathrm{SO}(d) \times \mathbb{Z}_2$ is orthogonal. For $\{M_d : \ M^\dagger M = \mathbb{1}\}$, then $(\det(M))^2 = 1$, $\det(M) = \pm 1$. This means that S can be special for $\det(M) = +1$. While Z_2 have two $\{+1, -1\}$.

We have a Euclidian group $\{\hat{\Omega}_\theta\} \leftarrow G = E(d) \rightarrow \{h_\theta\}$ corresponding to all the operators.

$$\underset{(G\circlearrowright\mathbb{V})}{\overset{\mathbb{V}=\{|\boldsymbol{r}\rangle\}}{\{\hat{\Omega}_\theta\}}} \xleftarrow[\substack{\Omega_1\leftarrow g_1,\ \Omega_2\leftarrow g_2 \\ \Omega_1\Omega_2\leftarrow g_1\cdot g_2}]{\text{homomorphism}} \underset{\substack{\| \\ E(d)}}{G} \xrightarrow{\text{homo}} \underset{(G\circlearrowright\mathbb{R}^d)}{\overset{\mathbb{R}=\{\boldsymbol{r}\}}{\{\hat{h}_\theta\}}}, \quad G \longrightarrow GL(V), \quad \Omega : V \rightarrow V \tag{3.18}$$

where "homomorphism" means the same shape and form, h_θ acts on $\boldsymbol{r}$ while $\hat{\Omega}_\theta$ acts on $|\boldsymbol{r}\rangle$. They form *Group Action*: Representation.

Translation group We start from the translation group $T(d)$. Consider

$$T_{\boldsymbol{a}} \cdot T_{\boldsymbol{b}} = T_{\boldsymbol{a}+\boldsymbol{b}=\boldsymbol{b}+\boldsymbol{a}}$$

we call it the *Abelian Group*. In Hilbert space of this case, $V = \mathrm{span}(\{|\boldsymbol{r}\rangle\})$. Then, the operator $\hat{T}_{\boldsymbol{a}}$ on this space

$$\hat{T}_{\boldsymbol{a}} = \mathrm{e}^{-\mathrm{i}\boldsymbol{a}\cdot\hat{\boldsymbol{k}}}$$

where $\hat{g}_{T_i} = \hat{k}_i$ for $i = 1, 2, 3$.

Quiz Now, consider

$$T_{\boldsymbol{a}} \xlongequal{k\to\mathrm{i}\nabla} \mathrm{e}^{-\boldsymbol{a}\cdot\nabla}$$

Calculate

$$\langle \boldsymbol{r}|\hat{T}_a|\psi\rangle = (T_{\boldsymbol{a}}\psi)(\boldsymbol{r}) = \psi(\boldsymbol{r}-\boldsymbol{a}).$$

By Foruier transform , where one can have the eigenvalue Equation

$$\nabla\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = -\,\mathrm{i}\boldsymbol{k}\,\mathrm{e}$$

and in Foruier transform

$$\psi(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{k}\tilde{\psi}(\boldsymbol{k})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$$

we can have

$$f(\nabla)\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = f(\mathrm{i}\boldsymbol{k})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \quad \mathrm{e}^{-\boldsymbol{a}\cdot\nabla}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{a})}$$

Due to the property of the transform operator

$$\mathrm{e}^{-\boldsymbol{a}\cdot\nabla}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r}-\boldsymbol{a})$$

substitute the identities above

$$\mathrm{e}^{-\boldsymbol{a}\cdot\nabla}\psi(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{k}\tilde{\psi}(\boldsymbol{k})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{a})} = \psi(\boldsymbol{r}-\boldsymbol{a})$$

For Abelian group, we have the commutative generator

$$[\hat{k}_i, \hat{k}_j] = 0$$

(a) $V = \{|\boldsymbol{k},\sigma\rangle|\hat{\boldsymbol{k}}|\boldsymbol{k},\sigma\rangle = \boldsymbol{k}|\boldsymbol{k},\sigma\rangle, \boldsymbol{k}\in\mathbb{R}^3\}$. Now, the Hilbert space becomes a direct sum

$$V = \bigoplus_{\boldsymbol{k}\in\mathbb{R}^3} V_{\boldsymbol{k}}, \quad \text{where} \quad V_{\boldsymbol{k}_0} = \mathrm{span}(\{|\boldsymbol{k}_\sigma,\sigma\rangle\})$$

(b) $[\hat{H},\hat{\boldsymbol{k}}] = 0, \forall\boldsymbol{a}$. The Hamiltonian operator also becomes

$$\hat{H} = \bigoplus_{\boldsymbol{k}\in\mathbb{R}^3} \hat{H}_{\boldsymbol{k}} = \begin{pmatrix} H_{\boldsymbol{k}_1} & & \\ & H_{\boldsymbol{k}_2} & \\ & & \ddots \end{pmatrix}$$

where

$$\hat{H}_{\boldsymbol{k}} = P_{\boldsymbol{k}} \hat{H} P_{\boldsymbol{k}}, \quad \text{and} \quad P_{\boldsymbol{k}} = \sum_{\sigma} |\boldsymbol{k}, \sigma\rangle\langle\boldsymbol{k}, \sigma|$$

Then, $V_{\boldsymbol{k}} = P_{\boldsymbol{k}} V$, the so-called *Bloch Theorem*[1].

Non-abelian Group

Example 3.3.2. $\mathrm{SO}(d)$ for $d > 2$

Example 3.3.3 (Dihedred Group for n-gon)**.** The elements

$$\{e,\ R,\ R^2, \rho_0, \rho_1,\ \rho_2\} = \langle R, \rho = \rho_0| \quad \text{(generators)}$$

where

(a) $R^2 = \bar{R}$

(b) $\rho_i = \bar{\rho}_i$

(c) $R^3 = e = \rho_i$

(d) $R\rho_i\bar{R} = \rho_{i+1}$

(e) $\rho R \bar{\rho}_0 = \bar{R}$

In summary

(a) $R\rho_0\bar{R} = \rho_{R(0)}$

(b) $\rho_0 R \bar{\rho}_0 = R_{\text{flip}} = \bar{R}$

(c) $\rho_i\rho_{i+1} = R$

(d) $\rho_{i+1}\rho_i = \bar{R}$

From $\rho_a\rho_b = T_{2(a+b)}$, we have

$$\rho_i\rho_{i\pm 1} = T_{\mp 2} = T_{\pm 1} = R^2$$

and from $\rho_a\rho_b\rho_c = \rho_{a-b+c}$, we have

$$\rho_0\rho_1\bar{\rho}_0 = \rho_{0-1+0} = \rho_{-1} = \rho_2$$

$$R\rho_0 = \rho_2\rho_0\rho_0 = \rho_2, \quad R^2\rho_0 = \rho_1$$

Cayley Table (Group Multiplication Table)

$$\{e,\ R,\ R^2, \rho_0, \rho_1,\ \rho_2\} = \langle \underbrace{R, \rho = \rho_0}_{\text{generators}} | \underbrace{R^3 = \rho^2 = e, \rho R = R^2\rho}_{\text{relations}} \rangle$$

where R^{n_1}, ρ^{m_1}, R^{n_2}, ρ_{m_2} will appear in the group. We can always switch R and ρ since

$$\rho R = R^2 \rho$$

Similar for D_n.
Now, we can define two operators

$$\hat{R}|i\rangle = |R(i)\rangle = |i+1\rangle, \quad \text{and} \quad \hat{\rho}|i\rangle = |\rho(i)\rangle = |-i\rangle$$

[1] In the lattice, we need to change $\boldsymbol{a} \in \mathbb{R}^3 \to \mathbb{Z}^3$

on Hilbert space $V = \mathrm{span}(\{|0\rangle, |1\rangle, |2\rangle\})$. The Hamiltonian

$$\hat{H} = \sum_{i,j=0,1,2} |i\rangle h_{ij} \langle j|$$

where $h_{ij} = h_{ji}^*$. So,

$$\forall \hat{g} \in D_3,\ [\hat{H}, \hat{g}] = 0 \Rightarrow ?$$

Since $\hat{R}\hat{H}\hat{R}^{-1} = \sum_{ij} |i+1\rangle h_{ij} \langle j+1| = \hat{H}$, then

$$h_{ij} = h_{i+1,j+1}, \quad h_{ij} = h_{-i,-j}$$

we have

$$\hat{H} = \begin{pmatrix} \epsilon & t & t \\ t & \epsilon & t \\ t & t' & \epsilon \end{pmatrix} = \begin{pmatrix} 0 & t & t \\ t & 0 & t \\ t & t' & 0 \end{pmatrix}$$

The eigenvalue and eigenvector, the basis are $|0\rangle$, $|1\rangle$, $|2\rangle$.

$$\hat{H} = t(\hat{R} + \hat{R}^2)$$

we know $\hat{R}^3 = 1$, then the eigenvalue should be $\lambda_n = \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}}$

$$\hat{R}|\psi_n\rangle = \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}n} |\psi_n\rangle, \quad n = 0,\ 1,\ 2$$

Then eigenvalues are

$$E_{\psi_0} = 2t, \quad E_{\psi_1} = E_{\psi_2} = t(\omega + \omega^*)$$

we arrive at the degeneracy. Now, write the operators $\hat{R}$ and $\hat{\rho}$ into the basis

$$\{|\psi_0\rangle,\ |\psi_1\rangle,\ |\psi_2\rangle\}$$

R_ψ in the ψ basis, it is diagonal

$$R_\psi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \bar{\omega} \end{pmatrix}$$

Calculate how $\hat{R}(\hat{\rho}|\psi_0\rangle)$ acts.

$$\hat{R}(\hat{\rho}|\psi_0\rangle) = \hat{\rho}\hat{R}^2|\psi_0\rangle \xlongequal{\hat{R}|\psi_0\rangle = |\psi_0\rangle} \hat{\rho}|\psi_0\rangle$$

So, $\langle\psi_i|\hat{\rho}|\psi_0\rangle = \delta_{i,0}$. For $|\psi_1\rangle$,

$$\hat{R}(\hat{\rho}|\psi_1\rangle) = \hat{\rho}\hat{R}^2|\psi_1\rangle = \bar{\omega}\hat{\rho}|\psi_1\rangle$$

So, in matrix

$$R_\psi = \begin{pmatrix} 1 & & 0 \\ & \omega & \\ 0 & & \bar{\omega} \end{pmatrix}, \quad \rho_\psi = \begin{pmatrix} 1 & 0 & \\ 0 & & 1 \\ & 1 & \end{pmatrix}$$

In the new basis, the Hilbert space

$$V = V_{\psi_0} \oplus V_{\{\psi_1,\psi_2\}}, \quad g = g_{\psi_0} \oplus g_{\{\psi_1,\psi_2\}}$$

and

$$0 = \langle \psi_1 | \hat{\rho} | \psi_1 \rangle$$

This is why the degeneracy occurs.

$$\hat{H}|\psi\rangle = E|\psi\rangle, \quad \hat{H}(\hat{\rho}|\psi\rangle) = \hat{\rho}\hat{H}|\psi\rangle = E(\hat{\rho}|\psi\rangle).$$

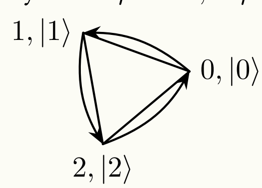
Quick Review of Group Representation Starting from

$$\underset{\text{Group}}{G} \ \underset{\text{acts on}}{\overset{\tau}{\circlearrowleft}} \ \underset{\text{linear space}}{V}, \quad \tau : G \to \underset{\text{Linear operator space on } V}{\overset{\text{opened}}{G}\overset{\text{linear}}{L}(V)}$$

where τ is homomorphism:

$$\begin{array}{l} \forall g_{1,2} \in G, \quad (g_1 \circ g_2) \longmapsto A_1 A_2 \\ \quad \downarrow \\ \quad A_{1,2} \end{array}$$

Example 3.3.4. For the group $D_3 = \{e, R, R^2, \rho_0, \rho_1, \rho_2\} \cong S_3$ which satisfy $R^3 = \rho^2 = e,\ R\rho = \rho R^2$.



$$(\quad),\ (012) = (120) = (201),\ (021),\ (12),\ (20),\ (01)$$

For example, $(12)(12) = (\quad)$, $(012)(12) = (10)$.

Then, for the group multiplication

$$(12)(012) = (12)(120) = (12)(12)(20) = (20), \quad (12)(021) = (12)(210) = (12)(21)(10) = (10)$$

Consider taking $i \mapsto |i\rangle$, basis of Hilbert space V ($\{|0\rangle, |1\rangle, |2\rangle\}$). Then, the identities become

$$\hat{R}|i\rangle = |R(i)\rangle, \quad \hat{R}\rho|i\rangle = |\rho(i)\rangle.$$

Then, we can say $\{e, R, R^2, \rho_0, \rho_1, \rho_2\} \subset V$. The Hilbert space can be composed into two parts

$$V = V_{\psi_0} \oplus V_{\{\psi_1,\psi_2\}}$$

where $|\psi_n\rangle$ means $\hat{R}|\psi_n\rangle = \omega^n|\psi_n\rangle$, $\omega = \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}}$. So, the subspace

$$V_{\psi_0} = \mathrm{span}(\{\psi_0\}),\ V_{\{\psi_1,\psi_2\}} = \mathrm{span}(\{\psi_1, \psi_2\})$$

$\forall \hat{g} \in \hat{D}_3$,

$$g = \begin{array}{c c} \begin{array}{c} |\psi_0\rangle \\ |\psi_1\rangle \\ |\psi_2\rangle \end{array} & \begin{pmatrix} \blacksquare & O & \\ O & \blacksquare & \\ & & \end{pmatrix} \\ & \begin{array}{ccc} \langle\psi_0| & \langle\psi_1| & \langle\psi_2| \end{array} \end{array}$$

where the generator

$$R = \left(\begin{array}{c|cc} 1 & & O \\ \hline \multirow{2}{*}{O} & \omega & \\ & & \omega^* \end{array}\right), \quad \rho = \left(\begin{array}{c|cc} 1 & & O \\ \hline \multirow{2}{*}{O} & & 1 \\ & 1 & \end{array}\right)$$

we label the subspace V_{ψ_0} as A_1, and label $V_{\{\psi_1,\psi_2\}}$ as E. Then

$$e_A = 1, \quad R_{A_1} = 1, \quad \rho_{A_1} = 1 \Rightarrow g_{A_1} = 1,$$

$$e_E = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix}, \quad R_E = \begin{pmatrix} \omega & \\ & \omega^* \end{pmatrix}, \quad \rho_E = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \text{(Equivalent Representations)}$$

The multiplication

$$R_E \rho_E = \begin{pmatrix} 0 & \omega \\ \omega^* & 0 \end{pmatrix} = \rho_E R_E^2 = \begin{pmatrix} & \omega \\ \omega^* & \end{pmatrix} \begin{pmatrix} \omega^* & \\ & \omega \end{pmatrix}.$$

For non-Abelian group, $\hat{R}\hat{\rho} \neq \hat{\rho}\hat{R}$.

<u>minimal</u> invariant subspace $\leftrightarrow$ <u>irreducible</u> (sub)representation

Now, consider the Hilbert space becomes

$$\operatorname{opan}(\{|0\pm\rangle, |1\pm\rangle, |2\pm\rangle\}).$$

Induce

$$i\pm \mapsto |i\pm\rangle, \quad \hat{R}|i,s\rangle = |i+1,s\rangle, \; \hat{\rho}|i,s\rangle = |-i,-s\rangle$$

Consider the Hamiltonian

$$\hat{H} = \sum_{j,s,j',s'} |j,s\rangle h_{js;j's'} \langle j's'|$$

which satisfies

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

$$\{\text{Transformations on Real Space}\}$$
$$\text{def} \downarrow\uparrow \text{ represent}$$
$$G$$
$$\downarrow \text{represent}$$
$$\{\text{Transformations on } \underset{\text{HS } V \text{ represent}\{\text{Transformations on Operator Space}\}}{\text{Function Space}}\}, \quad \{V \to V\}$$

For invariant subspace W (group action): $\forall g \in G$, $|w\rangle \in W$, we have

$$\hat{g}(= \tau(g))|w\rangle \in W$$

Now, minimal invariant subspace $\leftrightarrow$ irreducible representation. Choose $|\psi_1\rangle$, which satisfies

$$\hat{H}|\psi_1\rangle = E|\psi_1\rangle$$

Then, $|\psi_2\rangle = \hat{\rho}|\psi_1\rangle$, and they are orthogonal to each other $\langle\psi_2|\psi_1\rangle = 0$, then

$$\hat{H}\hat{\rho}|\psi_1\rangle = E\hat{\rho}|\psi_1\rangle$$

Schur's Lemma In irrepresentation τ, if $[\hat{H}_\tau, \hat{g}_\tau] = 0\ \forall g \in G$, then it is the irrepresentation of G. Then, $\hat{H}_\tau = E\mathbb{1}_\tau$, which call $\dim(V_\tau) = \#\text{Degeneracy}$.

Space Inversion & Time Reversal

Classical	$\mathcal{I} = \rho_x\rho_y\rho_z$	$\mathcal{T}$
	$\boldsymbol{r} \to -\boldsymbol{r}$, $t \to t$	$t \to -t$, $\boldsymbol{r} \to \boldsymbol{r}$
	$\boldsymbol{p} \to -\boldsymbol{p}$	$\boldsymbol{p} \to -\boldsymbol{p}$
Polar (Vector)	$\boldsymbol{E} \to -\boldsymbol{E}$	$\boldsymbol{E} \to \boldsymbol{E}$
Axial (Pseudo vector)	$\boldsymbol{B} \to \boldsymbol{B}$	$\boldsymbol{B} \to -\boldsymbol{B}$
$\boldsymbol{E} = -\nabla\varphi$	$\varphi \to \varphi$	$\varphi \to \varphi$
$\boldsymbol{A} = \nabla \times \boldsymbol{B}$	$\boldsymbol{A} \to -\boldsymbol{A}$	$\boldsymbol{A} \to \boldsymbol{A}$

Quantum:

$\hat{I}$	$\hat{T}$
$\hat{I}\hat{\boldsymbol{r}}\hat{I}^{-1} = -\hat{\boldsymbol{r}}$	$\hat{T}\hat{\boldsymbol{r}}\hat{T}^{-1} = \hat{\boldsymbol{r}}$
$\hat{I}\hat{\boldsymbol{p}}\hat{I}^{-1} = -\hat{\boldsymbol{p}}$	$\hat{T}\hat{\boldsymbol{p}}\hat{T}^{-1} = -\hat{\boldsymbol{p}}$
$\hat{I}[\hat{x}, \hat{p}_x]\hat{I}^{-1} = [-\hat{x}, -\hat{p}_x] = \mathrm{i}$	$\hat{T}[\hat{x}, \hat{p}_x]\hat{T}^{-1} = [\hat{x}, -$

For $\hat{f}$ anti-linear

$$\hat{f}(a|\psi\rangle + b|\chi\rangle = a^*\hat{f}|\varphi\rangle + b^*\hat{f}|\chi\rangle)$$

Norm-preserving

$$\langle\hat{f}\psi|\hat{f}\psi\rangle = \langle\psi|\psi\rangle$$

Quiz Prove that $\forall\psi,\ x_i$, $\langle\hat{f}\psi|\hat{f}\chi\rangle = \langle x|\psi\rangle = \langle\psi|\chi\rangle^*$. BTW, when it is satisfied, f is called anti-unitary. We already have for $\hat{I}$: $\{e, I\}$, $I^2 = e$; and for T: $\{e, T\}$, $T^2 = e$. Combine irreps of $\{e, i\}$, and $i^2 = e$ called involution.

$$|\psi\rangle \sim \mathrm{e}^{\mathrm{i}\theta}|\psi\rangle \in V,$$

then

$$\hat{e}|\psi\rangle = |\psi\rangle, \quad \hat{i}|\psi\rangle = |\chi\rangle, \quad \hat{i}^2|\psi\rangle = \hat{i}|\chi\rangle = \mathrm{e}^{\mathrm{i}\theta}|\psi\rangle.$$

Take $|\chi\rangle \propto |\psi\rangle$, then $\langle\psi|\chi\rangle = 0$. Start with $\hat{i}$ be unitary with $\hat{I}$ is unitary. We can always construct another state with a linear combination

$$|\phi\rangle = a|\psi\rangle + b|\chi\rangle,$$

Then,

$$|\phi\rangle \propto \hat{i}_\pm|\phi\rangle = a_\pm|\chi\rangle + b\,\mathrm{e}^{\mathrm{i}\theta}|\psi\rangle$$

Rearrange it

$$\frac{b\,\mathrm{e}^{\mathrm{i}\theta}}{a} = \frac{a}{b}, \quad \left(\frac{a}{b}\right)^2 = \mathrm{e}^{\mathrm{i}\theta}, \quad g = 1,\ a_\pm = \pm\,\mathrm{e}^{\mathrm{i}\theta}$$

For anti-unitary, we need to

$$|\phi\rangle \propto \hat{i}|\phi\rangle = a^*|\chi\rangle + b^*\,\mathrm{e}^{\mathrm{i}\theta}|\psi\rangle$$

Rearrange it

$$\frac{b^*\,\mathrm{e}^{\mathrm{i}\theta}}{a} = \frac{a^*}{b} \Rightarrow |a|^2 = |b|^2\,\mathrm{e}^{\mathrm{i}\theta}$$

If $|a|^2 = |b|^2$, $\mathrm{e}^{\mathrm{i}\theta} = 1$.

3.3.2 Degeneracies

3.4 Angular momentum, Lie algebra

3.5 Gauge

Lecture #1 Review

Problem 1.1. Solve the Schrödinger equation (i.e., find the eigenvalues and eigenstates, then plot typical eigenstates) with the following 1D Hamiltonians

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

where

1. $V(x) = \frac{1}{2}m\omega^2 x^2$; (25') 2. $V(x) = V_0\delta(L/2 - |x|)$ with $\delta(x)$ the Heavisine step function; (15')
3. $V(x) = V_0[\delta(x + L/2) + \delta(x - L/2)]$ with $\delta(x)$ the Dirac delta function. (15')

Solution.

(a) Under this potential, the system appears as a Harmonic oscillator. Substitute the Hamiltonian into the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(x) = E\psi(x).$$

where $\hat{p} = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}$. We define

i. $\alpha = \sqrt{m\omega/\hbar}$ ii. $\xi = \alpha x$, $x = \xi/\alpha$ iii. $\psi(x) = u(\xi)$ iv. $\lambda = 2E/\hbar\omega$

for simplification. Consider the asymptotic behavior of this ODE first

$$\frac{\mathrm{d}^2 u(\xi)}{\mathrm{d}\xi^{2^2}} + (\lambda - \xi^2)u(\xi) = 0 \xRightarrow{|\xi|\to\infty} \frac{\mathrm{d}^2 u(\xi)}{\mathrm{d}\xi^{2^2}} - \xi^2 u(\xi) = 0,$$

and its asymptotic solution is $u(\xi) = \mathrm{e}^{-\xi^2/2}$ (Since $\mathrm{e}^{+\xi^2/2}$ blows up, so it is discarded). Now, insert a polynomial $H(\xi)$ to obtain its solution in common solution

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

then substitute it into the ODE, and simplify it

$$H'' - 2\xi H' + (\lambda - 1)H = 0.$$

It is so-called *Hermit Polynomial*. We assume the expansion of $H(\xi)$ is a power series

$$H(\xi) = \sum_{n=0}^{\infty} a_n \xi^n,$$

and then substitute it into the ODE

$$\sum_{n=2}^{\infty} a_n n(n-1)\xi^{n-2} - 2\xi\sum_{n=1}^{\infty} a_n n\xi^{n-1} + (\lambda - 1)\sum_{n=0}^{\infty} a_n \xi^n = 0.$$

We have to combine the three sum terms. Since in the 2nd derivation of $H(\xi)$ the top 2 terms disappers, while in the 1st derivation of $H(\xi)$, the first term disappers, so the expansion can be

$$\sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)\xi^n - 2\sum_{n=0}^{\infty} a_n n\xi^n + (\lambda - 1)\sum_{n=0}^{\infty} a_n \xi^n = 0.$$

Since there is a term contains single "n", so we need to discuss respectively.

i. For $n = 0$, we have $2a_2 + \lambda - 1 = 0$, and $a_2 = -(1-\lambda)a_0/2$

ii. For $n \geq 1$, we have $a_{n+2} = [2n - (\lambda - 1)]/[(n+2)(n+1)]a_n$.

Apply *d'Alembert's Judgement* to the nth and the $n+2$th terms of $H(\xi)$

$$\lim_{n\to\infty} \frac{a_{n+2}\xi^{n+2}}{a_n\xi^n} = \lim_{n\to\infty} \frac{2n-(\lambda-1)}{(n+2)(n+1)}\xi^2 \sim \frac{2}{n}\xi^2,$$

means that $H(\xi)$ will divergent. To avoid this, the series needs to be cut off at nth term (n is finite), let

$$a_{n+2} = [2n - (\lambda-1)]a_n/[(n+2)(n+1)] = 0,$$

since $a_n \neq 0$, so $2n - (\lambda - 1) = 0$, that is

$$\lambda = 2n + 1 = 2E/\hbar\omega, \quad \text{and} \quad E = \hbar\omega(n + 1/2).$$

From the limitation of wave function, we arrive at the discrete energy level. Now, normalize it

$$\langle\psi(x)|\psi(x)\rangle = \int_{\mathbb{R}} [H_n(\xi)]^2 \,\mathrm{e}^{-2}\,\mathrm{d}\xi/\alpha = 1,$$

using the orthogonality property of Hermit polynomial

$$\int_{\mathbb{R}} H_m(\xi)H_n(\xi)\,\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi = \sqrt{\pi}2^n n!\delta_{mn},$$

we arrive at the normalized wave function

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right), \quad \text{or} \quad \psi_n(\xi) = \sqrt{\frac{\alpha}{\sqrt{\pi}2^n n!}}H_n(\xi)\,\mathrm{e}^{-\xi^2/2}.$$

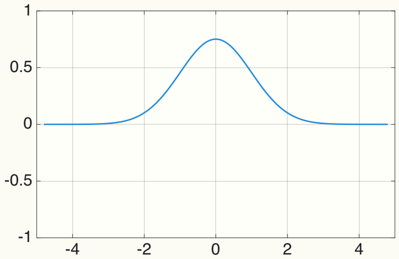
For the typical state:

i. $\psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\,\mathrm{e}^{-\alpha^2x^2/2}$, is a Gaussian distribution.

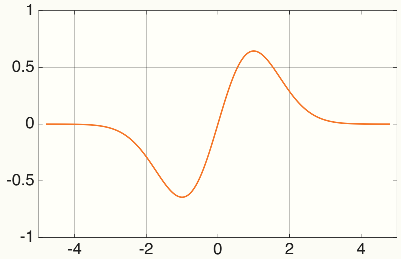
ii. $\psi_1(x) = \sqrt{\frac{\alpha}{2\sqrt{\pi}}}(2\alpha x)\,\mathrm{e}^{-\alpha^2x^2/2}$, is odd.

iii. $\psi_2(x) = \sqrt{\frac{\alpha}{8\sqrt{\pi}}}(4\alpha^2x^2 - 2)\,\mathrm{e}^{-\alpha^2x^2/2}$, is even.

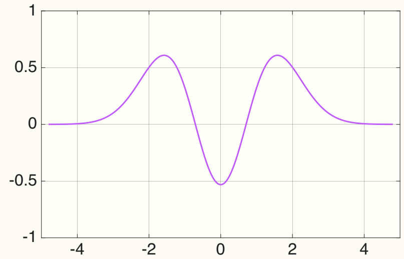
The figures of the typical eigenstates: Ground state ($n = 0$), first excited state ($n = 1$), and second excited state ($n = 2$) plotted by MATLAB are listed as follows



(a) Ground state $\psi_0(x)$



(b) 1st excited state $\psi_1(x)$



(c) 2nd excited state $\psi_2(x)$

The MATLAB source code for the three eigenstates is also attached as follows.

```
%#ok<*CLALL>; hw0_fig1.m
clear all; close all; clc

x = linspace(-4.8, 4.8, 2400); n = 3; c = lines(2*n);

for i = 0:n - 1
  figure('Visible', 'off');
  set(gca, 'Color',  '#fffff9', 'GridColor', 'black', ...
           'XColor', '#1f1f1f', 'YColor', '#1f1f1f');
  box on; grid on; hold on; fontsize(33, "points");
  psi = sqrt(1/(sqrt(pi) * 2^i * factorial(i))) ... normalization const.
      * hermiteH(i, x) .* exp(-x.^2/2);
  plot(x, psi, 'LineWidth', 3, 'Color', c(i + floor(i/2) + 1, :));
  xlim([-5, 5]); xticks([-4 -2 0 2 4]); ylim([-1, 1]); yticks([-1 -.5 0 .5 1]);
  hold off;
  exportgraphics(gcf, 'hw0_fig1.pdf', 'ContentType', 'vector', ...
                 'BackgroundColor', 'none', 'Append', i > 0);
  close(gcf);
end
```

(b) Under this potential, the system appears as a potential barrier and can be divided into three regions:

i. Region I and III ($|x| > L/2$): the wave function decays exponentially.

ii. Region II ($|x| \le L/2$): the wave function behaves oscillatory.

The Hamiltonian is

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + V_0\delta(L/2 - |x|),$$

where $\hat{p} = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}$. The Schrödinger equation for the system is

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) &= E\psi(x), && \text{Region I and III} \\ \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_0\right)\psi(x) &= E\psi(x), && \text{Region II} \end{aligned}$$

Case 1 Energy above the barrier ($E > V_0$)
Define

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad \text{and} \quad \kappa = \sqrt{\frac{2m(E - V_0)}{\hbar^2}},$$

the Schrödinger equation becomes

$$\begin{aligned} \psi''(x) + k^2\psi(x) &= 0, && \text{Regions I and III} \\ \psi''(x) + \kappa^2\psi(x) &= 0, && \text{Regions II} \end{aligned}$$

and its the solution in the three regions is

$$
\begin{aligned}
\psi_{\mathrm{I}}(x) &= \mathrm{e}^{\mathrm{i}kx} + r\,\mathrm{e}^{-\mathrm{i}kx}, && \text{Region I: Incident \& reflected waves} \\
\psi_{\mathrm{III}}(x) &= t\,\mathrm{e}^{\mathrm{i}kx}, && \text{Region III: Transmitted wave} \\
\psi_{\mathrm{II}}(x) &= C\,\mathrm{e}^{\mathrm{i}\kappa x} + D\,\mathrm{e}^{-\mathrm{i}\kappa x}, && \text{Region II: Transmitted \& reflected wave inside the barrier}
\end{aligned}
$$

To find the eigenstates, apply the boundary conditions at $x = \pm L/2$, that is

$$\psi_{\mathrm{I}}^{(0,1)}(-L/2) = \psi_{\mathrm{II}}^{(0,1)}(-L/2), \quad \text{and} \quad \psi_{\mathrm{III}}^{(0,1)}(L/2) = \psi_{\mathrm{II}}^{(0,1)}(L/2).$$

We get a Quaternion linear equation system. By canceling C and D, we derived the transmission coefficient $T = |t|^2$ and reflection coefficient $R = |r|^2$

$$T = \frac{4k^2\kappa^2\cos^2(\kappa L)}{(k^2-\kappa^2)^2\sin^2(\kappa L) + 4k^2\kappa^2\cos^2(\kappa L)}, \quad \text{and} \quad R = \frac{(k^2-\kappa^2)^2\sin^2(\kappa L)}{(k^2-\kappa^2)^2\sin^2(\kappa L) + 4k^2\kappa^2\cos^2(\kappa L)}.$$

Case 2 Energy below the Barrier ($E_0 < V_0$)
This case can be considered as $\kappa \to \mathrm{i}\kappa$. Reusing the conclusion from case $E > V_0$, the wave function

$$\psi_{\mathrm{I}}(x) = \mathrm{e}^{\mathrm{i}kx} + r\,\mathrm{e}^{-\mathrm{i}kx},\ \psi_{\mathrm{III}}(x) = t\,\mathrm{e}^{\mathrm{i}kx},\ \psi_{\mathrm{II}}(x) = C\,\mathrm{e}^{-\kappa x} + D\,\mathrm{e}^{\kappa x},$$

and the transmission & reflection coefficient

$$T = \frac{4k^2\kappa^2\,\mathrm{ch}^2(\kappa L)}{(k^2+\kappa^2)^2\,\mathrm{sh}^2(\kappa L) + 4k^2\kappa^2\,\mathrm{ch}^2(\kappa L)}, \quad \text{and} \quad R = \frac{(k^2+\kappa^2)^2\,\mathrm{sh}^2(\kappa L)}{(k^2+\kappa^2)^2\,\mathrm{sh}^2(\kappa L) + 4k^2\kappa^2\,\mathrm{ch}^2(\kappa L)}.$$

here used the identities for hyperbolic functions: $\sin(\mathrm{i}x) = -\mathrm{i}\,\mathrm{sh}(x)$, $\cos(\mathrm{i}x) = \mathrm{ch}(x)$.

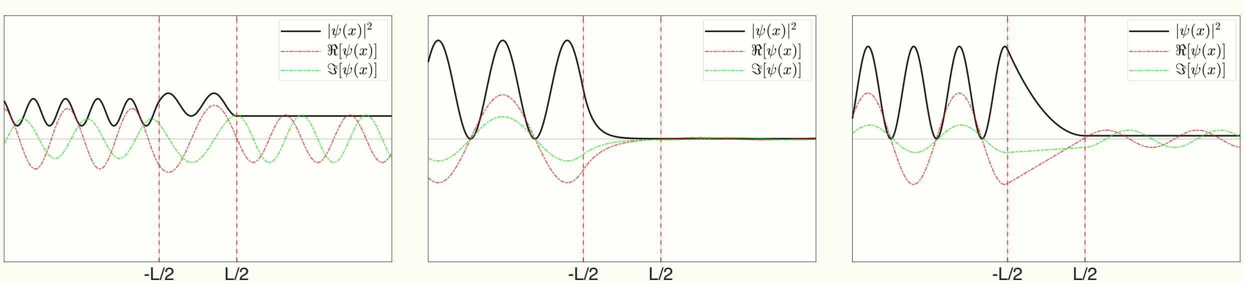
Case 3 Energy equal to the barrier ($E = V_0$)
Now, $\kappa = 0$. So, in Region II

$$\psi''(x) = 0, \quad \psi_{\mathrm{II}}(x) = Cx + D,$$

while the expression of the wave function in Region I and Region III remains unchanged. Concerning the transmission & reflection coefficient, we can calculate the limitation directly

$$\lim_{\kappa\to 0} T = \frac{4}{4 + (kL)^2}, \quad \text{and} \quad \lim_{\kappa\to 0} R = \frac{(kL)^2}{4 + (kL)^2}.$$

The figures of the typical eigenstates: Propagation wave function ($E > V_0$), Tunneling wave function ($E < V_0$), and the Critical Wave Function ($E = V_0$) are plotted by MATLAB and listed as follows



(a) $E > V_0$ (b) $E < V_0$ (c) $E = V_0$

The MATLAB source code for the three situations is also attached as follows.

```
%#ok<*CLALL>; hw0_fig2.m
clear all; close all; clc

eV = 1.6022e-19; m = 9.1093837e-31; hbar = 1.054571817e-34; au = 1e-10;
V0 = 6.8*eV; L = 4*au; a = L/2; x = linspace(-10*au, 10*au, 1e4);
E = [13.6 3.4 V0*(1+eps)/eV]*eV;
u = @(E) sqrt(2 * m * E) / hbar;        p = @(E) 1i * u(E) * a;
v = @(E) sqrt(2 * m * (E - V0)) / hbar; q = @(E) 1i * v(E) * a;
r = @(E) exp(-2*p(E)) * (u(E)^2 - v(E)^2) * (1 - exp(4*q(E))) / ...
         ((u(E) + v(E))^2 - (u(E) - v(E))^2 * exp(4*q(E)));
t = @(E) 4 * u(E) * v(E) * exp(-2*(p(E)-q(E))) / ...
         (u(E) * (1 - exp(2*q(E))) + v(E) * (1 + exp(2*q(E))))/ ...
         (u(E) * (1 + exp(2*q(E))) + v(E) * (1 - exp(2*q(E))));
c = @(E) t(E) * (u(E) + v(E)) * exp(p(E) - q(E)) / 2 / v(E);
d = @(E) -c(E) * exp(2*q(E)) * (u(E) - v(E)) / (u(E) + v(E));
psi = @(E,x) arrayfun(@(xi) ...
  (xi < -a)      .* (exp(1i*u(E)*xi) + r(E) * exp(-1i*u(E)*xi)) + ...
  (abs(xi) <= a) .* (c(E) * exp(1i*v(E)*xi) + d(E) * exp(-1i*v(E)*xi)) + ...
  (xi > a)       .* (t(E) * exp(1i*u(E)*xi)), x);

for i = 1:3
  PSI = psi(E(i),x);
  figure('Visible','off');
  set(gca, 'Color',  '#fffff9', 'GridColor', 'black', ...
           'XColor', '#1f1f1f', 'YColor', '#1f1f1f');
  box on; grid on; hold on; fontsize(33, "points");
  plot(x, abs(PSI).^2,     'LineWidth', 3, 'Color', [.1, .1, .1]);
  plot(x, real(PSI), '-.', 'LineWidth', 2, 'Color', [.9, .1, .1, .75]);
  plot(x, imag(PSI), '-.', 'LineWidth', 2, 'Color', [.1, .9, .1, .75]);
  xticks([-a a]); xline([-a a], 'r--', 'LineWidth', 2, 'Alpha', 0.7);
  yticks([]);     yline(0, 'k-', 'Alpha', .3);
  xticklabels({'-L/2' 'L/2'}); ylim([-5, 5]);
  legend('\ $|\psi(x)|^2$', '\ $\Re[\psi(x)]$', '\ $\Im[\psi(x)]$',...
         'Interpreter', 'latex', 'IconColumnWidth', 75, ...
         'BackgroundAlpha', .5, 'Color', 'w', 'TextColor', 'k');
  hold off;
  exportgraphics(gcf, 'hw0_fig2.pdf', 'ContentType', 'vector', ...
                 'BackgroundColor', 'none', 'Append', i > 1);
  close(gcf);
end
```

(c) Firstly, discuss the sign of V_0.

i If $V_0 > 0$, the δ-functions are repulsive (barriers). There are no bound states.

ii If $V_0 < 0$, the δ-functions are attractive (wells), then bound states exist.

So, we assume $V_0 < 0$, for bound states. Let $V_0 = -|V_0|$, so the potential is attractive

$$V(x) = -|V_0|[\delta(x + L/2) + \delta(x - L/2)].$$

which has divided the system into three regions

Region I: $x < -L/2$ Region II: $|x| < L/2$ Region III: $x > L/2$

Under this potential, the system appears as a double δ-well with the strength of V_0. The Schrödinger equation for the range $\mathbb{R}\backslash\{\pm L/2\}$ becomes

$$\psi''(x) - k^2\psi(x) = 0,$$

where $k = \sqrt{-2mE/\hbar^2}$ ($E < 0$ for bound states). Due to symmetry, the solutions should

$$\begin{aligned}
&\psi_{\mathsf{I}}(x) = A\,\mathrm{e}^{kx}, && \psi_{\mathsf{II}}(x) = B(\mathrm{e}^{kx} + \mathrm{e}^{-kx}) = B\,\mathrm{ch}(kx), && \psi_{\mathsf{III}}(x) = A\,\mathrm{e}^{-kx}, && \text{Even Parity}\\
&\psi_{\mathsf{I}}(x) = -A\,\mathrm{e}^{kx}, && \psi_{\mathsf{II}}(x) = B(\mathrm{e}^{kx} - \mathrm{e}^{-kx}) = B\,\mathrm{sh}(kx), && \psi_{\mathsf{III}}(x) = A\,\mathrm{e}^{-kx}, && \text{Odd Parity}
\end{aligned}$$

To get the continuity of the wave function's 1st derivative at $x_0 = \pm L/2$, integrate from x_0^- to x_0^+

$$-\frac{\hbar^2}{2m}[\psi'(x_0^-) - \psi'(x_0^+)] - |V_0|\psi(x_0) = E\psi \cdot 2\epsilon \approxeq 0, \quad \psi'(x_0^+) - \psi'(x_0^-) = -\frac{2m|V_0|}{\hbar^2}\psi(x_0).$$

Then we can substitute the solutions to the boundary conditions.

Even Parity Expand the continuous conditions at $x = L/2$

$$A\,\mathrm{e}^{-kL/2} = B\,\mathrm{ch}(kL/2), \quad \text{and} \quad -kA\,\mathrm{e}^{-kL/2} - kB\,\mathrm{sh}(L/2) = -\frac{2m|V_0|}{\hbar^2}\psi(L/2).$$

(Due to the symmetry, it is equal to expand at $x = -L/2$.) Combine the conditions, and defint $\lambda = 2m|V_0|/\hbar^2$, we have

$$k + k\,\mathrm{th}\left(\frac{kL}{2}\right) = \frac{2m|V_0|}{\hbar^2} = \lambda,$$

Odd Parity Similar to even parity, at $x = L/2$, we have

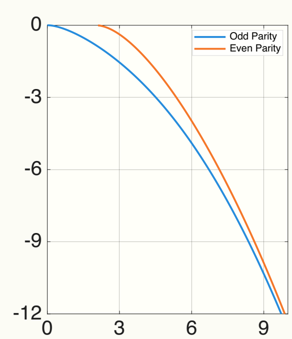
$$A\,\mathrm{e}^{-kL/2} = B\,\mathrm{sh}(kL/2),$$

$$-kA\,\mathrm{e}^{-kL/2} - kB\,\mathrm{ch}(kL/2) = -\frac{2m|V_0|}{\hbar^2}\psi(L/2).$$

Combine them, and we have

$$k + k\,\mathrm{cth}(kL/2) = \lambda,$$

where $\lambda = 2m|V_0|/\hbar^2$.



Mingyu Xia (Westlake ID: 20251202247) «xiamingyu@westlake.edu.cn»

The MATLAB source code for the boundary conditions of two parities is also attached as follows.

```
%#ok<*CLALL>; hw0_fig3.m
clear all; close all; clc

x       = linspace(-13.6, 0, 2400);
k       = sqrt(-2 * x);
lambda  = [k + k .* tanh(k/2); k + k .* coth(k/2)];

figure('Visible', 'off');
set(gca, 'Color',  '#fffff9', 'GridColor', 'black', ...
         'XColor', '#1f1f1f', 'YColor', '#1f1f1f');
box on; grid on; hold on; axis equal;
plot(lambda(1,:), x, 'LineWidth', 3);
plot(lambda(2,:), x, 'LineWidth', 3);
fontsize(32, "points");
lh = legend({' Odd Parity', ' Even Parity'}, 'Color', 'white', ...
             'TextColor', 'k', 'BackgroundAlpha', .8, 'FontSize', 16);
lh.IconColumnWidth = 50;
xlim([0, 10]);  xticks([0 3 6 9]); ylim([-12, 0]); yticks([-12 -9 -6 -3 0]);
hold off;
exportgraphics(gcf, 'hw0_fig3.pdf', 'ContentType', 'vector', ...
               'BackgroundColor', 'none');
close(gcf);
```

Problem 1.2. Describe the following experiments (drawing pictures is recommended) and interpret the observations:

1. Double-slit experiment with *single* particles (e.g. photons, electrons, atoms, molecules, etc.); (15')
2. Stern-Gerlach experiment; (15')
3. Aharonov-Bohm effect. (15')

Solution.

(a) Double-slit experiment.

Experiment Description A coherent particle source (such as an electron gun) is directed toward a barrier with two parallel slits. Then, a screen behind the barrier will show the result pattern.

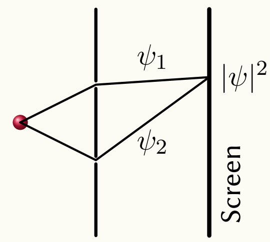
In people's classical thoughts, one particle will pass one of the slits and then leave a mark on the screen every time, and finally there will be two distinct bands on the screen corresponding to the slit geometries.

But the actual pattern on the screen is an interference pattern, consisting of multiple alternating light and dark fringes. And this pattern will build gradually as more particles arrive at the screen.

Interpretation

i. Wave-particle duality: Every single particle behaves as a wave when passing through the slits, and interfering with itself; However, every single particle is detected as a discrete point on the screen, which behaves as particle.

ii. Superposition state: Each particle effectively passes through both slits as superposition states. The probability of detection at a point on the screen is determined by the square of the magnitude of the total wavefunction, consisting of the probability amplitudes from both paths. Mathematically

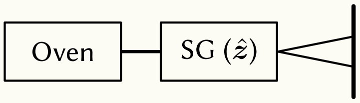


$$P(x) = \langle \psi(x) | \psi(x) \rangle = |\psi_1|^2 + |\psi_2|^2 + 2\,\mathrm{Re}[\langle \psi_1 | \psi_2 \rangle]$$

The last term represents the interference between the two paths and is responsible for the pattern.

(b) Stern-Gerlach experiment.

Experiment Description Silver atoms are heated in an oven, then some of them escape from a small hole in the oven. The silver atom beam goes through a collimator and is then subjected to an inhomogeneous magnetic field.

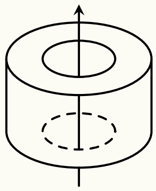


Since the atoms in the oven are randomly oriented, people expect a continuous bundle of beams to come out of the magnetic field in the Stern-Gerlach apparatus. However, what the experiment observed is that the SG apparatus *splits the original silver beam* from the oven *into two distinct components*.

Interpretation The discrete deflection reveals that the electron spin is quantized. The magnetic moment of electrons (and thus atoms) can only take discrete values relative to any measurement axis. For electrons, the measurement of the spin component along any axis yields only one of two possible values: $+\hbar/2$ (spin up) or $-\hbar/2$ (spin down).

(c) Aharonov-Bohm effect.

Experiment Description A beam of electrons is split into two paths (e.g., using a double-slit setup) that encircle a region containing a long solenoid that produces a confined magnetic field. The magnetic field $\boldsymbol{B}$ is zero outside the solenoid, but the magnetic vector potential $\boldsymbol{A}$ is non-zero outside. The two beams are recombined to produce interference fringes on a screen.



When a current is passed through the solenoid, creating a magnetic flux Φ inside it, the interference pattern shifts *even though the electrons travel in regions where the magnetic field is zero.*

Interpretation The effect highlights the non-local nature of quantum mechanics: electrons are influenced by the vector potential without entering the magnetic field region. The measured phase shift is gauge-invariant, depending on the enclosed magnetic flux, not the non-measurable potential itself.

Problem 1.3 (Optional, 30'). Solve the hydrogen atom model:

$$\mathcal{H} = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}.$$

Solution. Assume the wave function of hydrogen atom is $\Psi(r,t) = \psi(r)\,\mathrm{e}^{-\mathrm{i}\omega t}$. Substitute the time-independent wave function to Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi).$$

Since the given hydrogen atom's potential is central, that is depends only on r, the Laplacian operator becomes

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}.$$

Referring to *Mathematical Methods in Physics*, we have

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y_{lm}(\theta,\phi) = -l(l+1)Y_{lm}(\theta,\phi).$$

then we can separate the variables again. Let

$$\psi(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi),$$

where $R_l(r)$ is the *Radial Wave Function*, and $Y_{lm}(\theta,\phi)$ is the spherical function. Substitute $\psi(r,\theta,\phi)$ to Schrödinger equation, we have

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R_{nl}(r)}{\mathrm{d}r}\right) + \frac{\hbar^2 l(l+1)}{2mr^2}R_{nl}(r) - \frac{e^2}{4\pi\varepsilon_0 r}R_{nl}(r).$$

Let $R_{nl}(r) = \chi_l(r)/r$, then substitute it to the Schrödinger equation,

$$\chi''(r) + \left[\frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right) - \frac{l(l+1)}{r^2}\right]\chi_l(r) = 0.$$

To solve it, consider its asymptotic behavior first.

i When $r \to 0$, we have

$$\chi_l''(r) - \frac{l(l+1)}{r^2}\chi_l(r) = 0.$$

and we take the solution $\chi_l^0(r) = r^{l+1}$ ($\chi_l^0(r) = r^{-l}$ is discard to avoid divergent).

ii When $r \to \infty$, we have

$$\chi_l''(r) + \frac{2m}{\hbar^2}E\chi_l(r) = 0$$

and we take the solution $\chi_l^\infty(r) = \mathrm{e}^{-kr}$, where $k = \sqrt{2mE/\hbar^2}$ ($\chi_l^\infty(r) = \mathrm{e}^{kr}$ is also discard).

To obtain the general solution, let

$$\chi_l(r) = \chi_l^0(r)\chi_l^\infty(r)u_l(r).$$

and substitute it to the Schrödinger equation

$$\xi^2\frac{\mathrm{d}^2u_l(\xi)}{\mathrm{d}\xi^2} + [2(l+1)-\xi]\frac{\mathrm{d}u_l(\xi)}{\mathrm{d}\xi} - \frac{2(L+1)k - \frac{2me^2}{4\pi\varepsilon_0\hbar^2}}{2k}u_l(\xi) = 0,$$

which suits the Laguerre polynomial

$$\xi\frac{\mathrm{d}^2u_l(\xi)}{\mathrm{d}\xi^2} + (\gamma-\xi)\frac{\mathrm{d}u_l(\xi)}{\mathrm{d}\xi} - \alpha u_l(\xi) = 0,$$

compare with it, we have

$$\gamma = 2(l+1), \quad \text{and} \quad \alpha = l+1-\frac{me^2}{4\pi\varepsilon_0 k\hbar^2}.$$

Since the solution of this equation at $\xi = 0$ can be expanded into a series

$$F_{\gamma,\alpha}(\xi) = 1 + \sum_{n=1}^{\infty}\left\{\left[\frac{(\alpha+n-1)!}{(\alpha-1)!}\xi^n\right]\Big/\left[\frac{(\gamma+n-1)!}{(\gamma-1)!}n\right]\right\}.$$

Apply *d'Alembert's Judgement* to the nth and the $n+1$th terms of $F_{\gamma,\alpha}(\xi)$

$$\lim_{n\to\infty}\frac{f_{n+1}(\xi)}{f_n(\xi)} = \frac{\xi}{n},$$

means that $F_{\gamma,\alpha}(\xi)$ will divergent. To avoid this, the series needs to be cut off at the n'th term (n' is finite), let $n' = -\alpha$, that is

$$l+1-\frac{me^2}{4\pi\varepsilon_0 k\hbar^2} = n', \quad n \equiv l+1+n' = \frac{me^2}{4\pi\varepsilon_0 k\hbar^2},$$

since $k = \sqrt{2mE/\hbar^2}$, we obtain the energy of hydrogen atom

$$E_n = -\frac{me^4}{32\pi\varepsilon_0\hbar^2}\frac{1}{n^2} = -\frac{E_0}{n^2},$$

and the basic state wave function is

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a_0^3}}\,\mathrm{e}^{-r/a_0}.$$

where $a_0 = 4\pi\varepsilon_0\hbar^2/me^2$ is Bohr radius.

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Lecture #2 Hilbert Space

Problem 2.1 (Function space). A square-integrable function, or L^2 function, is a real- or complex-valued function for which the integral of the square of the absolute value is finite. Let us consider the set of complex-valued, continuous L^2 functions on the real line $\mathbb{R}$ (or on a subset $A \subset \mathbb{R}$). The set $L^2(A) = \{\psi : A \to \mathbb{C} | \int_A |\psi(x)|^2 \, \mathrm{d}x < \infty\}$ is naturally a complex vector space, called *function space*.

(a) Show that the integral $\int_A \varphi(x)^* \psi(x) \, \mathrm{d}x$ with $\varphi, \psi \in L^2(A)$ defines an *inner product* $\langle \varphi | \psi \rangle$.

(b) $L^2(A)$ is a Hilbert space with the above definition of inner product. Find at least two different orthonormal bases (excluding δ-functions) for each of the three cases

i. $A = (-\infty, +\infty)$; ii. $A = [-1, 1]$; iii. $A = (0, +\infty)$.

Demonstrate the orthonormality and the completeness explicitly. (Hint: One choice can be our familiar Fourier basis and the other from a polynomial expansion by virtue of *Weierstrass's theorem*). Also see Problem 1.2.

Solution.

(a) *Proof.* To show that the integral defines an inner product, we check the axioms of an inner product on a complex vector space.

i. Conjugate symmetry: $\langle \varphi | \psi \rangle = \int_A \varphi^* \psi = \overline{\int_A \psi^* \varphi} = \overline{\langle \psi | \varphi \rangle}$.

ii. Linearity: For $\alpha, \beta \in \mathbb{C}$, in the second argument,

$$\langle \varphi | (\alpha\psi_1 + \beta\psi_2) \rangle = \int_A \varphi^* (\alpha\psi_1 + \beta\psi_2) = \alpha \langle \varphi | \psi_1 \rangle + \beta \langle \varphi | \psi_2 \rangle.$$

Conjugate-linearity in the first argument follows similarly.

iii. Positive-definiteness: $\langle \psi | \psi \rangle = \int_A |\psi(x)|^2 \, \mathrm{d}x \geq 0$, also for φ.

Hence, $\langle \varphi | \psi \rangle$ is an inner product on $L^2(A)$. □

(b) i. $A = (-\infty, +\infty)$

Case 1 Hermite functions

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi} 2^n n!}} H_n(x) \, \mathrm{e}^{-x^2/2}, \quad n = 0, 1, 2, \ldots,$$

where H_n is the $n-$th Hermite polynomial, belong to $L^2(\mathbb{R})$. Using the orthonormality of the Hermite polynomial, we get the orthonormality of the function

$$\int_A \psi_m(x) \psi_n(x) \, \mathrm{d}x = \delta_{mn}.$$

From Sturm-Liouville theory, $\{\psi_n\}_{n \geq 0}$ form a basis for $L^2(\mathbb{R})$. So it is complete.

Case 2 Haar basis

$$\psi_{n,k}(x) = 2^{n/2}\psi_{0,0}(2^n x - k), \quad x \in \mathbb{R},$$

ψ is a compactly supported mother wavelet chosen so that the family is orthonormal in $L^2(\mathbb{R})$

$$\int_A \psi_{n,k}(x)\psi_{n',k'}(x)\,\mathrm{d}x = \delta_{nn'}\delta jj'.$$

The Haar system on the real line is an orthonormal basis in $L^2(\mathbb{R})$, so it is complete.

ii. $A = [-1, 1]$

Case 1 Fourier basis

$$\psi_n(x) = \frac{1}{\sqrt{2}}\,\mathrm{e}^{\mathrm{i}n\pi x}, \quad n \in \mathbb{Z},$$

its orthonormality

$$\int_{-1}^{1} \psi_m(x)\psi_n(x)\,\mathrm{d}x = \frac{1}{2}\int_{-1}^{1} \mathrm{e}^{\mathrm{i}(m-n)\pi x}\,\mathrm{d}x = \delta_{mn},$$

It is standard Fourier series theory, which satisfies completeness.

Case 2 Legendre polynomials

$$\psi_n(x) = \sqrt{n + \frac{1}{2}}P_n(x), \quad n = 0, 1, 2, \ldots,$$

its orthonormality

$$\int_{-1}^{1} \psi_m(x)\psi_n(x)\,\mathrm{d}x = \frac{2n+1}{2}\int_{-1}^{1} P_m(x)P_n(x)\,\mathrm{d}x = \delta_{mn}.$$

Due to Weierstrass' theorem, polynomials are dense in A in the sup norm, hence complete in L^2.

iii. $A = (0, +\infty)$

Case 1 Laguerre functions

$$\psi_n(x) = \mathrm{e}^{-x/2}L_n(x), \quad \text{where} \quad L_n(x) = \mathrm{e}^x\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^n\,\mathrm{e}^{-x}),$$

its orthonormality

$$\int_A \psi_m(x)\psi_n(x)\,\mathrm{d}x = \int_A \mathrm{e}^{-x}L_m(x)\,\mathrm{d}x = \delta_{mn}.$$

The Laguerre polynomials (with the $\mathrm{e}^{x/2}$ factor) are eigenfunctions of a self-adjoint Sturm-Liouville operator on $(0, \infty)$ and form a complete orthonormal set in $L^2(0, \infty)$.

Case 2 Consider the mapping $\varphi : A \to (0, 1), t \mapsto \frac{2}{\pi}\arctan(t)$. Then use the sine functions in x-space

$$\psi(x) = \sqrt{2}\sin(n\pi t(x)),$$

it is trivial that sine functions are orthonormal and complete.

Problem 2.2 (Sturm-Liouville theory). Many physics problems involve second-order, linear differential equations of the general form: $\alpha(x)y'' + \beta(x)y' + \gamma(x)y = \lambda y$, where α, β, and γ are real functions, and λ is a constant. Such an ODE can be rewritten in a *Sturm-Liouville* form $\mathcal{L}y = \lambda y$ with a proper choice (cf. (a)) of the *weight function* $\omega(x)$ in the linear second-order differential operator

$$\mathcal{L} = \omega^{-1}\frac{\mathrm{d}}{\mathrm{d}x}\left(\omega\alpha\frac{\mathrm{d}}{\mathrm{d}x}\right) + \gamma.$$

This, combined with suitable boundary conditions (cf. (b)), renders $\mathcal{L}$ a self-adjoint operator if the inner product is defined to be

$$\langle u|v\rangle = \int_{x_1}^{x_2} u^*(x)v(x)\omega(x)\,\mathrm{d}x.$$

Hence, the Sturm-Liouville problem becomes an eigenvalue problem with the solutions being the eigenvalues and the corresponding λ's being the eigenvalues. The Sturm-Liouville theory provides a connection between a second-order, linear differential equation and Hilbert space $\mathcal{L}^2([x_1, x_2])$ by establishing the normalized eigenvectors of the former (in its Sturm-Liouville form) as a complete orthonormal basis of the latter.

(a) Find the general expression of $\omega(x)$ that permits the rewriting of the original ODE in its Sturm-Liouville form. Compute $\omega(x)$ for the following ODEs

$$\begin{aligned} &\text{(i)} && -y'' + 2xy' = \lambda y && \text{(Hermite)} \\ &\text{(ii)} && -(1-x^2)y'' + 2xy' = \lambda y && \text{(Legendre)} \\ &\text{(iii)} && -xy'' - (1-x)y' = \lambda y && \text{(Laguerre)} \end{aligned}$$

(b) Find the general boundary condition $\mathcal{L}$ to be self-adjoint in $[x_1, x_2]$ with respect to the above-defined inner product, namely, $\langle u|\mathcal{L}v\rangle = \langle \mathcal{L}u|v\rangle$. Note that u and v can, in general, be complex functions. Check that the boundary condition is satisfied when

i. $x_1 = -\infty$, $x_2 = +\infty$ for Hermite equation.

ii. $x_1 = -1$, $x_2 = 1$ for Legendre equation.

iii. $x_1 = 0$, $x_2 = +\infty$ for Laguerre equation.

(c) With $\mathcal{L}$ being self-adjoint in $[x_1, x_2]$, show that if $\mathcal{L}v_i = \lambda_i v_i$ $(i = 1, 2)$ and $\lambda_1 \neq \lambda_2$, then $\langle v_1|v_2\rangle = 0$.

Solution.

(a) Apply $\mathcal{L}$ to a test function y, we have

$$\mathcal{L}y = \frac{1}{\omega}[(\omega\alpha)'y' + \omega\alpha y''] + \gamma y = \alpha y'' + \frac{(\omega\alpha)'}{\omega}y' + \gamma y,$$

Comparing with the original $\alpha y'' + \beta y' + \gamma y$, we require

$$\beta(x) = \frac{(\omega\alpha)'}{\omega} = \alpha'(x) + \alpha(x)\frac{\omega'(x)}{\omega(x)}.$$

Then, we can solve ω'/ω

$$\frac{\omega'}{\omega} = \frac{\beta(x) - \alpha'(x)}{\alpha(x)}, \quad \omega(x) = C \exp\left(\int_A \frac{\beta(x') - \alpha'(x')}{\alpha(x')}\,\mathrm{d}x'\right),$$

where C is an arbitrary positive constant, and A is the integral range for the following different types.

Hermite: $-y'' + 2xy' = \lambda y$

To compare with, we have $\alpha = -1$, $\beta = 2x$, $\alpha' = 0$. Then

$$\omega'/\omega = (2x - 0)/(-1) = -2x, \quad \omega(x) = C\,\mathrm{e}^{-x^2}.$$

Legendre: $-(1 - x^2)y'' + 2xy' = \lambda y$

To compare with, we have $\alpha = -(1 - x^2)$, $\beta = 2x$, $\alpha' = 2x$. Then

$$\omega'/\omega = (2x - 2x)/(-1), \quad \omega(x) = C.$$

Laguerre: $-xy'' - (1 - x)y' = \lambda y$

To compare with, we have $\alpha = -x$, $\beta = -(1 - x) = x - 1$, $\alpha' = -1$. Then

$$\omega'/\omega = [(x - 1) - (-1)]/(-x) = -1, \quad \omega(x) = C\,\mathrm{e}^{-x}.$$

(b) Using the inner product

$$\langle u|v\rangle = \int_{x_1}^{x_2} u^*(x)v(x)\omega(x)\,\mathrm{d}x.$$

to compute the difference $\langle u|\mathcal{L}v\rangle - \langle \mathcal{L}u|v\rangle$. We have

$$\langle u|\mathcal{L}v\rangle = \int_{x_1}^{x_2} u^*\Big[\omega^{-1}(\omega\alpha v')' + \gamma v\Big]\omega\,\mathrm{d}x = \int_{x_1}^{x_2} u^*(\omega\alpha v')'\,\mathrm{d}x + \int_{x_1}^{x_2} u^* v\gamma\omega\,\mathrm{d}x,$$
$$\langle \mathcal{L}u|v\rangle = \int_{x_1}^{x_2} \Big[\omega^{-1}(\omega\alpha(u^*)')' + \gamma u^*\Big]v\omega\,\mathrm{d}x = \int_{x_1}^{x_2} (\omega\alpha(u^*)')'v\,\mathrm{d}x + \int_{x_1}^{x_2} \gamma u^* v\omega\,\mathrm{d}x.$$

Then the difference can be expressed as

$$\langle u|\mathcal{L}v\rangle - \langle \mathcal{L}u|v\rangle = [\omega(x)\alpha(x)(u^*(x)v'(x) - u'^*(x)v(x))]_{x_1}^{x_2}.$$

If it is zero, then $\mathcal{L}$ is adjoint under the corresponding interval. Now, substitute the three boundary conditions into the difference.

i. Hermite: $x \in (-\infty, +\infty)$, $\omega = e^{-x^2}$, $\alpha = -1$. Boundary term: $[-e^{-x^2}(u^*v' - u'^*v)]_{-\infty}^{+\infty} = 0$.

ii. Legendre: $x \in [-1, 1]$, $\omega = 1$, $\alpha = -(1 - x^2)$. Boundary term $\left[-(1 - x^2)(u^*v' - u'^*v)\right]_{-1}^{1} = 0$.

iii. Laguerre: $x \in [0, \infty)$, $\omega = e^{-x}$, $\alpha = -x$. Boundary term $[-xe^{-x}(u^*v' - u'^*v)]_0^{\infty} = 0$.

So, $\mathcal{L}$ is self-adjoint in the three domain.

(c) *Proof.* Using self-adjointness for $i = 1$ and $i = 2$

$$\lambda_2\langle v_1|v_2\rangle = \langle v_1|\mathcal{L}v_2\rangle = \langle \mathcal{L}v_1|v_2\rangle = \lambda_1\langle v_1|v_2\rangle.$$

Rearranging, we can obtain

$$(\lambda_2 - \lambda_1)\langle v_1|v_2\rangle = 0.$$

Since $\lambda_1 \neq \lambda_2$, then $\langle v_1|v_2\rangle = 0$. □

Problem 2.3 (Linear map). Let V and W be vector spaces over the same field $\mathbb{K}$. A map $f : V \to W$ is called a *linear map* if $f(au + bv) = af(u) + bf(v)$ for all $a, b \in \mathbb{K}$ and $u, v \in V$.

(a) Show that the set $L(V, W)$ of linear maps from V to W itself forms a vector space over $\mathbb{K}$.

(b) Consider finite dimensional vector spaces V and W. Let $\{v_1, v_2, \ldots, v_n\}$ be a basis of V, and $\{w_1, w_2, \ldots, w_n\}$ be a basis of W. Does the set of equations $f(v_i) = \sum_{j=1}^{m} \omega_j F_{ji}$ with $i = 1, 2, \ldots, n$ and $F_{ij} \in \mathbb{K}$ uniquely determine the $m \times n$ matrix F? Why? Conversely, does any $m \times n$ matrix F over $\mathbb{K}$ uniquely determine a linear map f by the same set of equations? Why?

(c) Following (a) and (b), find a basis of $L(V, W)$.

⋆ (d) (optional) Define the *kernel* of f to be $\ker(f) = \{v \in V | f(v) = 0\}$ and the *image* of f to be $\mathrm{im}(f) = \{\omega \in W | \omega = f(v), v \in V\}$. Both the kernel and the image of f are vector spaces with their dimensions called *nullity* $= \dim(\ker(f))$ and $\mathrm{rank} = \dim(\mathrm{im}(f))$, respectively. Prove that

$$\dim(\ker(f)) + \dim(\mathrm{im}(f)) = \dim(V).$$

Solution.

(a) *Proof.* Define addition and scalar multiplication on $L(V, W)$ by

$$(f + g)(v) = f(v) + g(v), \quad (\alpha f)(v) = \alpha(f(v)),$$

for all $f, g \in L(V, W)$, $\alpha \in \mathbb{K}$, $v \in V$.

Closure and linearity If f, g are linear, then for all $a, b \in \mathbb{K}$ and $u, v \in V$,

$$(f + g)(au + bv) = f(au + bv) + g(au + bv) = a(f + g)(u) + b(f + g)(v),$$

so $f + g$ is linear. Similarly,

$$(\alpha f)(au + bv) = \alpha(f(au + bv)) = \alpha(af(u) + bf(v)) = a(\alpha f)(u) + b(\alpha f)(v),$$

so αf is linear.

Vector space axioms Associativity, commutativity of addition, existence of the zero map $0 : V \to W$ with $0(v) = 0_W$, additive inverses $(-f)(v) = -f(v)$, and scalar multiplication axioms all follow from the corresponding properties in W. Thus $L(V, W)$ is a vector space over $\mathbb{K}$. □

(b) Let $\dim V = n$ with basis $\{v_1, \ldots, v_n\}$, and $\dim W = m$ with basis $\{w_1, \ldots, w_m\}$, then

$$f(v_i) = \sum_{j=1}^{m} F_{ji} w_j, \quad i = 1, \ldots, n.,$$

which defines an $m \times n$ matrix $F = (F_{ji})$.

i. For fixed i, the coefficients $F_{1i}, \ldots, F_{mi}$ are the unique coordinates of $f(v_i)$ in the basis $\{w_j\}$. So $f(v_i) = \sum_j F_{ji} w_j$ uniquely determine F.

ii. Define f on basis vectors by $f(v_i) = \sum_{j=1}^m F_{ji} w_j$, and extend linearly: for $v = \sum_{i=1}^n a_i v_i$, define

$$f(v) = \sum_{i=1}^n a_i f(v_i) = \sum_{i=1}^n \sum_{j=1}^m a_i F_{ji} w_j.$$

This is well-defined and linear, and uniquely determined by F. So, any $m \times n$ matrix F uniquely determine a linear map f, and there is a bijection between $L(V, W)$ and $m \times n$ matrices over $\mathbb{K}$ once bases are fixed.

(c) Under the identification $L(V, W) \cong \mathbb{K}^{m\times n}$, define for each $1 \le p \le m$, $1 \le q \le n$ the linear map $E^{(p,q)} : V \to W$ by

$$E^{(p,q)}(v_q) = w_p, \quad E^{(p,q)}(v_k) = 0 \quad \text{for} \quad k \neq q,$$

extended linearly. The matrix of $E^{(p,q)}$ has a 1 in the (p, q) entry and 0 elsewhere. These mn maps are linearly independent and span $L(V, W)$, hence form a basis. Thus

$$\dim L(V, W) = mn = \dim V \cdot \dim W.$$

(d) *Proof.* Let $f : V \to W$ be linear, $\dim V = n$; and let $\dim(\ker f) = k$, and choose a basis $\{u_1, \dots, u_k\}$ of $\ker f$. Extend to a basis $\{u_1, \dots, u_k, u_{k+1}, \dots, u_n\}$ of V. Let $S = \{f(u_{k+1}), \dots, f(u_n)\} \subset \operatorname{im} f$.

Span For any $v \in V$, write $v = \sum_{i=1}^n a_i u_i$. Then

$$f(v) = \sum_{i=1}^n a_i f(u_i) = \sum_{i=k+1}^n a_i f(u_i),$$

since $f(u_1) = \cdots = f(u_k) = 0$. So $\operatorname{im} f \subseteq \operatorname{span}(S)$.

Linear independence Suppose $\sum_{i=k+1}^n b_i f(u_i) = 0$. Then

$$f\left(\sum_{i=k+1}^n b_i u_i\right) = 0,$$

so $\sum_{i=k+1}^n b_i u_i \in \ker f$. Since $\{u_1, \dots, u_k\}$ is a basis of $\ker f$

$$\sum_{i=k+1}^n b_i u_i = \sum_{i=1}^k c_i u_i,$$

for some c_i. By linear independence of the full basis, all $b_i = 0$. So S is linearly independent. Thus S is a basis of $\operatorname{im} f$, and $|S| = n - k$. Hence

$$\dim(\ker f) + \dim(\operatorname{im} f) = k + (n - k) = n = \dim V.$$

which is the rank-nullity theorem. $\square$

Problem 2.4 (Coherent states). A coherent state $|\alpha\rangle$ is defined as an eigenstate of the annihilation operator $\hat{a}$ with a complex eigenvalue α:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle.$$

(a) Show that $|\alpha\rangle = \mathcal{N}\,\mathrm{e}^{\alpha\hat{a}^\dagger}|0\rangle$, where $\mathcal{N}$ is a normalization constant and $|0\rangle$ is the ground state such that $\hat{a}|0\rangle = 0$ (review the solution of a quantum harmonic oscillator if needed). Compute $\mathcal{N}$ and $\langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle$. Further show that $|\alpha\rangle = \mathrm{e}^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}|0\rangle$ up to a phase factor. $D(\alpha) \equiv \mathrm{e}^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}$ is a unitary operator called the displacement operator because it displaces the ground state $|0\rangle$ to $|\alpha\rangle$ (note that $|0\rangle$ is a special coherent state with $\alpha = 0$).

(b) Show that the set $\{|\alpha\rangle|\alpha \in \mathbb{C}\}$ form an overcomplete basis of the Hilbert space by computing $\langle\alpha|\beta\rangle$ for generic α and β, and proving

$$\int \frac{\mathrm{d}^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = \mathbb{1},$$

where $\mathrm{d}^2\alpha = \mathrm{d}\,\mathrm{Re}\,\alpha\,\mathrm{d}\,\mathrm{Im}\,\alpha = r_\alpha\,\mathrm{d}r_\alpha\,\mathrm{d}\varphi_\alpha$ ($\alpha = \mathrm{Re}\,\alpha + \mathrm{i}\,\mathrm{Im}\,\alpha = r_\alpha\,\mathrm{e}^{\mathrm{i}\varphi_\alpha}$). (Hint: Consider the matrix elements of the above operator in the orthonormal basis $\{|n\rangle\}$.)

(c) In the context of a quantum harmonic oscillator, $\hat{a} = (l_0^{-1}\hat{x} + \mathrm{i}l_0\hat{k})/\sqrt{2}$, where $l_0 \equiv \sqrt{\hbar/m\omega}$. Find the wavefunction (in real space) of a coherent state $\langle x|\alpha\rangle$, and compare this wavefunction with the Gaussian wave packet we have learned in our class. (Hint: Consider the real-space representation of the defining equation $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$.)

(d) Compute $\hat{U}^{-1}(t,0)\hat{a}\hat{U}(t,0)$ with $\hat{U}(t,0) = \exp[-\mathrm{i}(\hat{a}^\dagger\hat{a} + 1/2)\omega t]$, and use the result to derive $\hat{U}(t,0)|\alpha\rangle$. Interpret the result in the context of a quantum harmonic oscillator. (Hint: What is the physical meaning of $\mathrm{Re}\,\alpha$ and $\mathrm{Im}\,\alpha$?)

Solution.

(a) *Proof.* Expand the coherent state $|\alpha\rangle$ in terms of number state $|n\rangle$

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle.$$

Here, we merge the normalization factor into c_n to simplify, and it will be released at the end. Act $\hat{a}$ on the expand expression of $|\alpha\rangle$, due to the property of annihilation operator

$$\hat{a}|\alpha\rangle = \sum_{n=0}^{\infty} c_n\hat{a}|n\rangle = \sum_{n=1}^{\infty} c_n\sqrt{n}|n-1\rangle = \alpha\sum_{n=0}^{\infty} c_n|n\rangle,$$

the third term summing from $n = 1$ is due to $\hat{a}|0\rangle = 0$, which $n = 0$ make no sence. To uniform the lower limit of n, shift the summation index

$$\hat{a}|\alpha\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle = \alpha\sum_{n=0}^{\infty} c_n|n\rangle,$$

then we obtain the expression of the expansion coefficient

$$c_{n+1}\sqrt{n+1} = \alpha c_n, \quad \text{or} \quad c_n = \frac{\alpha}{\sqrt{n}}c_{n-1} = \frac{\alpha}{\sqrt{n}}\frac{\alpha}{\sqrt{n-1}}c_{n-2} = \cdots = \frac{\alpha^n}{\sqrt{n!}}c_0,$$

thus

$$|\alpha\rangle = c_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle = c_0 \sum_{n=0}^{\infty} \frac{(\alpha \hat{a}^\dagger)^n}{n!} |0\rangle = c_0 \, \mathrm{e}^{\alpha \hat{a}^\dagger} |0\rangle,$$

where $|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle$. To get the expression of c_0, normalize it

$$1 = \langle\alpha|\alpha\rangle = |c_0|^2 \langle 0|\mathrm{e}^{\alpha^* \hat{a}} \, \mathrm{e}^{\alpha \hat{a}^\dagger}|0\rangle = |c_0|^2 \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \langle n|n\rangle = |c_0|^2 \, \mathrm{e}^{|\alpha|^2}.$$

Hence, we prove that

$$|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2} \, \mathrm{e}^{\alpha \hat{a}^\dagger} |0\rangle = \mathcal{N} \, \mathrm{e}^{\alpha \hat{a}^\dagger} |0\rangle,$$

where $\mathcal{N} = c_0 = \mathrm{e}^{-|\alpha|^2/2}$. And the “exception value” of $\hat{a}^\dagger \hat{a}$ under the coherent state

$$\langle\alpha|\hat{a}^\dagger \hat{a}|\alpha\rangle = \alpha^* \alpha \langle\alpha|\alpha\rangle = |\alpha|^2,$$

where $\langle\alpha|\hat{a}^\dagger = \alpha^* \langle\alpha|$. The displacement operator can be written as

$$D(\alpha) = \mathrm{e}^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} \xlongequal[{[\alpha \hat{a}^\dagger, -\alpha^* \hat{a}] = |\alpha|^2}]{\text{BCH identity}} \mathrm{e}^{-|\alpha|^2/2} \, \mathrm{e}^{\alpha \hat{a}^\dagger} \, \mathrm{e}^{-\alpha^* \hat{a}},$$

when it acts on the vacuum $|0\rangle$, to calculate it, we need to expand the last term $\mathrm{e}^{-\alpha^* \hat{a}}$

$$\mathrm{e}^{-\alpha^* \hat{a}} |0\rangle = \sum_{k=0}^{\infty} \frac{(-\alpha^*)^k}{k!} \hat{a}^k |0\rangle = |0\rangle.$$

Due to every $\hat{a}$ annihilates $|0\rangle$, so only the $k = 0$ term survives. So the result of the displacement operator acting on the vacuum is

$$D(\alpha)|0\rangle = \mathrm{e}^{-|\alpha|^2/2} \, \mathrm{e}^{\alpha \hat{a}^\dagger} |0\rangle \equiv |\alpha\rangle.$$

i.e., the overall phase convention. □

(b) *Proof.* Firstly, we need to calculate some identities for preparation.

- Verify $D(\alpha)$ is a unitary operator.

$$D^\dagger(\alpha) = \mathrm{e}^{\alpha \hat{a} - \alpha^* \hat{a}^\dagger} = D(-\alpha) = D^{-1}(\alpha). \tag{A}$$

- Calculate $\langle 0|\mathrm{e}^{\gamma \hat{a}^\dagger}|0\rangle$

$$\langle 0|\mathrm{e}^{\gamma \hat{a}^\dagger}|0\rangle = \sum_{k=0}^{\infty} \frac{\gamma^k}{k!} \langle 0|(\hat{a}^\dagger)^k|0\rangle = \frac{\gamma^0}{0!}\langle 0|0\rangle + \sum_{k=1}^{\infty} \frac{\gamma^k}{k!} \sqrt{k} \langle 0|k\rangle + \cdots = 1. \tag{B}$$

  Since $\langle m|n\rangle = \delta_{m,n}$, only $k = 0$ term survives.

- Calculate $\langle m|\alpha\rangle$ and $\langle\alpha|n\rangle$. Expand $|\alpha\rangle$ in terms of number basis

$$|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2} \, \mathrm{e}^{\alpha \hat{a}^\dagger} |0\rangle = \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{a^n}{n!} (\hat{a}^\dagger)^n |0\rangle \xlongequal[\text{Property of creation O.P.}]{(\hat{a}^\dagger)^n = \sqrt{n!}|n\rangle} \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{a^n}{\sqrt{n!}} |n\rangle.$$

  Now we obtain the inner product

$$\langle m|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{a^n}{\sqrt{n!}} \delta_{mn} = \mathrm{e}^{-|\alpha|^2/2} \frac{a^m}{\sqrt{m!}}, \quad \text{similarly} \quad \langle\alpha|n\rangle = \mathrm{e}^{-|\alpha|^2/2} \frac{(a^*)^n}{\sqrt{n!}}. \tag{C}$$

Now, calculate $\langle\alpha|\beta\rangle$. Write them in terms of the displacement operator

$$\langle\alpha|\beta\rangle = \langle 0|D^\dagger(\alpha)D(\beta)|0\rangle = \langle 0|D(-\alpha)D(\beta)|0\rangle \xlongequal{\text{BCH identity}} \mathrm{e}^{\frac{1}{2}(\alpha^{(}\beta-\alpha\beta^*))}\langle 0|D(\beta-\alpha)|0\rangle,$$

where we used Eq. (A). Denote $\gamma=\beta-\alpha$ for simplification, using Eq. (B)

$$\langle 0|D(\beta-\alpha)|0\rangle = \langle 0|D(\gamma)|0\rangle \xlongequal{\text{BCH identity}} \mathrm{e}^{-|\gamma|^2/2}\langle 0|\mathrm{e}^{\gamma\hat{a}^\dagger}|0\rangle = \mathrm{e}^{-|\gamma|^2/2}.$$

Substitute this equation to $\langle\alpha|\beta\rangle$, we have

$$\langle\alpha|\beta\rangle = \mathrm{e}^{\frac{1}{2}(\alpha^*\beta-\alpha\beta^*)}\,\mathrm{e}^{-|\beta-\alpha|^2/2} = \mathrm{e}^{-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2+\alpha^*\beta}.$$

Surround $\langle m|n\rangle$ to the integral kernel $|\alpha\rangle\langle\alpha|$. The integral becomes

$$I = \langle m|\left(\textstyle\int \frac{\mathrm{d}^2\alpha}{\pi}\right)|\alpha\rangle\langle\alpha|n\rangle.$$

Substitute Eq. (C) to the left and right bra-ket group, respectively

$$I = \int\frac{\mathrm{d}^2\alpha}{\pi}\,\mathrm{e}^{-|\alpha|^2}\frac{\alpha^m(\alpha^*)^n}{\sqrt{m!n!}} \xlongequal[m=n]{\alpha=r\mathrm{e}^{\mathrm{i}\theta}} \frac{2}{n!}\int_0^\infty r^{2n+1}\,\mathrm{e}^{-r^2}\,\mathrm{d}r = 1, \quad \text{and} \quad \int\frac{\mathrm{d}^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = \mathbb{1},$$

where the matrix element equals δ_{mn}, then the operator equals the identity on the number basis. □

(c) Denote the position-space wavefunction $\psi_\alpha(x)=\langle x|\alpha\rangle$. Act $\hat{a}$ on it to write the eigenvalue equation

$$\frac{1}{\sqrt{2}}\left(\frac{x}{l_0}+l_0\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_\alpha(x) = \alpha\psi_\alpha(x),$$

based on $\hat{a}|\alpha\rangle=\alpha|\alpha\rangle$. Simplify the ODE

$$\psi_\alpha' - \left(\frac{\sqrt{2}\alpha}{l_0}-\frac{x}{l_0^2}\right)\psi_\alpha = 0, \quad \psi_\alpha(x) = A\exp\left(\frac{\sqrt{2}\alpha}{l_0}x-\frac{x^2}{2l_0^2}\right).$$

Consider the real-space representation, let $\alpha=\alpha_1+\mathrm{i}\alpha_2$, and normalize it. We can obtain

$$\psi_\alpha(x) = \frac{1}{(\pi l_0^2)^{1/4}}\exp\left[-\frac{(x-x_0)^2}{2l_0^2}+\mathrm{i}\frac{p_0x}{\hbar}\right],$$

where $x_0=\sqrt{2}\operatorname{Re}\alpha l_0$, $p_0=\sqrt{2}\hbar\operatorname{Im}\alpha/l_0$. To compare with the Gaussian wave packet: the coherent-state wavefunction is a Gaussian wave packet centered at x_0 with momentum p_0 and width l_0.

(d) Apply the BCH identity, we can obtain

$$\hat{U}^{-1}(t,0)\hat{a}\hat{U}(t,0) = \mathrm{e}^{\mathrm{i}\theta\hat{N}}\hat{a}\,\mathrm{e}^{-\mathrm{i}\theta\hat{N}} = \hat{a}+[\mathrm{i}\theta\hat{N},\hat{a}]+\frac{1}{2!}[\mathrm{i}\theta\hat{N},[\mathrm{i}\theta\hat{N},\hat{a}]]+\cdots = \hat{a}\sum_{n=0}^\infty\frac{(-\mathrm{i}\theta)^n}{n!} = \mathrm{e}^{-\mathrm{i}\theta}\hat{a}.$$

where $\hat{N}=\hat{a}^\dagger\hat{a}$, $\theta=\omega t$, $[\hat{N},\hat{a}]=-\hat{a}$. Concerning $\hat{U}|\alpha\rangle$, which I think a violent expansion is better :-)

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

where $\hat{a}^\dagger\hat{a}|n\rangle=n|n\rangle$ and use the expression of the expansion of $|\alpha\rangle\to|\alpha\,\mathrm{e}^{-\mathrm{i}\omega t}\rangle$. The interpretation of the result said that the complex index $\alpha(t)=\alpha(0)\,\mathrm{e}^{-\mathrm{i}\omega t}$ is the phase-space coordinate, i.e.

$$\langle x(t)\rangle = \sqrt{2}l_0\operatorname{Re}[\alpha(t)] = x_0\cos\theta+\frac{p_0}{m\omega}\sin\theta,\ \langle p(t)\rangle = \frac{\sqrt{2}\hbar}{l_0}\operatorname{Im}[\alpha(t)] = p_0\cos\theta-m\omega x_0\sin\theta,$$

enable the coherent-state center follows the classical harmonic-oscillator trajectory $(x(t),p(t))$ with frequency ω.

Problem 2.5 (Perturbed harmonic oscillator). Consider the following Hamiltonian:

$$\hat{H} = \frac{\hbar^2 \hat{k}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 + \mathcal{E}(t)\hat{x},$$

where the last term is assumed to be a perturbation.

(a) For time-independent $\mathcal{E}(t) = \mathcal{E}_0$, compute the ground state energy and wavefunction up to the second-order correction with perturbation theory. Solve the model exactly and compare the exact result with the perturbative result.

(b) For time-dependent $\mathcal{E}(t)$, compute the transition probability (as a function of t) from the unperturbed ground state $|0^{(0)}\rangle$ to an unperturbed excited state $|n^{(0)}\rangle$ up to the second order pertubation. Further apply the general result to the case of $\mathcal{E}(t) = \mathcal{E}_0 \sin \Omega t$, interpret what you obtain.

⋆ (c) (optional) Solve the time-dependent model exactly and compare the exact result with the perturbative result. (Hint: Consider $\hat{a}(t)$ and $\hat{n}(t)$ in the Heisenberg picture, also see Problem 3(d) above.)

Solution.

(a) **Perturbation theory**

The coordinate operator can be written in terms of annihilation and creation operators

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger).$$

i. First-order energy

$$E_0^{(1)} = \langle 0^{(0)}|\mathcal{E}_0\hat{x}|0^{(0)}\rangle = 0.$$

where $\langle 0|\hat{a}|0\rangle = \langle 0|\hat{a}^\dagger|0\rangle = 0$.

ii. Second-order energy

$$E_0^{(2)} = \sum_{k\neq 0} \frac{|\langle k^{(0)}|\mathcal{E}_0\hat{x}|0^{(0)}\rangle|^2}{E_0^{(0)} - E_k^{(0)}} \xlongequal{\text{only } k=1 \text{ survives}} \frac{\mathcal{E}_0^2\hbar}{2m\omega} \frac{|\langle 1^{(0)}|1^{(0)}\rangle|^2}{\frac{1}{2}\hbar\omega - \frac{3}{2}\hbar\omega} = -\frac{\mathcal{E}_0^2}{2m\omega^2}.$$

So, the perturbative result of the ground state energy up to second order gives

$$E_0 \approx \frac{1}{2}\hbar\omega + 0 - \frac{\mathcal{E}_0^2}{2m\omega^2} = \frac{1}{2}\hbar\omega - \frac{\mathcal{E}_0^2}{2m\omega^2}.$$

The perturbative result of the ground state wavefunction up to second order gives

$$\begin{aligned}
|0\rangle \approx |0^{(0)}\rangle &+ \underbrace{\sum_{k\neq 0}|k^{(0)}\rangle \frac{\langle k^{(0)}|\mathcal{E}_0\hat{x}|0^{(0)}\rangle}{E_0^{(0)} - E_k^{(0)}}}_{k=1 \text{ survives}} + \underbrace{\sum_{k\neq 0}\sum_{l\neq 0}|k^{(0)}\rangle \frac{\langle k^{(0)}|\mathcal{E}_0\hat{x}|l^{(0)}\rangle\langle l^{(0)}|\mathcal{E}_0\hat{x}|0^{(0)}\rangle}{(E_0^{(0)} - E_k^{(0)})(E_0^{(0)} - E_l^{(0)})}}_{l=1,\,k=2 \text{ survive}} \\
&- \underbrace{\sum_{k\neq 0}|k^{(0)}\rangle \frac{\langle k^{(0)}|\mathcal{E}_0\hat{x}|0^{(0)}\rangle\langle 0^{(0)}|\mathcal{E}_0\hat{x}|0^{(0)}\rangle}{(E_0^{(0)} - E_k^{(0)})^2}}_{\text{Vanish}} - \underbrace{\frac{1}{2}|0^{(0)}\rangle \sum_{k\neq 0} \frac{|\langle k^{(0)}|\mathcal{E}_0\hat{x}|0^{(0)}\rangle|^2}{(E_0^{(0)} - E_k^{(0)})^2}}_{k=1 \text{ survives}} \\
&= |0\rangle - \alpha|1\rangle - \frac{\alpha^2}{\sqrt{2}}|2\rangle - \frac{\alpha^2}{2}|0\rangle,
\end{aligned}$$

where $\alpha = \frac{\mathcal{E}_0}{\sqrt{2m\hbar\omega^3}}$.

Exact solution

The Hamiltonian can be written as

$$\hat{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(\hat{x} + \frac{\mathcal{E}_0}{m\omega^2}\right)^2 - \frac{\mathcal{E}_0^2}{2m\omega^2}.$$

shows that under this perturbation term, the spectrum is that of an H.O. center at $x_0 = -\frac{\mathcal{E}_0}{m\omega^2}$, and the eigenvalue shifted a constant of $-\frac{\mathcal{E}_0^2}{2m\omega^2}$. So, the exact ground state energy and wavefunction are

$$E_0^{\text{exact}} = \frac{1}{2}\hbar\omega - \frac{\mathcal{E}_0^2}{2m\omega^2}, \quad \psi_0^{\text{exact}}(x) = \phi_0\left(x + \frac{\mathcal{E}_0}{m\omega^2}\right) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{m\omega}{2\hbar}\left(x + \frac{\mathcal{E}_0}{m\omega^2}\right)^2\right],$$

where $\phi_0(x)$ is the unperturbed H.O. ground-state wavefunction (centered at $x = 0$).

Comparison

The exact and perturbative (up to second order) energies agree. The exact wavefunction is the H.O. ground state shifted by $-\frac{\mathcal{E}_0}{2\omega^2}$ and the perturbative corrections reproduce the expansion of that displacement.

(b) The system starts in the unperturbed ground state $|\psi(0)\rangle = |0^{(0)}\rangle$. $|\psi(t)\rangle$ can be expanded as

$$|\psi(t)\rangle = \sum_n |n^{(0)}\rangle\langle n^{(0)}|\psi(t)\rangle \xlongequal{\text{Interaction picture}} \sum_n c_n(t)\, \mathrm{e}^{-\mathrm{i}E_n^{(0)}t/\hbar}|n^{(0)}\rangle.$$

Thus, the probability to find the system in the unperturbed eigenstate $|n^{(0)}\rangle$ at time t is The probability is the square of the projection of $|n^{(0)}\rangle$ to $|\psi(t)\rangle$

$$P_{0\to n}(t) = |\langle n^{(0)}|\psi(t)\rangle|^2 = |c_n(t)|^2.$$

where $c_n(t)$ satisfies the Dyson series

$$c_n(t) = c_n^{(0)}(t) + c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots,$$

we need to calculate the first and second orders.

i. The first order term $c_n^{(1)}(t)$

Substitute the expansion of $|\psi(t)\rangle$ to the Schrödinger equation, then inner product with $\langle m|$, we can obtain

$$\mathrm{i}\hbar\dot{c}_m(t) = \sum_n V_{mn}(t)\,\mathrm{e}^{\mathrm{i}\omega_{mn}t}c_n(t),$$

where $V_{mn}(t) = \langle m|\hat{V}(t)|n\rangle$, $\omega_{mn} \equiv (E_m - E_n)/\hbar$, and the relation $\hat{H}_0|n\rangle = E_n|n\rangle$ and the orthonormality are applied. Since we need to keep the order of V the same on LHS and RHS, i.e., handle the map of different orders of corrections from LHS to RHS, we insert the parameter λ

$$c_n(t) = \sum_{k\geq 0} \lambda^k c_n^{(k)}(t).$$

Then substitute it into the Schrödinger equation, we can have

$$\mathrm{i}\hbar\sum_{k\geq 0}\lambda^k\dot{c}_n^{(k)}(t) = \sum_{l\geq 0}\lambda^{l+1}\sum_m V_{nm}(t)\,\mathrm{e}^{\mathrm{i}\omega_{nm}t}c_m^{(l)}(t).$$

Since $c_n(0) = \langle n|0\rangle = \delta_{n0} \equiv c_n^{(0)}(t)$, for the coefficient of λ^1

$$\mathrm{i}\hbar\dot{c}_n^{(1)}(t) = \sum_m V_{nm}(t)\,\mathrm{e}^{\mathrm{i}\omega_{nm}t}c_m^{(0)}(t) = V_{n0}(t)\,\mathrm{e}^{\mathrm{i}\omega_{n0}t}.$$

Integral over t, we can obtain

$$c_n^{(1)}(t) = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' V_{n0}(t')\,\mathrm{e}^{\mathrm{i}\omega_{n0}t'} \xlongequal{\hat{V}(t)=\mathcal{E}(t)\hat{x}} -\frac{\mathrm{i}}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}\int_0^t \mathrm{d}t'\mathcal{E}(t')\,\mathrm{e}^{\mathrm{i}\omega t'} \equiv c_1^{(1)}(t),$$

and the first-order transition probability to $|n\rangle = |1\rangle$ is

$$P_{0\to 1}^{(1)}(t) = |c_n^{(1)}(t)|^2 = \frac{1}{2m\omega\hbar}\left|\int_0^t \mathrm{d}t'\mathcal{E}(t')\,\mathrm{e}^{\mathrm{i}\omega t'}\right|^2,$$

where due to $\langle n|\hat{x}|0\rangle$ is nonzero only for $n = 1$.

ii. The second order term $c_n^{(2)}(t)$

Similarly, the general second-order amplitude is

$$c_n^{(2)}(t) = -\frac{1}{\hbar^2}\sum_m \langle n|\hat{x}|m\rangle\langle m|\hat{x}|0\rangle \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\mathcal{E}(t')\mathcal{E}(t'')\,\mathrm{e}^{\mathrm{i}\omega_{nm}t'}\,\mathrm{e}^{\mathrm{i}\omega_{m0}t''}.$$

Since $m = 1$, and n can be valued as 0 or 2, then we have

$$c_2^{(2)}(t) = \frac{1}{\sqrt{2}m\hbar\omega}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\mathcal{E}(t')\mathcal{E}(t'')\,\mathrm{e}^{\mathrm{i}\omega(t'+t'')},$$
$$c_0^{(2)}(t) = \frac{1}{2m\hbar\omega}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\mathcal{E}(t')\mathcal{E}(t'')\,\mathrm{e}^{-\mathrm{i}\omega(t'-t'')}.$$

and the corresponding second-order transition probabilities are

$$P_{0\to 2}^{(2)} = |c_2^{(2)}(t)|^2 = \frac{1}{2(m\hbar\omega)^2}\left|\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\mathcal{E}(t')\mathcal{E}(t'')\,\mathrm{e}^{\mathrm{i}\omega(t'+t'')}\right|^2,$$
$$P_{0\to 0}^{(2)} = |c_0^{(2)}(t)|^2 = \frac{1}{(2m\hbar\omega)^2}\left|\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\mathcal{E}(t')\mathcal{E}(t'')\,\mathrm{e}^{-\mathrm{i}\omega(t'-t'')}\right|^2.$$

Now apply $\mathcal{E}(t) = \mathcal{E}_0\sin(\Omega t)$, the first-order and second-order amplitude to $|1\rangle$ are

$$c_1^{(1)}(t) = -\frac{\mathcal{E}_0}{2\hbar}\sqrt{\frac{\hbar}{2m\omega}}\left[\frac{\mathrm{e}^{\mathrm{i}(\omega+\Omega)t}-1}{\omega+\Omega} - \frac{\mathrm{e}^{\mathrm{i}(\omega-\Omega)t}-1}{\omega-\Omega}\right],$$
$$c_2^{(2)}(t) = \frac{\sqrt{2}\mathcal{E}_0^2}{8m\hbar\omega}\left[\frac{\mathrm{e}^{\mathrm{i}(\omega-\Omega)t}-1}{\omega-\Omega} - \frac{\mathrm{e}^{\mathrm{i}(\omega+\Omega)t}-1}{\omega+\Omega}\right]^2,$$
$$c_0^{(2)}(t) = \frac{\mathcal{E}_0^2}{8m\hbar\omega(\omega^2-\Omega^2)}\Bigg\{2\omega t + \frac{\mathrm{i}}{2\Omega}\Big[(\omega+\Omega)\,\mathrm{e}^{-2\mathrm{i}\Omega t} - (\omega-\Omega)\,\mathrm{e}^{2\mathrm{i}\Omega t} - 2\Omega\Big]$$
$$+ 2\,\mathrm{i}\Omega\left(\frac{1-\mathrm{e}^{-\mathrm{i}(\omega+\Omega)t}}{\omega+\Omega} - \frac{1-\mathrm{e}^{-\mathrm{i}(\omega-\Omega)t}}{\omega-\Omega}\right)\Bigg\}.$$

Interpretation If $\Omega \approx \omega$, then we will find that $|c_1^{(1)}|, |c_2^{(2)}| \propto t^2$ at short times. In the long-time limit, this becomes the usual resonance: the transition rate arrives at the maximum value. Of course, we can know the trend of $c_0^{(2)}$ from the relation $|c_0^{(2)}|^2 \approx 1 - |c_1^{(1)}|^2 - |c_2^{(2)}|^2$.

(c) The Heisenberg EOM for $\hat{a}(t)$ is

$$\frac{\mathrm{d}\hat{a}}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{a}] = -\mathrm{i}\omega\hat{a} + \frac{\mathrm{i}}{\hbar}[\mathcal{E}(t)\hat{x}, \hat{a}] = -\mathrm{i}\omega\hat{a} - \mathrm{i}\frac{\mathcal{E}(t)}{\sqrt{2m\hbar\omega}},$$

where $[\hat{x}, \hat{a}] = -\sqrt{\frac{\hbar}{2m\omega}}$. So, the solution is

$$\hat{a}(t) = \hat{a}(0)\,\mathrm{e}^{-\mathrm{i}\omega t} - \frac{\mathrm{i}}{\sqrt{2m\hbar\omega}}\int_0^t \mathrm{d}t'\mathcal{E}(t')\,\mathrm{e}^{-\mathrm{i}\omega(t-t')}.$$

In Heisenberg picture, the state is fixed at $|0\rangle$, but $\hat{a}(t)$ is time-dependent; In Schrödinger picture, the state evolves. For a linear driving term, the ground state evolves into a coherent state $|\alpha(t)\rangle$ satisfying

$$\hat{a}|\psi(t)\rangle = \alpha(t)|\psi(t)\rangle,$$

where $\alpha(t)$ is the expectation value $\langle\hat{a}(t)\rangle$ in the Heisenberg picture with initial state $|0\rangle$

$$\alpha(t) = \langle 0|\hat{a}(t)|0\rangle = -\frac{\mathrm{i}}{\sqrt{2m\hbar\omega}}\,\mathrm{e}^{-\mathrm{i}\omega t}\int_0^t \mathcal{E}(t')\,\mathrm{e}^{\mathrm{i}\omega t'}\,\mathrm{d}t'.$$

Then, the probability is expressed as

$$P_{0\to n}(t) = |\langle n|\alpha(t)\rangle|^2 = \left|\mathrm{e}^{-|\alpha|^2/2}\sum_{k=0}^{\infty}\frac{a^k}{\sqrt{k!}}\langle n|k\rangle\right|^2 = \mathrm{e}^{-|\alpha(t)|^2}\frac{|\alpha(t)|^{2n}}{n!}.$$

For small $\mathcal{E}_0$, $\alpha(t)$ is small, so

$$P_{0\to 1} \approx |\alpha(t)|^2, \quad \text{and} \quad P_{0\to 2} \approx \frac{1}{2}|\alpha(t)|^4.$$

So perturbation theory to second order matches the exact expansion after expanding in terms of $\alpha(t)$.

Problem 2.6 (Quantum foundations). Referring to the reading material "Addressing the quantum measurement problem" by Sean M. Carroll (attached below), which of the following types of theories is your favorite? (Maybe tell me why? Or do you have your own alternative theory?) 1. epistemic; 2. hidden-variable; 3. objective-collapse; 4. Everett's many-worlds.

Solution. My favorite theory is **Everett's Many-Worlds theory**.
What makes this interpretation most appealing is its simplicity and consistency. It treats the wavefunction as a complete description of reality that always evolves according to the Schrödinger equation—no mysterious collapses or hidden mechanisms are required. In this view, measurement is just a physical interaction that entangles a system with its environment, causing the universal wavefunction to branch into different components, each corresponding to a possible outcome.
Of course, the idea of a constantly branching multiverse may initially sound extravagant. However, modern decoherence theory makes it more tangible by explaining why these branches become effectively independent and why we only experience one of them. I also appreciate that Many-Worlds doesn't add extra postulates—rather, it takes quantum mechanics at face value and follows its logic wherever it leads.
Nonetheless, this interpretation isn't free of problems. The biggest challenge is the probability issue: if every outcome occurs somewhere, how do we make sense of the Born rule? And although it's admittedly strange to think there could be countless versions of ourselves living in parallel worlds, I still find Many-Worlds the most compelling. It offers a clean and coherent picture of quantum reality and addresses the measurement problem head-on, without compromise.

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Problem 2.1 (Function space).

Solution (By TA).

(a)

$$\int_A |\psi(x)|^2 \, \mathrm{d}x$$

To prove the three properties: Conjugate, Linearity, and Positive-definiteness.

(b) Fourier bases.

i. $(-\infty, +\infty)$, the wavefunction $\{\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}kx}\}$, $\alpha \sim k \in \mathbb{R}$. The normalization

$$\int_{-\infty}^{+\infty} \psi_k(x)^* \psi_k(x) \, \mathrm{d}x = \delta(k - k'),$$

The orthonormality

$$\int_{-\infty}^{+\infty} \psi_k(x) \psi_k(x') \, \mathrm{d}k = \delta(x - x')$$

Remark (For $\{|\alpha\rangle\}$). Orthonormality

$$\langle \alpha|\alpha'\rangle = \delta_{\alpha\alpha'} \to \int \mathrm{d}x \alpha^*(x)\alpha'(x) = \delta_{\alpha\alpha'}$$

Completeness

$$\sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{1} \to \sum_\alpha \langle x|\alpha\rangle\langle\alpha|x'\rangle = \delta(x - x')$$

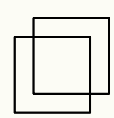
Remark (Or Haar basis:).

$$\phi(x) = \begin{cases} 1, & 0 \le x \le 1, \\ 0, & \text{otherwise} \end{cases}, \quad \psi(x) = \begin{cases} 1, & 0 \le x \le \frac{1}{2}, \\ -1, & \frac{1}{2} \le x < 1, \\ 0, & \text{otherwise} \end{cases}, \quad \psi_{j,k}(x) = 2^{j/2}\psi(2^j x - k), \quad j, k \in \mathbb{Z}$$

ii. $[-1, 1]$

The wavefunction

$$\mathrm{e}^{\mathrm{i}kx}$$



Δx

Then, $k \cdot \Delta x = n \cdot 2\pi$, $k_n = n\pi$. The basis

$$\left\{ \frac{1}{\sqrt{2}} \mathrm{e}^{\mathrm{i}n\pi x} \right\}, \quad \alpha \sim n$$

iii. $(0, +\infty)$. The basis

$$\left\{ \sqrt{\frac{2}{\pi}} \cos(kx), \quad \alpha \sim k \in \mathbb{R}^+ \right\}$$

Problem 2.2 (Strum-Liouville theory).

Solution (By TA).

(a) Actually, the problem is something like

$$\langle u|v\rangle = \int_{x_1}^{x_2} u^*(x)v(x)\omega(x)\,\mathrm{d}x, \quad \text{where} \quad \alpha(x),\ \beta(x),\ \gamma(x) \in \mathbb{R}$$

The operator

$$\mathcal{L} = \omega^{-1}\frac{\mathrm{d}}{\mathrm{d}x}\left(\omega\alpha\frac{\mathrm{d}}{\mathrm{d}x}\right) + \gamma = \alpha\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \omega^{-1}\frac{\mathrm{d}}{\mathrm{d}x}(\omega\alpha) + \gamma$$

Then,

$$\alpha(x)y'' + \beta(x)y' + \gamma(x)y = \lambda y, \quad \beta(x) = \omega^{-1}\frac{\mathrm{d}}{\mathrm{d}x}(\omega\alpha) \Rightarrow \frac{\beta\omega\alpha}{\alpha} = \frac{\mathrm{d}(\omega\alpha)}{\mathrm{d}x}, \Rightarrow \omega = \frac{C}{\alpha}\,\mathrm{e}^{\int\frac{\beta}{\alpha}\mathrm{d}x}$$

Or, it can be a extension of the inner product.

i. $\omega(\alpha) = C\,\mathrm{e}^{-x^2} \sim \mathrm{e}^{-x^2}$ ii. $\omega(x) = C \sim 1.$ iii. $\omega(x) = C\,\mathrm{e}^{-x} \sim \mathrm{e}^{-x}.$

(b) Calculate directly

$$\langle u|\mathcal{L}v\rangle = \langle\mathcal{L}u|v\rangle, \quad \omega \in \mathbb{R}$$

Then, we will obtain

$$\omega\alpha(u^*v' - u'^*v)\big|_{x_1}^{x_2}, \quad \omega(x_2)\alpha(x_2) = \omega(x_1)\alpha(x_1) = 0$$

i. $(-\infty, +\infty)$

$$H_n(x) = (-1)^n\,\mathrm{e}^{x^2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\,\mathrm{e}^{-x^2}, \quad \mathrm{e}^{-t^2+2xt} = \sum_{n=0}^{\infty}\frac{k\ln(x)}{n!}t^n$$

ii. $[-1, 1]$

$$P_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}}{\mathrm{d}x}(x^2-1)^n, \quad \frac{1}{\sqrt{t^2-2xt+1}} = \sum_{n=0}^{\infty}P_n(x)t^n$$

iii.

$$L_n(x) = \frac{1}{n!}\,\mathrm{e}^x\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(\mathrm{e}^{-x}x^n\right), \quad \frac{1}{1-t}\,\mathrm{e}^{-\frac{tx}{1-t}} = \sum_{n=0}^{\infty}\ln(x)t^n$$

(c) Write the eigenfunctions

$$\mathcal{L}v_i = \lambda_i v_i, \quad \langle\mathcal{L}v_1|v_2\rangle = \langle v_1|\mathcal{L}v_2\rangle$$

then,

$$(\lambda_1-\lambda_2)\langle v_1|v_2\rangle = 0, \quad \lambda_1 \neq \lambda_2, \Rightarrow \langle v_1|v_2\rangle = 0$$

Remark. Actually, an arbitrary function can be exapnded as

$$f(x) = c_0 1 + c_1 x + c_2 x^2 + \cdots + c_n x^n + \cdots$$

when one write it, he assumed that

$$\{1, x, x^2, x^3, \cdots, x^n, \cdots\}$$

has constructed a basis of $f(x)$. But they are not orthonormal. We need to make the orthonormality between every two elements by Scimet orthonormality, for example, in range $[0,1]$

$$\int_{A\sim\mathbb{R}} \mathrm{d}x\varphi^*(x)\chi(x) = \langle\varphi|\chi\rangle$$

If the range is $\mathbb{R}$, the integral $\int_{\mathbb{R}} x^{n+m}$ makes no sense. We need to make it square integral on the real axis by multiplying, it would be something like a Gaussian function $\omega(x) \sim \mathrm{e}^{-x^2}$. Then, the integral becomes

$$\int_{\infty} \mathrm{d}x\omega(x)x^{n+m} = 0$$

To "kill" the functioin on both sides, or add the weight function $\omega = \mathrm{e}^{-x}$ to kill the function on one side.

Problem 2.3 (Linear map).

Solution (By TA).

(a) $L:\ V \to W$. Vector space $f(u)$

  i. $+$: identity, inverse, commutativity; associativity: $(f_1+f_2)+f_3 = \cdots$

  ii. $\times$: $a(bf_1) = (ab)f_1$

  iii. $+\times$: $a(f_1+f_2)$, $(a+b)f_1$

(b) V and W are two matrix, the transformation between is a matrix, actually, a linear map. The matrix is JUST A TOOL.

$$\boldsymbol{v} = \sum_{i=1}^{\dim(V)} c_i\boldsymbol{v}_i$$

The core formula is

$$f(v_i) = \sum_{j=1}^{n} w_i F_{ji} \equiv \boldsymbol{u}_i$$

Which can be written into matrix

$$(w_1, w_2, \cdots, w_n)\begin{pmatrix} F_{11} & \cdots & F_{1n} \\ \vdots & \ddots & \vdots \\ F_{m1} & \cdots & F_{mn} \end{pmatrix} = (u_1, u_2, \cdots, u_n)$$

Uniqueness: The two vectors are unique, then, the matrix is unique.

(c) For example

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \sum_{i=1}^{4} f_i M_i = a\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + b\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + d\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

We can write

$$A = \{F^{kl}, 1 \le k \le n,\ 1 \le l \le m\}, \quad F^{kl}(\boldsymbol{V}_i) = \boldsymbol{W}_j\delta_{ik}\delta_{jl}$$

(d) By definition

$$\ker(f) = \{v \in V | f(v) = 0\}$$
$$\mathrm{im}(f) = \{w \in W | w = f(v), v \in V\}$$
$$\dim(\ker(f)) = s, \quad \dim(\mathrm{im}(f)) = m, \quad \dim(V) = g$$

and prove $s + m = g$. We can write

$$S = \{v_1, v_2, \ldots, v_s\},\ f(v) = 0, \quad M = \{v_{s+1}, \ldots, v_g\},\ f(v) = w$$

For arbitrary v, $f(v) = 0$, it means a linear combination

$$v = \sum_{i=1}^{s} c_i v_i, \quad v_i \in S$$

Then, $f(v) = w \in W \Rightarrow v = \sum_{i=g+1}^{g} c_i v_i$, $v_i \,\mathrm{im}\, M$. Substitute

$$f(\boldsymbol{v}) = f\left(\sum_{i=s+1}^{g} c_i \boldsymbol{v}_i\right) = \sum_{i=s+1}^{g} c_i f(\boldsymbol{v}_i) = \sum_{i=s+1}^{g} c_i \underbrace{f(\boldsymbol{v}_2)}_{w_i}$$

Then, consider v_{1--3} and w_{1--3}. Let

$$w_1 = a w_2 + b w_3, \quad f(v_1) = a f(v_2) + b f(v_3), \quad = v_1 = a v_2 + b v_3$$

Then, we can prove the dim of W-space. $s + m = g$.

Interuption

$$(w_1, w_2, \cdots, w_n) \begin{pmatrix} F_{11} & \cdots & F_{1n} \\ \vdots & \ddots & \vdots \\ F_{m1} & \cdots & F_{mn} \end{pmatrix} = (u_1, u_2, \cdots, u_n)$$

where the top three cols of F is 0.

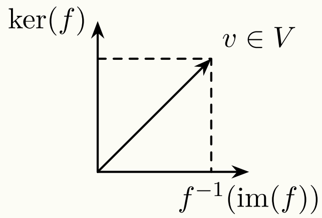
Remark. $f : V \to W$. The kernel.

$$\ker(f) = \{v \in V | f(v) = 0_w\}$$

conduct the linear space. The linear space always is

$$(v, F) = (+, \times)$$

about elements or operations. If v_1, $v_2 \in \ker(f)$ then $a v_1 + b v_2 \in \ker(f)$, a, $b \in F$. i.e., $\ker$ is a linear space, also, the $\mathrm{im}(f) = \{w \in W | \exists u \in V, w = f(u)\} < w$. Also, we can separate an arbitrary vector in V



Problem 2.4 (Coherent states).

Solution (By TA).

Baker-Campbell-Hausdorff

$$D(\alpha) \equiv \mathrm{e}^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = \mathrm{e}^{\alpha\hat{a}^\dagger}\,\mathrm{e}^{-\alpha^*\hat{a}}\,\mathrm{e}^{-\frac{1}{2}[\alpha\hat{a}^\dagger, \alpha^*\hat{a}]}$$

(a) By definition

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

Expand it

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_i|n\rangle$$

Then,

$$\hat{a}|\alpha\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle = \alpha\sum_{n=0}^{\infty} c_n|n\rangle$$

The coefficients

$$c_{n+1}\sqrt{n+1} = \alpha c_n, \quad c_n = \frac{\alpha^n}{\sqrt{n!}}c_0$$

Then, the coherent state can be written as the sum of fork basis

$$|\alpha\rangle = N\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

where

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

So,

$$|\alpha\rangle = N\sum_{n=0}^{\infty}\frac{(\alpha\hat{a}^\dagger)^n}{n!}|0\rangle$$

(b) Normalization $\langle\alpha|\alpha\rangle_\alpha = 1$, insert the operator

$$\langle\hat{a}^\dagger\hat{a}|\alpha\rangle = (\hat{a}|\alpha\rangle)^\dagger\hat{a}|\alpha\rangle = |\alpha|^2$$

Then,

$$|\alpha\rangle = D(\alpha)|0\rangle$$

Finally,

$$\mathrm{e}^{-\frac{1}{2}|\alpha|^2}\mathrm{e}^{\alpha\hat{a}^\dagger}\cancelto{\mathbb{1}}{\mathrm{e}^{-\alpha^*\hat{a}}}|0\rangle \to \mathbb{1} + \hat{a}$$

(c) $\{|\alpha\rangle|\alpha\in\mathbb{C}\}$ overcomplete. $\langle\alpha|\beta\rangle \neq 0$, $\int\frac{\mathrm{d}^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = \mathbb{1}$.

$$\langle n|\int\frac{\mathrm{d}^2\alpha}{\pi}|\alpha\rangle\langle\alpha|m\rangle = \delta_{nm} = \frac{1}{\pi}\frac{1}{\sqrt{n!m!}}\int_0^\infty \mathrm{d}r r^{n+m+1}\,\mathrm{e}^{-r^2}\int_0^{2\pi}\mathrm{d}\varphi\,\mathrm{e}^{\mathrm{i}\varphi(n-m)} = 2\pi\delta_{nm} \xlongequal{n=m} \delta_{nm}$$

(d) $\psi_\alpha(x) = \langle x|\alpha\rangle$.

$$\langle x|\hat{a}|\alpha\rangle = \alpha\psi_\alpha(x) = \frac{1}{\sqrt{2}}\left(\frac{x}{l_0} + l_0\,\partial_x\right)\psi_\alpha(x)$$

It is an ODE. The solution is

$$\psi_\alpha(x) = k\exp\left\{\left(-\frac{1}{2}\frac{x}{l_0} - \sqrt{2}\,\mathrm{Re}[\alpha]\right)^2 + \mathrm{i}\sqrt{2}\,\mathrm{Im}[\alpha]\frac{x}{l_0}\right\}$$

where $k = (\pi l_0^2)^{-1/4}$.

The exponitional term

$$\mathrm{e}^{\frac{(x-x_0)^2}{2\sigma^2} + \mathrm{i}\frac{p_0}{\hbar}x}$$

The first part means the center of the wavefunction is x_0; The second term: By Fourier transformation

$$\tilde{\psi}_\alpha(p) = N\int_{-\infty}^{\infty}\psi_\alpha(x)\,\mathrm{e}^{-\mathrm{i}px/\hbar}\,\mathrm{d}x \propto \mathrm{e}^{-\frac{(p-p_0)^2}{2\sigma_p^2} + \mathrm{i}x_0\frac{p}{\hbar}}$$

Means that in the momentum space, centered with p_0. The position and momentum is closely connected with each other.

Actually, for coherent state, it should be $\mathrm{e}^{-\frac{1}{2a}(x-x_c)^2}$ where $a = \Delta x$, corresponding to Δp. If define $l_0 = \sqrt{\frac{\hbar}{m\omega}}$, then $x \sim l_0$, $k \sim l_0^{-1}$.

Coherent state vs squeezed state. Usually, $\langle\alpha|\beta\rangle \neq 0$, then define $P(\alpha) = |\langle\alpha|\alpha_0\rangle|^2$. The wavepack's centre is (the real part of on x axis, or the image part of k axis) α_0.

Problem 2.5 (Perturbed harmonic oscillator).

Solution (By Li Jian).

(a) Time-independent: $V = \epsilon_0\hat{x} = \frac{\epsilon_0}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger)$. We can consider it as an electric field: the oscillator have a positive charge, then the electric potential is gradient.

In classical situation, just change the equilibirum point. In quantum situation, to the exact solution, just merge

$$H = \frac{1}{2}m\omega^2(x - x_0)^2 + C$$

Denote $\hat{\tilde{x}} = \hat{x} - x_0$, then $[\hat{\tilde{x}}, \hat{k}] = \mathrm{i}$. The annihilation operator

$$\hat{\tilde{a}} = (\hat{x} + \mathrm{i}\hat{k})/\sqrt{2}, \quad \hat{\tilde{a}}|0\rangle = 0, \quad (a^\dagger)^n|0\rangle \sim |n\rangle$$

The matrix element

$$V_{mn} = \langle m|\hat{V}|n\rangle = V_0(\sqrt{n}\delta_{m+1,n} + \sqrt{m}\delta_{m,n+1})$$

After pertubation, the state from ground state

$$|0\rangle \to |g\rangle = |0\rangle + |g^{(1)}\rangle + |g^{(2)}\rangle + \cdots$$

The energy

$$E_g = E_0 + E_g^{(1)} + E_g^{(2)} + \cdots$$

where $E_0 = \frac{1}{2}\hbar\omega$. The result

$$
\begin{aligned}
E_g^{(1)} &= V_{00} = \langle 0|\hat{V}|0\rangle = 0, \quad \text{Since the 00-matrix element is excluded} \\
E_g^{(2)} &= \sum_{n=1}^{\infty} -\frac{V_{00}V_{n0}}{E_n - E_0} = -\frac{V_0^2}{\hbar\omega} \\
|g^{(1)}\rangle &= \sum_{n=1}^{\infty} |n\rangle\left(-\frac{V_{n0}}{E_n - E_0}\right) = -\frac{V_0}{\hbar\omega}|1\rangle \\
|g^{(2)}\rangle &= \sum_{n=1}^{\infty} |n\rangle\left[-\frac{1}{E_n - E_0}\left(\frac{V_{n0}V_{00}}{E_n - E_0} - \sum_{n=1}^{\infty}\frac{V_{nm}V_{mn}}{E_m - E_0}\right)\right] = \frac{1}{\sqrt{2}}\left(\frac{V_0}{\hbar\omega}\right)^2|2\rangle
\end{aligned}
$$

The exact solution: Since the Hamiltonian

$$
\hat{H} = \frac{1}{2}\hbar\omega\left[\left(\frac{\hat{x}}{l_0}\right)^2 + (l_0\hat{k})^2\right] + \sqrt{2}V_0\frac{\hat{x}}{l_0} = \frac{1}{2}\hbar\omega\left[\left(\frac{\hat{x}}{l_0} + \sqrt{2}\frac{V_0}{\hbar\omega}\right)^2 + (l_0\hat{k})^2\right] - \frac{V_0^2}{\hbar\omega}
$$

where $l_0 = \sqrt{\frac{\hbar}{m\omega}}$, $V_0 = l_0\epsilon_0/\sqrt{2}$. The ground energy of this Hamiltonian is

$$
\tilde{E}_0 = \underbrace{\frac{1}{2}\hbar\omega}_{E_0} - \frac{V_0^2}{\hbar\omega}
$$

We can consider $|0\rangle$ as a coherent state

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

The wave function $\mathrm{e}^{-\frac{1}{2}(x-0)^2}$, $(a^\dagger)^2|0\rangle = \sqrt{2}|2\rangle$.

$$
|g\rangle = |\alpha = -?\frac{V_0}{\hbar\omega}\rangle = \mathrm{e}^{\alpha\hat{a}^\dagger}|0\rangle = \mathrm{e}^{-\frac{V_0}{\hbar\omega}a^\dagger}|0\rangle = |0\rangle + \left(-\frac{V_0}{\hbar\omega}|1\rangle\right) + \frac{1}{2}\left(-\frac{V_0}{\hbar\omega}\right)^2\sqrt{2}|2\rangle
$$

, i.e., the coherent state which center is shifted, and the exact solutions and pertubation solutions are corresponding.

(b) To simplify, we need to use the interaction picture

$$
V^{\mathsf{I}}(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}\hat{V}^{\mathsf{S}}(t)\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t} = \hbar V(t)(\hat{a}\,\mathrm{e}^{-\mathrm{i}\omega t} + \hat{a}^\dagger\,\mathrm{e}^{\mathrm{i}\omega t})
$$

where $\hat{H}_0$ contains $a^\dagger a$ and $\hat{V}^{\mathsf{S}}(t)$ contains $\hat{a} + \hat{a}^\dagger$, $v(t) = \frac{\epsilon(t)l_0}{\sqrt{2}\hbar}$. The coefficient

$$
\underset{0\to n}{c_n^{(1)}}(t) = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\langle n|\hat{V}^{\mathsf{I}}(t')|0\rangle = -\,\mathrm{i}\mu_\omega(t)\delta_{n,1}
$$

where $\mu_\omega(t) = \int_0^t \mathrm{d}t' v(t')\,\mathrm{e}^{\mathrm{i}\omega t'}$. The amplitude of second jump is

$$
c_n^{(2)}(t) = (-\frac{\mathrm{i}}{\hbar})^2\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\langle n|\hat{V}^{\mathsf{I}}(t_1)\hat{V}^{\mathsf{I}}(t_2)|0\rangle = -\left[\frac{1}{2}|\mu_\omega(t)|^2 - \mathrm{i}C\right]\delta_{n,0} + (-\,\mathrm{i})^2\frac{\mu_\omega^2(t)}{\sqrt{2}}\delta_{n,2}
$$

At $t = 0$, the evolution of $|0\rangle$ under $\hat{U}(t)$

$$
|0\rangle \xrightarrow{\hat{U}(t)} |?\rangle
$$

Since the Heisenberg time-dependent operator

$$\hat{a}(t) \equiv \hat{U}(t)\hat{a}\hat{U}(t)^{-1} \equiv f_t(\hat{a})$$

To solve it, back to the Heisenberg equation

$$\frac{\mathrm{d}}{\mathrm{d}t} f_t(\hat{a}) = g_t(\hat{a})$$

where $\mathrm{i}\frac{\mathrm{d}U(t)}{\mathrm{d}t} = HU$, $-\mathrm{i}\left.\frac{\mathrm{d}U(t)}{\mathrm{d}t}\right|^{-1} = U(t)^{-1}H(t)$. It tells

$$\hat{a}\hat{U}(t) = \hat{U}(t)f_t(\hat{a})$$

Consider

$$\hat{a}(\hat{U}(t)|0\rangle) = \hat{U}(t)f_t(\hat{a})|0\rangle = f_t(0)(\hat{U}(t)|0\rangle)$$

i.e., the exact solution $|\alpha\rangle = |\alpha = f_t(0)\rangle$, and it can also be expanded $\sum_n (c_n)|n\rangle$. The eigenvalue of unperturbed state is time-dependent $\alpha(t) = -\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\omega t}\mu_\omega(t)$.

Perturbation Theory

Consider Hamiltonian of the following form

$$\hat{H}(t) = \hat{H}^{(0)} + \hat{H}^{(1)}(t), \tag{1}$$

where $\hat{H}^{(0)}$ is time-independent and is regarded as being solved with a full set of (eigenvalue, eigenstate) pairs

$$\hat{H}^{(0)} \left|\psi_n^{(0)}\right\rangle = \epsilon_n^{(0)} \left|\psi_n^{(0)}\right\rangle, \tag{2}$$

and $\|\hat{H}^{(1)}\| \ll \delta\epsilon^{(0)}$ with $\delta\epsilon^{(0)}$ being the energy level spacing of the unperturbed spectrum [1]. To keep track of the order of the corrections due to $\hat{H}^{(1)}$, we rewrite Eq. (1) as

$$\hat{H}(t,\lambda) = \hat{H}^{(0)} + \lambda\hat{H}^{(1)}(t), \tag{3}$$

and later use λ as an expansion parameter.

Our goal is to find, up to the j-th order correction in λ:

- when $\hat{H}^{(1)}$ is *time-independent*, the (eigenvalue, eigenstate) pairs of the full Hamiltonian:

$$\hat{H}(\lambda) \left|\psi_n(\lambda)\right\rangle = \epsilon_n(\lambda) \left|\psi_n(\lambda)\right\rangle \tag{4}$$

  (λ is set to 1 at the end);

- when $\hat{H}^{(1)}(t)$ is *time-dependent*, the transition probability between unperturbed eigenstates $p_{m\leftarrow n}(t) \equiv \left|\left\langle \psi_m^{(0)}\right| \hat{U}(t,0) \left|\psi_n^{(0)}\right\rangle\right|^2$.

[1] The case of degenerate spectrum will be treated separately based on the nondegenerate solution.

1 Time-independent case

We start from formal expansions

$$\epsilon_n(\lambda) = \epsilon_n^{(0)} + \lambda\epsilon_n^{(2)} + \lambda^2\epsilon_n^{(2)} + \cdots, \tag{5}$$

$$\left|\psi_n(\lambda)\right\rangle = \left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle + \cdots, \tag{6}$$

where the above kets are not necessarily normalized (which does not affect the validity of Eq. (4)). We will fix, however, $\left|\psi_n^{(0)}\right\rangle$ to be always normalized such that $\left\langle \psi_m^{(0)} | \psi_n^{(0)} \right\rangle = \delta_{mn}$, and in addition $\left|\psi_n^{(j>0)}\right\rangle$ to be always orthogonal to $\left|\psi_n^{(0)}\right\rangle$ such that $\left\langle \psi_n^{(0)} | \psi_n^{(j>0)} \right\rangle = 0$. The latter condition can be seen as absorbing all possible $\left|\psi_n^{(0)}\right\rangle$ components in $\left|\psi_n^{(j>0)}\right\rangle$ into the zero-th order $\left|\psi_n^{(0)}\right\rangle$ (and then renormalize it). The normalization of $\left|\psi_n(\lambda)\right\rangle$ comes as the final step by taking $\left|\psi_n(\lambda)\right\rangle_{\text{normalized}} = \left|\psi_n(\lambda)\right\rangle / \sqrt{\left\langle \psi_n(\lambda) | \psi_n(\lambda) \right\rangle}$ and keeping the result up to $O(\lambda^j)$. For example,

$$\text{for } j=1: \quad \left|\psi_n(\lambda)\right\rangle_{\text{normalized}} \simeq \left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle; \tag{7}$$

$$\text{for } j=2: \quad \left|\psi_n(\lambda)\right\rangle_{\text{normalized}} \simeq \left(1 - \frac{\lambda^2}{2}\left\langle \psi_n^{(1)} | \psi_n^{(1)} \right\rangle\right)\left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle. \tag{8}$$

With the given problem, $\{\left|\psi_n^{(0)}\right\rangle\}$ is obviously "the" basis to work with. Let us use the un-hatted $H^{(0,1)}$ for the matrix representation of $\hat{H}^{(0,1)}$ in this basis:

$$H_{mn}^{(0,1)} = \left\langle \psi_m^{(0)} \right| \hat{H}^{(0,1)} \left|\psi_n^{(0)}\right\rangle, \tag{9}$$

and define matrices $E^{(j)}$ and $\Psi^{(j)}$ with their elements given by

$$E_{mn}^{(j)} = \epsilon_n^{(j)}\delta_{mn}, \quad \Psi_{mn}^{(j)} = \left\langle \psi_m^{(0)} | \psi_n^{(j)} \right\rangle. \tag{10}$$

Note that $E^{(j)}$ *is always diagonal whereas* $\Psi^{(j>0)}$ *always has a vanishing diagonal.*

It follows that Eq. (4) becomes

$$\begin{aligned}&(H^{(0)} + \lambda H^{(1)})(\Psi^{(0)} + \lambda\Psi^{(1)} + \lambda^2\Psi^{(2)} + \cdots) \\ &= (\Psi^{(0)} + \lambda\Psi^{(1)} + \lambda^2\Psi^{(2)} + \cdots)(E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots),\end{aligned} \tag{11}$$

where, by construction,

$$H^{(0)} = E^{(0)}, \quad \Psi^{(0)} = \mathbb{1}. \tag{12}$$

Eq. (11) is the core of the time-independent perturbation theory. Let us break it down order by order:

$$\lambda^0: \quad H^{(0)}\Psi^{(0)} = \Psi^{(0)}E^{(0)}; \tag{13}$$

$$\lambda^1: \quad H^{(0)}\Psi^{(1)} + H^{(1)}\Psi^{(0)} = \Psi^{(0)}E^{(1)} + \Psi^{(1)}E^{(0)}; \tag{14}$$

$$\lambda^2: \quad H^{(0)}\Psi^{(2)} + H^{(1)}\Psi^{(1)} = \Psi^{(0)}E^{(2)} + \Psi^{(1)}E^{(1)} + \Psi^{(2)}E^{(0)}; \tag{15}$$

$$\lambda^j: \quad H^{(0)}\Psi^{(j)} + H^{(1)}\Psi^{(j-1)} = \sum_{i=0}^{j}\Psi^{(i)}E^{(j-i)}. \tag{16}$$

As a consequence of the chosen basis, Eq. (13) is as trivial as $E^{(0)}\mathbb{1} = \mathbb{1}E^{(0)}$. Higher order equations become useful. Eq. (14) can be decoupled into diagonal and off-diagonal parts (note that $H^{(0)}\Psi^{(j>0)}$ and $\Psi^{(i>0)}E^{(i')}$ always have vanishing diagonals):

$$\text{diag}(H^{(1)}) = E^{(1)} \quad \text{or} \quad \epsilon_n^{(1)} = H_{nn}^{(1)}; \tag{17}$$

$$\text{offdiag}(E^{(0)}\Psi^{(1)} + H^{(1)}) = \text{offdiag}(\Psi^{(1)}E^{(0)}) \quad \text{or} \quad \Psi_{mn}^{(1)}\big|_{m\neq n} = -\frac{H_{mn}^{(1)}}{\epsilon_m^{(0)} - \epsilon_n^{(0)}}. \tag{18}$$

Similarly, Eq. (15) produces

$$\epsilon_n^{(2)} = \sum_{m\neq n} H_{nm}^{(1)}\Psi_{mn}^{(1)}; \tag{19}$$

$$\Psi_{mn}^{(2)}\big|_{m\neq n} = \frac{\Psi_{mn}^{(1)}H_{nn}^{(1)} - \sum_l H_{ml}^{(1)}\Psi_{ln}^{(1)}}{\epsilon_m^{(0)} - \epsilon_n^{(0)}}. \tag{20}$$

Or, generically,

$$\epsilon_n^{(j)} = (H^{(1)}\Psi^{(j-1)})_{nn} = \left\langle \psi_n^{(0)} \right| \hat{H}^{(1)} \left|\psi_n^{(j-1)}\right\rangle; \tag{21}$$

$$\Psi_{mn}^{(j)}\big|_{m\neq n} = \frac{(\sum_{i=1}^{j-1}\Psi^{(i)}E^{(j-i)} - H^{(1)}\Psi^{(j-1)})_{mn}}{\epsilon_m^{(0)} - \epsilon_n^{(0)}}. \tag{22}$$

The normalization of $\Psi = \sum_{i=0}^{j}\lambda^i\Psi^{(i)}$ is important but straightforward.

2 Time-dependent case

In this section, we shall write $\hat{V}(t) \equiv \hat{H}^{(1)}(t)$ and drop λ because the power of V already indicates the order of the correction. In the interaction picture, with the basis chosen to be $\{\left|\psi_n^{(0)}(t)\right\rangle\}$ with $\left|\psi_n^{(0)}(t)\right\rangle = \hat{U}^{(0)}(t)\left|\psi_n^{(0)}\right\rangle = \exp(-i\hat{H}^{(0)}t)\left|\psi_n^{(0)}\right\rangle = \exp(-i\epsilon_n^{(0)}t)\left|\psi_n^{(0)}\right\rangle$, a transition probability amplitudes can be identified (up to a phase factor) with a matrix elements of the interaction time-evolution operator

$$U^I(t)_{mn} = \left\langle \psi_m^{(0)} \right| \hat{U}^I(t) \left|\psi_n^{(0)}\right\rangle = \left\langle \psi_m^{(0)}(t) \right| \hat{U}(t) \left|\psi_n^{(0)}\right\rangle, \tag{23}$$

where

$$\frac{d}{dt}U^I(t) = -iV^I(t)U^I(t), \tag{24}$$

with

$$V_{mn}^I(t) = \left\langle \psi_m^{(0)}(t) \right| \hat{V}(t) \left|\psi_n^{(0)}(t)\right\rangle = V_{mn}(t)e^{i(\epsilon_m^{(0)} - \epsilon_n^{(0)})t}. \tag{25}$$

Eq. (24) is formally solved by the Dyson series

$$U^I(t) = \mathbb{1} + (-i)\int_0^t dt_1 V^I(t_1) + (-i)^2\int_0^t dt_1 V^I(t_1)\int_0^{t_1} dt_2 V^I(t_2) + \cdots. \tag{26}$$

Eq. (26) is the core of the time-dependent perturbation theory.

To see it at work, let's study the example of the two-level (Rabi) model. In this case, $\epsilon_\pm^{(0)} = \pm\Omega/2$, and

$$V(t) = \begin{pmatrix} 0 & \gamma e^{-i\omega t} \\ \gamma e^{i\omega t} & 0 \end{pmatrix} \quad \Rightarrow \quad V^I(t) = \begin{pmatrix} 0 & \gamma e^{i(\Omega-\omega)t} \\ \gamma e^{-i(\Omega-\omega)t} & 0 \end{pmatrix}. \tag{27}$$

The first order term in Eq. (26) becomes

$$(-i)\int_0^t dt_1 V^I(t_1) = \begin{pmatrix} 0 & -\frac{\gamma}{\Omega-\omega}[e^{i(\Omega-\omega)t} - 1] \\ \frac{\gamma}{\Omega-\omega}[e^{-i(\Omega-\omega)t} - 1] & 0 \end{pmatrix}. \tag{28}$$

The second order term in Eq. (26) becomes

$$\begin{aligned}&(-i)^2\int_0^t dt_1 V^I(t_1)\int_0^{t_1} dt_2 V^I(t_2) \\ &= \begin{pmatrix} -i\frac{\gamma^2}{\Omega-\omega}t + (\frac{\gamma}{\Omega-\omega})^2[e^{i(\Omega-\omega)t} - 1] & 0 \\ 0 & i\frac{\gamma^2}{\Omega-\omega}t + (\frac{\gamma}{\Omega-\omega})^2[e^{-i(\Omega-\omega)t} - 1] \end{pmatrix}.\end{aligned} \tag{29}$$

A Exact solution of the two-level model

In a pre-chosen basis, the model Hamiltonian reads

$$H = \begin{pmatrix} \Omega/2 & \gamma e^{-i\omega t} \\ \gamma e^{i\omega t} & -\Omega/2 \end{pmatrix} \quad (\Omega, \gamma, \omega \geq 0). \tag{30}$$

Let us define

$$\Delta \equiv \sqrt{(\Omega/2)^2 + \gamma^2}, \quad \cos\theta \equiv \frac{\Omega/2}{\Delta}, \quad \sin\theta \equiv \frac{\gamma}{\Delta}, \tag{31}$$

such that

$$H = \Delta\begin{pmatrix} \cos\theta & \sin\theta e^{-i\omega t} \\ \sin\theta e^{i\omega t} & -\cos\theta \end{pmatrix}. \tag{32}$$

When $\omega = 0$ (i.e. H is time-independent), the eigenvalues and the corresponding eigenstates are

$$\epsilon_\pm = \pm\Delta, \quad \psi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}, \quad \psi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}. \tag{33}$$

If $\gamma \ll \Omega$, we can expand, up to $(\gamma/\Omega)^2$,

$$\Delta \simeq (\Omega/2)\left[1 + \frac{1}{2}\left(\frac{\gamma}{\Omega/2}\right)^2\right] \simeq \frac{\Omega}{2} + \frac{\gamma^2}{\Omega}, \tag{34}$$

$$\cos\frac{\theta}{2} = \sqrt{\frac{1}{2}(1 + \cos\theta)} = \sqrt{\frac{1}{2}(1 + \left[1 + \left(\frac{\gamma}{\Omega/2}\right)^2\right]^{-1/2})} \simeq 1 - \frac{1}{2}\left(\frac{\gamma}{\Omega}\right)^2, \tag{35}$$

$$\sin\frac{\theta}{2} = \sqrt{\frac{1}{2}(1 - \cos\theta)} = \sqrt{\frac{1}{2}(1 - \left[1 + \left(\frac{\gamma}{\Omega/2}\right)^2\right]^{-1/2})} \simeq \frac{\gamma}{\Omega}. \tag{36}$$

These expansions allow us to compare the exact solutions in Eq. (33) with a time-independent perturbation calculation.

When $\omega > 0$ (i.e. H is time-dependent), we aim to solve for the time-evolution operator $U(t) \equiv U(t,0)$ which satisfies

$$\frac{d}{dt}U(t) = -iH(t)U(t). \tag{37}$$

We first transform

$$\tilde{H} = \rho_\omega(t)H(t)\rho_\omega(t)^{-1} = \begin{pmatrix} \Omega/2 & \gamma \\ \gamma & -\Omega/2 \end{pmatrix}, \tag{38}$$

$$\tilde{U}(t) = \rho_\omega(t)U(t), \tag{39}$$

where

$$\rho_\omega(t) \equiv \begin{pmatrix} e^{i\omega t/2} & \\ & e^{-i\omega t/2} \end{pmatrix}. \tag{40}$$

Then Eq. (37) becomes

$$\frac{d}{dt}\tilde{U}(t) = -i(\tilde{H} - \frac{\omega}{2}\sigma_z)\tilde{U}(t). \tag{41}$$

Now we have a time-independent "effective" Hamiltonian such that we immediately obtain

$$\tilde{U}(t) = \exp[-i(\tilde{H} - \frac{\omega}{2}\sigma_z)t] \tag{42}$$

$$= \cos(\Delta_\omega t) - i\sin(\Delta_\omega t)(\cos\theta_\omega\sigma_z + \sin\theta_\omega\sigma_x), \tag{43}$$

where

$$\Delta_\omega \equiv \sqrt{(\frac{\Omega-\omega}{2})^2 + \gamma^2}, \quad \cos\theta_\omega \equiv \frac{(\Omega-\omega)/2}{\Delta_\omega}, \quad \sin\theta_\omega \equiv \frac{\gamma}{\Delta_\omega}. \tag{44}$$

If the initial state at $t = 0$ is given by $\psi(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, then

$$\psi(t) = U(t)\psi(0) = \begin{pmatrix} e^{-i\omega t/2}[\cos(\Delta_\omega t) - i\sin(\Delta_\omega t)\cos\theta_\omega] \\ -ie^{i\omega t/2}\sin(\Delta_\omega t)\sin\theta_\omega \end{pmatrix}. \tag{45}$$

It follows that the transition probability from the first component to the second is given by

$$p(t) = \sin^2(\Delta_\omega t)\sin^2\theta_\omega = \frac{\gamma^2}{(\frac{\Omega-\omega}{2})^2 + \gamma^2}\sin^2(\Delta_\omega t). \tag{46}$$