Summary of Lecture #1: fundamental concepts

Goals and Requirements:

- Reflect on what you have learned about the basic objects in quantum mechanics: wavefunctions & operators.
- Establish the basic picture about the math structure of quantum mechanics (NOTE: these are not mathematically rigorous)

Hilbert space $\mathcal{H}$	linear space equipped with an inner product
quantum states ('ket') $\lvert\psi\rangle$	elements in the linear space $\mathcal{H}$
'bra' $\langle\psi\rvert$	linear functionals defined on $\mathcal{H}$: $\mathcal{H} \mapsto \mathbb{C}$
quantum mechanical operators	linear mappings: $\mathcal{H}_1 \mapsto \mathcal{H}_2$.

- Be familiarized with the general description of a quantum state: the density matrix. Get some taste of quantum entropy and quantum entanglement if time permits.
- By the end of this lecture, you should feel comfortable about
  dealing with abstract quantum *states* without reference to the wavefunctions, and
  dealing with abstract quantum *operators* without reference to matrices.
- NOTE: statements with $\star$ are advanced topics/challenge questions/extra exercises (NOT required).

References:

J.J. Sakurai, *Modern Quantum Mechanics*, Chapter 1.

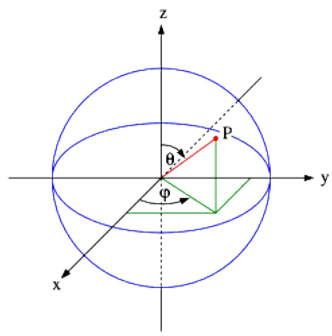
P.A.M. Dirac, *The Principle of Quantum Mechanics*, Sections I.5-6, Chapter III.

J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, Chapters I,II.

I. THE HILBERT SPACE

A. The Wavefunction

- $\psi(\boldsymbol{x})$ is a complex-valued function defined on some "coordinate" space V ($\boldsymbol{x} \in V$).
- Strictly speaking, $\psi(\boldsymbol{x})$ shall be normalizable: $\int |\psi(\boldsymbol{x})|^2 \, \mathrm{d}V < \infty$.
- Probability of the system being in "volume element" $\mathrm{d}V$ is $\frac{|\psi(\boldsymbol{x})|^2 \, \mathrm{d}V}{\int |\psi(\boldsymbol{x})|^2 \, \mathrm{d}V}$. – *Max Born.*
- Normalized $\psi(\boldsymbol{x})$ has "dimension"(unit) of "volume"$^{-1/2}$ (usually not dimensionless).
- Be careful when you parametrize the coordinate space. You might need to absorb the Jacobian into the wavefunction (depending on the definition of $\mathrm{d}V$), and/or introduce artificial "boundary conditions".
- We may need non-normalizable wavefunctions when the space V is not compact ($\int \mathrm{d}V = \infty$), *e.g.* plane waves in open space. We usually regularize this problem by first taking a finite V, and finally taking the limit that the volume goes to infinity.
- Most wavefunctions we will deal with are continuous, and (piecewise) smooth.
- Example:
  V is the unit sphere S^2 parametrized by polar and azimuth angles $\boldsymbol{x} = (\theta, \varphi) \in [0, \pi] \times [0, 2\pi]$, $\mathrm{d}V = \sin\theta \, \mathrm{d}\theta \mathrm{d}\varphi$,
  legitimate $\psi(\theta, \varphi)$ are normalizable complex functions
  ($\int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} |\psi(\theta, \varphi)|^2 \, \sin\theta \, \mathrm{d}\theta \mathrm{d}\varphi < \infty$)
  with the "boundary condition" $\psi(\theta, 0) = \psi(\theta, 2\pi)$, $\forall\theta$
  and $\psi(0, \varphi) = \psi(0, 0)$, $\psi(\pi, \varphi) = \psi(\pi, 0)$, $\forall\varphi$.
  A basis of such wavefunctions are spherical harmonics $Y_\ell^m(\theta, \phi)$.



B. The Hilbert Space

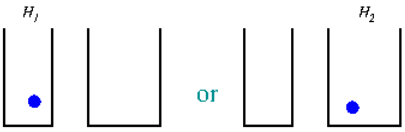
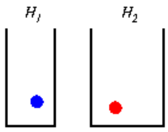
- The Hilbert space $\mathcal{H}(V)$ defined on a coordinate space V is the *complex linear* space formed by *normalizable* wavefunctions defined on V.
  - Being a linear space: if ψ_1 and ψ_2 are elements of $\mathcal{H}$ (legitimate wavefunc.), then so does $\lambda_1\psi_1 + \lambda_2\psi_2$, for any complex numbers λ_1 and λ_2. Exercise: prove this.

- There is a natural *inner product*("overlap") of two wavefunctions ϕ and ψ, $(\phi, \psi) = \int \phi^*(\boldsymbol{x})\, \psi(\boldsymbol{x})\, \mathrm{d}V$, satisfying the three important "axioms"
  - Hermiticity: $(\phi, \psi) = (\psi, \phi)^*$.
  - Linearity: $(\phi, \lambda_1\psi_1 + \lambda_2\psi_2) = \lambda_1 \cdot (\phi, \psi_1) + \lambda_2 \cdot (\phi, \psi_2)$, for $\lambda_1, \lambda_2 \in \mathbb{C}$.
    - Above two properties lead to, $(\lambda_1\phi_1 + \lambda_2\phi_2, \psi) = \lambda_1^* \cdot (\phi_1, \psi) + \lambda_2^* \cdot (\phi_2, \psi)$.
  - Positive definiteness: $(\psi, \psi) \geq 0$, and $(\psi, \psi) = 0$ if and only if "$\psi = 0$".
- One consequence: $(\sum_i \lambda_i\psi_i, \sum_j \lambda_j\psi_j) = \sum_{i,j} \lambda_i^* \cdot (\psi_i, \psi_j) \cdot \lambda_j \geq 0 \Rightarrow$ the Gram matrix (ψ_i, ψ_j) (where i is row-index, j is column-index) is Hermitian and positive semi-definite.
  - The Gram determinant $\det[(\psi_i, \psi_j)] \geq 0$.
  - $n = 2$ case is the Cauchy-Schwarz inequality, $(\psi_1, \psi_1)(\psi_2, \psi_2) \geq |(\psi_1, \psi_2)|^2$.
  - The states ψ_i are linearly dependent if and only if the matrix (ψ_i, ψ_j) is singular, or equivalently $\det[(\psi_i, \psi_j)] = 0$.

C. Combining Hilbert Spaces: Direct Sum & Tensor Product

- Direct sum of two Hilbert spaces $\mathcal{H}_1(V_1) \oplus \mathcal{H}_2(V_2)$:
  the wavefunction $(\psi_1 \oplus \psi_2)(\boldsymbol{x}) = \begin{cases} \psi_1(\boldsymbol{x}), & \boldsymbol{x} \in V_1; \\ \psi_2(\boldsymbol{x}), & \boldsymbol{x} \in V_2. \end{cases}$
  The inner product becomes $(\phi_1 \oplus \phi_2, \psi_1 \oplus \psi_2)_{V_1 \oplus V_2} = (\phi_1, \psi_1)_{V_1} + (\phi_2, \psi_2)_{V_2} = \int \phi_1^*\psi_1\, \mathrm{d}V_1 + \int \phi_2^*\psi_2\, \mathrm{d}V_2$.
  - Note: you need consistent definition of the "volumes" of $V_{1,2}$.
- Tensor product of two Hilbert spaces $\mathcal{H}_1(V_1) \otimes \mathcal{H}_2(V_2)$:
  the wavefunction $(\psi_1 \otimes \psi_2)(\boldsymbol{x}_1, \boldsymbol{x}_2) = \psi_1(\boldsymbol{x}_1) \cdot \psi_2(\boldsymbol{x}_2)$, for $\boldsymbol{x}_1 \in V_1$ and $\boldsymbol{x}_2 \in V_2$.
  The inner product becomes $(\phi_1 \otimes \phi_2, \psi_1 \otimes \psi_2)_{V_1 \otimes V_2} = (\phi_1, \psi_1)_{V_1} \cdot (\phi_2, \psi_2)_{V_2}$.
  - Entanglement: wavefunctions in $\mathcal{H}_1 \otimes \mathcal{H}_2$ may not be a direct product $\psi_1 \otimes \psi_2$.
  - Identical particles: will be treated later.

- Example:

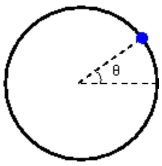
direct sum:	vs.	tensor product:
one particle in two potential wells		two inequivalent particles in two wells
need to know if it is in left **or** right		need to know **both** left & right particles' state
		
$\mathcal{H}_1 \oplus \mathcal{H}_2$		$\mathcal{H}_1 \otimes \mathcal{H}_2$

D. The Dirac Notation

- 'kets' $|\psi\rangle$: element(quantum state) in Hilbert space corresponding to wavefunction ψ.
- 'bras' $\langle\psi|$: linear functional defined on the Hilbert space: $\mathcal{H} \mapsto \mathbb{C}$, $\phi \mapsto (\psi, \phi)$.
  - Short-hand notation: $\langle\psi|\phi\rangle \equiv (\psi, \phi) = \int \psi^* \, \phi \, \mathrm{d}V$.
  - 'bra' is a linear functional: $\langle\psi|\lambda_1\phi_1 + \lambda_2\phi_2\rangle = \lambda_1\langle\psi|\phi_1\rangle + \lambda_2\langle\psi|\phi_2\rangle$.
  - 'bras' form an *anti-linear* space: $\lambda_1^*\langle\psi_1| + \lambda_2^*\langle\psi_2| = \langle\lambda_1\psi_1 + \lambda_2\psi_2|$.
  - Any 'continuous' linear functional $f\ :\ \mathcal{H} \mapsto \mathbb{C},\ \phi \mapsto f(\phi)$, corresponds to a wavefunction ψ_f so that $f = \langle\psi_f|$, $f(\phi) = (\psi_f, \phi)$. – *Riesz-Fréchet theorem.*
    With complete orthonormal basis $|\boldsymbol{e}_i\rangle$, $\langle\psi_f| = \sum_i f(\boldsymbol{e}_i)\,\langle\boldsymbol{e}_i|$,
    so $|\psi_f\rangle = \sum_i f(\boldsymbol{e}_i)^*\,|\boldsymbol{e}_i\rangle$.
- Short-hand notation: $|\psi_1\rangle + |\psi_2\rangle$ with $\psi_1 \in \mathcal{H}_1$, $\psi_2 \in \mathcal{H}_2$ means the direct sum state $\psi_1 \oplus \psi_2 \in \mathcal{H}_1 \oplus \mathcal{H}_2$.
- Short-hand notation: $|\psi_1\rangle|\psi_2\rangle$ with $\psi_1 \in \mathcal{H}_1$, $\psi_2 \in \mathcal{H}_2$ means the tensor product state $\psi_1 \otimes \psi_2 \in \mathcal{H}_1 \otimes \mathcal{H}_2$.
- Short-hand notation: $|\psi_1\rangle\langle\psi_2|$ with $\psi_1 \in \mathcal{H}_1$, $\psi_2 \in \mathcal{H}_2$ is a linear operator: $\mathcal{H}_2 \mapsto \mathcal{H}_1$, $\phi \mapsto (\psi_2, \phi)\psi_1 \equiv |\psi_1\rangle\langle\psi_2|\phi\rangle$.
- Other labels like quantum numbers or just an index, are often used in 'bras' & 'kets': *e.g.* $|L = 2, L_z = 0\rangle$, $|0\rangle$.

E. Complete Orthonormal Basis

- (Discrete) Orthonormal basis e_i $(i = 0, 1, \dots)$ satisfy $\langle e_i | e_j \rangle = \delta_{ij}$.
- Complete orthonormal basis: for any $\psi \in \mathcal{H}$, $|\psi\rangle = \sum_i |e_i\rangle\langle e_i|\psi\rangle$.
  - For finite dimensional Hilbert space, this is just
    'number of orthonormal basis'='dimension of Hilbert space'.
  - For infinite dimensional Hilbert space, completeness is usually very hard to prove.
- Resolution of identity: $\mathbb{1} = \sum_i |e_i\rangle\langle e_i|$, the sum is over a *complete orthonormal* basis.
  - We will see the resolution of identity in terms of *overcomplete* basis later.
  - Application: change of basis, for $|\psi\rangle = \sum_j \tilde{c}_j |\tilde{e}_j\rangle = \sum_i c_i |e_i\rangle = \sum_{i,j} c_i |\tilde{e}_j\rangle\langle\tilde{e}_j|e_i\rangle$, coefficients $\tilde{c}_j = \sum_i c_i \langle \tilde{e}_j | e_i \rangle$, where $\tilde{e}_j$ are another complete orthonormal basis.
    * The matrix $U_{ji} = \langle \tilde{e}_j | e_i \rangle$ is a unitary matrix. $(U \cdot U^\dagger)_{jk} = \sum_i U_{ji} (U^\dagger)_{ik} = \sum_i \langle \tilde{e}_j | e_i \rangle \langle e_i | \tilde{e}_k \rangle = \langle \tilde{e}_j | \tilde{e}_k \rangle$ (by resolution of identity) $= \delta_{jk} = (\mathbb{1})_{jk}$. Above relation is $\tilde{c}_j = \sum_i U_{ji} c_i$ or $\tilde{c} = U \cdot c$ in short form.
    * Conversely, given a unitary matrix U and complete orthonormal basis $|e_i\rangle$, then $|\tilde{e}_j\rangle \equiv \sum_i U_{ji} |e_i\rangle$ form a new set of complete orthonormal basis.
      Exercise: is the "U" here same as the "U" in previous item?
- Example: Fourier series.
  Particle moving on a ring parametrized by angle θ, legitimate wavefunctions are normalizable $\psi(\theta)$ with period 2π, $\psi(\theta + 2\pi) = \psi(\theta)$. A complete orthonormal basis is $e_n(\theta) = \frac{1}{\sqrt{2\pi}} \exp(\mathbb{i} n\theta)$ for $n \in \mathbb{Z}$.



- Basis of composite Hilbert space:
  if $|e_i\rangle$ $(i = 1, \dots, n)$ are the basis of $\mathcal{H}_1$, and $|e'_j\rangle$ $(j = 1, \dots, m)$ are the basis of $\mathcal{H}_2$,
  - the $(n + m)$ basis of $\mathcal{H}_1 \oplus \mathcal{H}_2$ can be chosen as
    $(|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle, |e'_1\rangle, |e'_2\rangle, \dots, |e'_m\rangle)$.
  - the $(n \times m)$ basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$ can be chosen as $|e_i\rangle \otimes |e'_j\rangle$, namely
    $(|e_1\rangle|e'_1\rangle, |e_1\rangle|e'_2\rangle, \dots, |e_1\rangle|e'_m\rangle, |e_2\rangle|e'_1\rangle, \dots, |e_2\rangle|e'_m\rangle, \cdots, |e_n\rangle|e'_1\rangle, \dots, |e_n\rangle|e'_m\rangle)$.

II. QUANTUM MECHANICAL OPERATORS

A. Quantum Mechanical Operators

- Linear operators: *linear* mappings between two (often the same) Hilbert spaces: $\hat{O}|\psi\rangle \in \mathcal{H}_2$ for $|\psi\rangle \in \mathcal{H}_1$, and $\hat{O}|\lambda_1\psi_1 + \lambda_2\psi_2\rangle = \lambda_1\hat{O}|\psi_1\rangle + \lambda_2\hat{O}|\psi_2\rangle$.

- Anti-linear operators: replace the last condition of linear operators by $\hat{O}|\lambda_1\psi_1 + \lambda_2\psi_2\rangle = \lambda_1^*\hat{O}|\psi_1\rangle + \lambda_2^*\hat{O}|\psi_2\rangle$.
  - Example: the operator of "taking complex conjugate" $\mathcal{K}$: $\phi(x) \mapsto \phi(x)^*$.

- Hermitian conjugate (adjoint) of linear operators: $\hat{O}^\dagger$ is a linear operator satisfying $(\hat{O}^\dagger\psi, \phi) = (\psi, \hat{O}\phi)$ for any ψ & ϕ, or $\langle\hat{O}^\dagger\psi| = \langle\psi|\hat{O}$ for any ψ.
  - $(\hat{O}^\dagger)^\dagger = \hat{O}$.
    "Proof": for *any* ψ & ϕ, by definitions of inner product and hermitian conjugate, $(\psi, ((\hat{O}^\dagger)^\dagger)\phi) = (((\hat{O}^\dagger)^\dagger)\phi, \psi)^* = (\phi, (\hat{O}^\dagger)\psi)^* = ((\hat{O}^\dagger)\psi, \phi) = (\psi, \hat{O}\phi)$. Then $((\hat{O}^\dagger)^\dagger)$ and $\hat{O}$ must be the same.
  - $(\lambda\hat{O})^\dagger = \lambda^*\hat{O}^\dagger$, $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.
    Exercise: try to "prove" these as the "proof" for the previous relation.
  - Hermitian operators: those satisfy $\hat{O}^\dagger = \hat{O}$.
    Anti-Hermitian operators: $\hat{O}^\dagger = -\hat{O}$.
  - Any operator is the sum of its Hermitian & anti-Hermitian part:
    $\hat{O} = \frac{\hat{O}+\hat{O}^\dagger}{2} + \frac{\hat{O}-\hat{O}^\dagger}{2}$, the 1st term is Hermitian, 2nd term is anti-Hermitian.

- Matrix representation: under a complete orthonormal basis $|n\rangle$, the operator $\hat{O}$ has 'matrix elements' $O_{mn} \equiv \langle m|\hat{O}|n\rangle$. $(O^\dagger)_{mn} = (O_{nm})^*$.
  - Matrix represention under non-orthogonal/overcomplete basis can also be useful.
  - Expectation value of $\hat{O}$ in state ψ: $\langle\psi|\hat{O}|\psi\rangle/\langle\psi|\psi\rangle$.

- Trace: $\mathrm{Tr}\hat{O} = \sum_n \langle n|\hat{O}|n\rangle$, summing over a complete orthonormal basis.
  The result of trace is *independent of the choice of basis*.
  Cyclic property: $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$, for 'finite' operators $\hat{A}, \hat{B}$ (*e.g.* finite dimensional)

- Eigenvalue λ and eigenstate $|\hat{O}=\lambda\rangle$ of operator $\hat{O}$: defined by $\hat{O}|\hat{O}=\lambda\rangle = \lambda|\hat{O}=\lambda\rangle$.
  - Eigenvalues of Hermitian operators are real.
- (Not required) Singular value decomposition (SVD):
  - Any operator can be written as $\hat{O} = \sum_n |\tilde{n}\rangle\, \rho_n\, \langle n|$, where n labels the singular value $\rho_n \geq 0$, and the two sets of orthonormal basis $|n\rangle$ & $|\tilde{n}\rangle$ are eigenstates of $\hat{O}^\dagger\hat{O}$ & $\hat{O}\hat{O}^\dagger$ respectively.
  - In complete orthonormal basis $|e_i\rangle$, the above relations becomes
    $O_{ij} = \langle e_i|\hat{O}|e_j\rangle = \sum_n \langle e_i|\tilde{n}\rangle\, \rho_n\, \langle n|e_j\rangle = (U\cdot\rho\cdot V^\dagger)_{ij}$,
    where the unitary matrices $U_{in} = \langle e_i|\tilde{n}\rangle$ and $V_{jn} = \langle e_j|n\rangle$,
    and the diagonal matrix ρ has diagonal elements ρ_n. And
    $(O^\dagger O)_{ij} = \langle e_i|\hat{O}^\dagger\hat{O}|e_j\rangle = \sum_n \langle e_i|n\rangle\, \rho_n^2\, \langle n|e_j\rangle = (V\cdot\rho^2\cdot V^\dagger)_{ij}$, and
    $(OO^\dagger)_{ij} = \langle e_i|\hat{O}\hat{O}^\dagger|e_j\rangle = \sum_n \langle e_i|\tilde{n}\rangle\, \rho_n^2\, \langle \tilde{n}|e_j\rangle = (U\cdot\rho^2\cdot U^\dagger)_{ij}$.
- Projection operators: operators $\hat{P}:\ \mathcal{H}\mapsto\mathcal{H}$, satisfying $\hat{P}\hat{P} = \hat{P}$.
  - Hermitian projection operators $\hat{P} = \sum_i |e_i\rangle\langle e_i|$, e_i are a set of orthonormal basis, and $\hat{P}$ have eigenvalues 1 and 0 only.
  - $\mathbb{1}-\hat{P}$ is also a projection operator. Exercise: check that $(\mathbb{1}-\hat{P})(\mathbb{1}-\hat{P}) = (\mathbb{1}-\hat{P})$.
- Inverse of an operator: $\hat{A}^{-1}$ must satisfy $\hat{A}^{-1}\cdot\hat{A} = \mathbb{1}$ and $\hat{A}\cdot\hat{A}^{-1} = \mathbb{1}$
  - $\star$ In infinite dimensional Hilbert space, there can be cases with $\hat{B}\hat{A} = \mathbb{1}$ while $\hat{A}\hat{B} \neq \mathbb{1}$, $\hat{B}$ shall not be called $\hat{A}^{-1}$.
- Unitary operators: linear operators with
  $(\hat{U}\psi, \hat{U}\phi) = (\psi, \phi)$, $\forall\psi,\phi$. Or equivalently $\hat{U}^\dagger\hat{U} = \mathbb{1}$.
  - Unitary operators are of the form $\sum_i |\tilde{e}_i\rangle\langle e_i|$, where e_i is a set of complete orthonormal basis, $\tilde{e}_i$ is another set of orthonormal basis.
  - If $\hat{H}$ is Hermitian, then $\exp(\mathbb{i}\hat{H})$ is unitary. Exercise: is the converse true?
- Anti-unitary operators: anti-linear operators with
  $(\hat{U}\psi, \hat{U}\phi) = (\psi, \phi)^*$, $\forall\psi,\phi$.

B. Abstract Calculations with Operators

- Commutator & anti-commutator of $\hat{A}$ & $\hat{B}$: $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$, $\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$.
  - For notation simplicity, define 'Lie derivative' $\mathcal{L}_{\hat{A}}\hat{B} \equiv [\hat{A}, \hat{B}]$.
- Elementary functions of operators may be defined by their power series expansion, *e.g.* $\exp(\hat{A}) = \sum_{n=0}^{\infty}(\hat{A})^n/n!$ (let's not worry about convergence).
  - Note: $\hat{A} \cdot f(\hat{B}) \cdot \hat{A}^{-1} = f(\hat{A} \cdot \hat{B} \cdot \hat{A}^{-1})$ for such functions f that can be defined as power series, because $\hat{A} \cdot (\hat{B})^n \cdot \hat{A}^{-1} = (\hat{A} \cdot \hat{B} \cdot \hat{A}^{-1})^n$.
- Jacobi identity: $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$. Or $[\mathcal{L}_{\hat{A}}, \mathcal{L}_{\hat{B}}]\hat{C} = \mathcal{L}_{[\hat{A},\hat{B}]}\hat{C}$.
- 'Leibniz's rule':
  $[\hat{A}, \hat{B}_1\hat{B}_2 \cdots \hat{B}_n] = [\hat{A}, \hat{B}_1]\hat{B}_2 \cdots \hat{B}_n + \hat{B}_1[\hat{A}, \hat{B}_2] \cdots \hat{B}_n + \cdots + \hat{B}_1\hat{B}_2 \cdots [\hat{A}, \hat{B}_n]$. Or
  $\mathcal{L}_{\hat{A}}(\hat{B}_1\hat{B}_2 \cdots \hat{B}_n) = (\mathcal{L}_{\hat{A}}\hat{B}_1)\hat{B}_2 \cdots \hat{B}_n + \hat{B}_1(\mathcal{L}_{\hat{A}}\hat{B}_2) \cdots \hat{B}_n + \cdots + \hat{B}_1\hat{B}_2 \cdots (\mathcal{L}_{\hat{A}}\hat{B}_n)$.
- Baker-Hausdorff formula: $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}]/1! + [\hat{A}, [\hat{A}, \hat{B}]]/2! + \ldots$
  Or formally $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \exp(\mathcal{L}_{\hat{A}})\hat{B}$.
  - A heuristic "proof":
    define $\hat{f}(t) = e^{t\hat{A}}\hat{B}e^{-t\hat{A}}$, then $\hat{f}(0) = \hat{B}$.
    Take derivative with respect to t, note that $\frac{\mathrm{d}}{\mathrm{d}t}e^{t\hat{A}} = \hat{A}e^{t\hat{A}} = e^{t\hat{A}}\hat{A}$,
    then $\frac{\mathrm{d}}{\mathrm{d}t}\hat{f}(t) = \hat{A} \cdot \hat{f}(t) - \hat{f}(t) \cdot \hat{A} = [\hat{A}, \hat{f}(t)] = \mathcal{L}_{\hat{A}}\hat{f}(t)$.
    The formal solution of this ordinary differential equation is then $\hat{f}(t) = e^{t\mathcal{L}_{\hat{A}}}\hat{f}(0)$,
    so $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{f}(1) = \exp(\mathcal{L}_{\hat{A}})\hat{B}$. □
- Direct sum & tensor product of operators are defined similarly to wavefunctions:
  for operator $\hat{A}$ defined on $\mathcal{H}_1$, and $\hat{B}$ defined on $\mathcal{H}_2$, $\hat{A} \otimes \hat{B}$ is an operator defined on $\mathcal{H}_1 \otimes \mathcal{H}_2$, such that $(\hat{A} \otimes \hat{B})|\psi \otimes \phi\rangle = (\hat{A}|\psi\rangle) \otimes (\hat{B}|\phi\rangle)$, for states $\psi \in \mathcal{H}_1$ and $\phi \in \mathcal{H}_2$.
  - $(\hat{A} \otimes \hat{B}) \cdot (\hat{C} \otimes \hat{D}) = \hat{A}\hat{C} \otimes \hat{B}\hat{D}$.
  - When $\hat{A}$ is referred to within $\hat{H}_1 \otimes \hat{H}_2$, it usually means $\hat{A} \otimes \mathbb{1}$. With this convention, $\hat{A} \otimes \hat{B}$ is usually written as $\hat{A}\hat{B}$, which means $(\hat{A} \otimes \mathbb{1}) \cdot (\mathbb{1} \otimes \hat{B}) = \hat{A} \otimes \hat{B}$.
  - $\mathrm{Tr}_{1\otimes 2}(\hat{A} \otimes \hat{B}) = \mathrm{Tr}_1(\hat{A}) \cdot \mathrm{Tr}_2(\hat{B})$, where the three different traces are taken in Hilbert spaces $\mathcal{H}_1 \otimes \mathcal{H}_2$, $\mathcal{H}_1$, $\mathcal{H}_2$, respectively.

- With complete orthonormal basis, $|e_i\rangle \in \mathcal{H}_1$ ($i = 1, \ldots, n$) and $|e'_j\rangle \in \mathcal{H}_2$ ($j = 1, \ldots, m$), the matrix representation of $\hat{A} \otimes \hat{B}$ is a $(n \times m)$-row $(n \times m)$-column matrix, $(\hat{A} \otimes \hat{B})_{(i,j)(i',j')} \equiv \langle e_i|\langle e'_j|\hat{A} \otimes \hat{B}|e_{i'}\rangle|e'_{j'}\rangle = \langle e_i|\hat{A}|e_{i'}\rangle \cdot \langle e'_j|\hat{B}|e'_{j'}\rangle = A_{ii'}B_{jj'}$. The combination $(i, j)[(i', j')]$ is the row[column] index ($i, i' = 1, \ldots, n$ and $j, j' = 1, \ldots, m$).

C. Back to Wavefunction

- The coordinate operator $\hat{x}$: $\phi(x) \mapsto x \cdot \phi(x)$. It is obviously Hermitian.
  - Worry #1: $x \cdot \phi(x)$ may not be normalizable!
  - Worry #2: What are the eigenstate wavefunctions of $\hat{x}$? Are they normalizable?
- Despite the above worries, denote the eigenstates of $\hat{x}$ by $|x\rangle$, *i.e.* $\hat{x}|x\rangle = x|x\rangle$.
  - 'Normalization': $\langle x'|x\rangle = \delta(x' - x)$, where δ is the Dirac-δ 'function'.
  - Resolution of identity: $\mathbb{1} = \int |x\rangle\langle x| \, \mathrm{d}x$.
  - The wavefunction $\psi(x)$: expansion coefficients of state ψ in the basis $|x\rangle$. $\psi(x) = \langle x|\psi\rangle$. And $|\psi\rangle = \int \psi(x)|x\rangle \, \mathrm{d}x$.
- The momentum operator $\hat{p}$: $\phi(x) \mapsto -\mathbb{i}\hbar\frac{\partial}{\partial x}\phi(x)$. It is not-so-obviously Hermitian.
  - Canonical commutation relation $[\hat{x}, \hat{p}] = \mathbb{i}\hbar$.
  - Similar worries as for the coordinate operator.
  - Nonetheless, denote the eigenstate of $\hat{p}$ as $|p\rangle$, $\hat{p}|p\rangle = p|p\rangle$.
  - 'Normalization': $\langle p'|p\rangle = \delta(p' - p)$.
  - Resolution of identity: $\mathbb{1} = \int |p\rangle\langle p| \, \mathrm{d}p$.
  - $\langle x|p\rangle = \frac{e^{\mathbb{i}px/\hbar}}{\sqrt{2\pi\hbar}}$ for 1D infinite space.
- $\star$ Construct examples of normalizable $\phi(x)$ so that $\hat{x}\,\phi(x)$ or $\hat{p}\,\phi(x)$ is not normalizable.
- IMPORTANT: $\hbar$ will be frequently omitted hereafter.

III. DENSITY MATRIX & ENTANGLEMENT

A. Density Matrix

- Density matrix of a *normalized* 'pure state' ψ: $\hat{\rho}_\psi = |\psi\rangle\langle\psi|$ is a projection operator.
  - Expectation value of $\hat{O}$ in ψ is $\langle\psi|\hat{O}|\psi\rangle = \mathrm{Tr}(\hat{\rho}_\psi\,\hat{O}) = \mathrm{Tr}(\hat{O}\,\hat{\rho}_\psi)$.
  - $\hat{\rho}$ is independent of the complex phase of $|\psi\rangle$, is a 'better' description of the state.
- Generic density matrix ρ: linear Hermitian non-negative operator of trace unity.
  $\hat{\rho}^\dagger = \hat{\rho}$; $\langle\phi|\hat{\rho}|\phi\rangle \geq 0$, $\forall\phi$; and $\mathrm{Tr}(\hat{\rho}) = 1$.
  - $\rho = \sum_i \lambda_i\,|e_i\rangle\langle e_i|$, with some orthonormal basis e_i, and $\lambda_i > 0$, $\sum_i \lambda_i = 1$.
  - Expectation value of $\hat{O}$ in generic 'mixed state' is $\mathrm{Tr}(\hat{\rho}\,\hat{O})$.
  - If $\hat{\rho}_j$ are density matrices, and $c_j > 0$, and $\sum_j c_j = 1$,
    then $\sum_j c_j\,\hat{\rho}_j$ is also a density matrix.
- The density matrix of Hamiltonian $\widehat{H}$ at finite temperature T:
  $\rho = \exp(-\widehat{H}/k_B T)/Z = \sum_{E_i} \frac{\exp(-E_i/k_B T)}{Z}|E_i\rangle\langle E_i|$,
  where E_i are eigenvalues, $|E_i\rangle$ are corresponding eigenstates,
  $Z = \mathrm{Tr}[\exp(-\widehat{H}/k_B T)] = \sum_{E_i} \exp(-E_i/k_B T)$.

B. $\star$ Some Quantum Information Basics (not required)

- von Neumann entropy of a density matrix $\hat{\rho}$: $S \equiv -\mathrm{Tr}(\hat{\rho}\,\ln\hat{\rho}) = -\sum_i \lambda_i\,\ln\lambda_i$.
  - Pure states have zero entropy & $\hat{\rho}^2 = \hat{\rho}$.
    Mixed states have positive entropy & $\hat{\rho}^2 < \hat{\rho}$.
  - In n(finite)-dimensional Hilbert space, $0 \leq S[\hat{\rho}] \leq \ln(n)$.
  - Rényi entropy: $S_n \equiv \frac{\ln[\mathrm{Tr}(\hat{\rho}^n)]}{1-n}$. Note: formally $\lim_{n\to 1} S_n = S$.
- $\star\star\star$ Concavity of von Neumann entropy: mixing two systems increases entropy.
  $S[\lambda\,\hat{\rho}_1 + (1-\lambda)\,\hat{\rho}_2] \geq \lambda\,S[\hat{\rho}_1] + (1-\lambda)\,S[\hat{\rho}_2]$,
  for two density matrices $\hat{\rho}_{1,2}$ and $0 < \lambda < 1$.

- Reduced density matrix: given a density matrix $\hat{\rho}$ on $\mathcal{H}_a \otimes \mathcal{H}_b$, reduced density matrix ρ_a on $\mathcal{H}_a$ is $\hat{\rho}_a = \mathrm{Tr}_b(\hat{\rho})$, obtained by taking partial trace over $\mathcal{H}_b$.
  - Meaning of partial trace: for any $\psi_{1,2} \in \mathcal{H}_a$, $\langle \psi_1 | \hat{\rho}_a | \psi_2 \rangle = \sum_i \langle \psi_1 \otimes \phi_i | \hat{\rho} | \psi_2 \otimes \phi_i \rangle$, and the sum is over a complete orthonormal basis ϕ_i of $\mathcal{H}_b$. The matrix elements of $\hat{\rho}_a$ under a orthonormal basis $\mathcal{H}_a$ can be computed by this relation.
  - $\star\star\star$ Subadditivity of entropy: information is 'lost' by separating two subsystems. $S_{a\otimes b}[\hat{\rho}] = \mathrm{Tr}_{a\otimes b}(-\hat{\rho} \ln \hat{\rho}) \leq S_a[\hat{\rho}_a] + S_b[\hat{\rho}_b] = \mathrm{Tr}_a(-\hat{\rho}_a \ln \hat{\rho}_a) + \mathrm{Tr}_b(-\hat{\rho}_b \ln \hat{\rho}_b) = S_{a\otimes b}[\hat{\rho}_a \otimes \hat{\rho}_b]$.

- Special case: $\hat{\rho} = |\psi\rangle\langle\psi|$ is for a normalized pure state $\psi \in \mathcal{H}_a \otimes \mathcal{H}_b$.
  - "Entanglement entropy": von Neumann entropy of reduced density matrix: $S_a = -\mathrm{Tr}_a(\hat{\rho}_a \ln \hat{\rho}_a)$, where $\hat{\rho}_a = \mathrm{Tr}_b(\hat{\rho})$.
  - The degrees of freedom of a and b are 'entangled' in this state ψ if $S_a > 0$.
  - The state ψ is a disentangled product state $\psi_a \otimes \phi_b$ if and only if $S_a = 0$.
  - Schmidt decomposition (just SVD): $|\psi\rangle = \sum_i \lambda_i \, |\phi_i\rangle \otimes |\varphi_i\rangle$,
    where $(\lambda_i)^2$ are eigenvalues of $\hat{\rho}_a$, ϕ_i (φ_i) are orthonormal eigenstates of $\hat{\rho}_a$ ($\hat{\rho}_b$).
  - $\star$ Reciprocity: define reduced density matrix $\hat{\rho}_b = \mathrm{Tr}_a(\hat{\rho})$ on $\mathcal{H}_b$.
    $S_b = \mathrm{Tr}_b(-\hat{\rho}_b \ln \hat{\rho}_b)$ equals to S_a above for a *pure state* in $\mathcal{H}_a \otimes \mathcal{H}_b$.

- Example: Bell state.
  $\mathcal{H}_a$ ($\mathcal{H}_b$) is 2-dimensional, with orthonormal basis $|0\rangle, |1\rangle$ ($|\tilde{0}\rangle, |\tilde{1}\rangle$).
  One of the Bell states is $\frac{1}{\sqrt{2}}(|0\rangle|\tilde{1}\rangle - |1\rangle|\tilde{0}\rangle)$.
  Exercise: write down the reduced density matrices $\hat{\rho}_a$ and $\hat{\rho}_b$. Compute the entanglement entropy.

IV. MEASUREMENT & THE UNCERTAINTY PRINCIPLE

A. Measurement

- Measurement can be done for a Hermitian operator $\hat{A}$ on pure or mixed states $\hat{\rho}$.
- The outcome of the measurement will be eigenvalues of $\hat{A}$.
- The probability of outcome λ is $P_\lambda = \mathrm{Tr}(\hat{P}_\lambda\,\hat{\rho})$, $\hat{P}_\lambda$ is the projection to eigenvalue-λ subspace. $\hat{P}_\lambda = \sum |\hat{A}=\lambda\rangle\langle\hat{A}=\lambda|$, summing over orthonormal eigenstates of $\hat{A}$ with eigenvalue λ.
  - If all eigenvalues λ' of $\hat{A}$ are known, then $\hat{P}_\lambda$ can be formally obtained by the "Lagrange interpolating polynomial", $\hat{P}_\lambda = \prod_{\lambda',\ \lambda'\neq\lambda}\left(\frac{\hat{A}-\lambda'\mathbb{1}}{\lambda-\lambda'}\right)$.
  - The statistical average of outcome is the expectation value of $\hat{A}$ in state $\hat{\rho}$, $\mathrm{Tr}(\hat{A}\,\hat{\rho}) = \mathrm{Tr}[(\sum_\lambda \lambda\,\hat{P}_\lambda)\,\hat{\rho}] = \sum_\lambda \lambda\,\mathrm{Tr}(\hat{P}_\lambda\,\hat{\rho}) = \sum_\lambda \lambda\,P_\lambda$.
    For pure state $\hat{\rho} = |\psi\rangle\langle\psi|$, this is $\langle\psi|\hat{A}|\psi\rangle$.
- The "collapse" postulate:
  if the measurement outcome is λ, the quantum state will "collapse" to $\frac{\hat{P}_\lambda\,\hat{\rho}\,\hat{P}_\lambda}{\mathrm{Tr}(\hat{P}_\lambda\,\hat{\rho})}$.
  - If eigenvalue-λ eigenstate is unique, this is the familiar statement
    that the system collapses to eigenstate $|\hat{A}=\lambda\rangle$.
- $\star\star\star$ Information is gained by measurement: 'entropy' decreases.
  $S[\hat{\rho}] \geq \sum_\lambda P_\lambda\,S[\hat{\rho}_\lambda]$, P_λ is the probability of outcome λ, $\hat{\rho}_\lambda$ is the collapsed state.
- An example:
  - Define Pauli matrices
    $\sigma_0 = \begin{pmatrix}1&0\\0&1\end{pmatrix}$, $\sigma_1 = \begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\sigma_2 = \begin{pmatrix}0&-\mathbb{i}\\ \mathbb{i}&0\end{pmatrix}$, $\sigma_3 = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$.
  - Consider a state described by the density matrix $\hat{\rho}$, represented in some basis as
    $$\hat{\rho} = \frac{1}{4}\begin{pmatrix}1&0&0&\mathbb{i}\\0&1&-\mathbb{i}&0\\0&\mathbb{i}&1&0\\-\mathbb{i}&0&0&1\end{pmatrix} = \frac{1}{4}\left[\mathbb{1}-\sigma_1\otimes\sigma_2\right].$$ Exercise: is this a pure state?

- Measure a Hermitian operator $\hat{A}$, represented in the same basis as $\hat{A} = \sigma_1 \otimes \sigma_3$.
- Eigenvalues of $\hat{A}$ are ± 1.
  Corresponding projection operators are $\hat{P}_{+1} = \frac{(-\mathbb{1})-\hat{A}}{(-1)-1}$ and $\hat{P}_{-1} = \frac{\mathbb{1}-\hat{A}}{1-(-1)}$.
- Outcome $+1$: probability $\mathrm{Tr}(\hat{\rho}\,\hat{P}_{+1}) = 1/2$,
  collapsed state is $\hat{\rho}_{+1} = (1/4)[\mathbb{1} + \sigma_1 \otimes \sigma_3]$.
  Outcome -1: probability $\mathrm{Tr}(\hat{\rho}\,\hat{P}_{-1}) = 1/2$,
  collapsed state is $\hat{\rho}_{-1} = (1/4)[\mathbb{1} - \sigma_1 \otimes \sigma_3]$.
- $\star$ Exercise: compute entropies $S[\hat{\rho}]$, $S[\hat{\rho}_{+1}]$ and $S[\hat{\rho}_{-1}]$, check if any information can be gained by this measurement, namely whether $S[\hat{\rho}] > (1/2)S[\hat{\rho}_{+1}] + (1/2)S[\hat{\rho}_{-1}]$?

B. The Uncertainty Principle

- For Hermitian $\hat{A}$ & $\hat{B}$, $(\langle \hat{A}^2\rangle - \langle \hat{A}\rangle^2)(\langle \hat{B}^2\rangle - \langle \hat{B}\rangle^2) \geq \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2$. – *W. Heisenberg*
  $\langle\cdot\rangle$ is the expectation value under a quantum state $\hat{\rho}$.
  - Rough description: product of variances of measurement outcomes for $\hat{A}$ & $\hat{B}$ is bounded below by the square of their commutator's expectation value.
  - Variances of measurement outcome: $\sum_\lambda P_\lambda\,(\lambda - \bar{\lambda})^2 = (\sum_\lambda P_\lambda\,\lambda^2) - \bar{\lambda}^2$, where λ are eigenvalues, P_λ is the probability of outcome λ, $\bar{\lambda} = \sum_\lambda P_\lambda\,\lambda$ is the 'average'.
  - Proof:
    Define the inner product of two operators $\hat{A}, \hat{B}$ as $(\hat{A},\hat{B}) = \langle \hat{A}^\dagger \hat{B}\rangle = \mathrm{Tr}(\hat{A}^\dagger \hat{B}\hat{\rho})$.
    Exercise: check that this indeed satisfies the "axioms" of inner product.
    Define two new operators $\hat{A}' = \hat{A} - \langle\hat{A}\rangle$, $\hat{B}' = \hat{B} - \langle\hat{B}\rangle$. For Hermitian $\hat{A}, \hat{B}$,
    $\frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2 = \frac{1}{4}|\langle[\hat{A}',\hat{B}']\rangle|^2 = \frac{1}{2}(\hat{A}',\hat{B}')(\hat{B}',\hat{A}') - \frac{1}{4}(\hat{A}',\hat{B}')^2 - \frac{1}{4}(\hat{B}',\hat{A}')^2$
    $= [\mathrm{Im}(\hat{A}',\hat{B}')]^2 \leq |(\hat{A}',\hat{B}')|^2 \leq (\hat{A}',\hat{A}')(\hat{B}',\hat{B}') = (\langle\hat{A}^2\rangle - |\langle\hat{A}\rangle|^2)(\langle\hat{B}^2\rangle - |\langle\hat{B}\rangle|^2)$.
    The last inequality used here is Cauchy-Schwarz. $\square$
  - Exercise: what is the condition for the equality to be true?
- Familiar case: $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$. $\langle \hat{x}^2 - \bar{x}^2\rangle\langle \hat{p}^2 - \bar{p}^2\rangle \geq \hbar^2/4$.

Appendix A: ⋆ About the Statements with ⋆ (not required)

- ⋆ In infinite dimensional Hilbert space, there can be cases with $\hat{B}\hat{A} = \mathbb{1}$ while $\hat{A}\hat{B} \neq \mathbb{1}$, $\hat{B}$ shall not be called $\hat{A}^{-1}$.
  - Example:

    Assume $|0\rangle, |1\rangle, \ldots$ are complete orthonormal basis.

    Define $\hat{A} = \sum_{n=0}^{\infty} |n+1\rangle\langle n| \;=\; |1\rangle\langle 0| + |2\rangle\langle 1| + \ldots.$

    Consider $\hat{B} = \sum_{n=0}^{\infty} |n\rangle\langle n+1|$, then $\hat{B}\cdot\hat{A} = \sum_{n=0}^{\infty} |n\rangle\langle n| = \mathbb{1}$.

    However $\hat{A}\cdot\hat{B} = \sum_{n=0}^{\infty} |n+1\rangle\langle n+1| = \mathbb{1} - |n=0\rangle\langle n=0| \;\neq\; \mathbb{1}$.

- ⋆ Construct examples of normalizable $\phi(x)$ so that $\hat{x}\,\phi(x)$ or $\hat{p}\,\phi(x)$ is not normalizable.
  - Example:

    $\phi(x) = \frac{\sin(x^3)}{x}$, defined on real axis of x.

    Check that ϕ is normalizable while both $\hat{x}\,\phi$ and $\hat{p}\,\phi$ are not.

- ⋆⋆⋆ Concavity of von Neumann entropy: $S[\lambda\,\hat{\rho}_1 + (1-\lambda)\,\hat{\rho}_2] \geq \lambda\,S[\hat{\rho}_1] + (1-\lambda)\,S[\hat{\rho}_2]$, for two density matrices $\hat{\rho}_{1,2}$ and $0 < \lambda < 1$.
  - Proof: see *e.g.*, M.A. Nielsen, I.L. Chuang, *Quantum Computation and Quantum Information*, section 11.3.5.

- ⋆ ⋆ ⋆ Subadditivity of entropy: $S_{a\oplus b}[\hat{\rho}] = \mathrm{Tr}_{a\oplus b}(-\hat{\rho}\,\ln\hat{\rho}) \leq S_a[\hat{\rho}_a] + S_b[\hat{\rho}_b] = \mathrm{Tr}_a(-\hat{\rho}_a\,\ln\hat{\rho}_a) + \mathrm{Tr}_b(-\hat{\rho}_b\,\ln\hat{\rho}_b) = S_{a\oplus b}[\hat{\rho}_a \otimes \hat{\rho}_b]$.
  - Proof: see H. Araki, E. H. Lieb, *Commun. Math. Phys.* **18**, 160 (1970).

- ⋆ Reciprocity: define reduced density matrices $\hat{\rho}_a = \mathrm{Tr}_b(\hat{\rho})$ & $\hat{\rho}_b = \mathrm{Tr}_a(\hat{\rho})$ on subspace $\mathcal{H}_a$ & $\mathcal{H}_b$ respectively, where $\rho = |\psi\rangle\langle\psi|$ is a *pure state* on $\mathcal{H}_a \otimes \mathcal{H}_b$. Then $S_b = \mathrm{Tr}_b(-\hat{\rho}_b\,\ln\hat{\rho}_b) = S_a = \mathrm{Tr}_a(-\hat{\rho}_a\,\ln\hat{\rho}_a)$.
  - Proof:

    This a simple consequence of the Schmidt decomposition of a pure state.

    $|\psi\rangle = \sum_i \lambda_i\,|e_i\rangle\otimes|\tilde{e}_i\rangle$, with orthonormal basis e_i for $\mathcal{H}_a$ and $\tilde{e}_i$ for $\mathcal{H}_b$, and real positive singular values λ_i. Then the reduced density matrix on $\mathcal{H}_a$ is $\sum_i \lambda_i^2\,|e_i\rangle\langle e_i|$, and on $\mathcal{H}_b$ is $\sum_i \lambda_i^2\,|\tilde{e}_i\rangle\langle\tilde{e}_i|$. So $S_a = -\sum_i \lambda_i^2 \ln(\lambda_i^2) = S_b$. $\square$

- $\star\star\star$ Information is gained by measurement: 'entropy' decreases.

  $S[\hat{\rho}] \geq \sum_\lambda P_\lambda\, S[\hat{\rho}_\lambda]$, P_λ is the probability of outcome λ, $\hat{\rho}_\lambda$ is the collapsed state.

  - Proof: see G. Lindblad, *Commun. Math. Phys.* **28**, 245 (1972).

Summary of Lecture #2: identical particles

Goals and Requirements:

- Get a clear picture of the *Fock space*:
  direct sum of identical particle Hilbert spaces for all possible particle numbers.
  $\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots$.

- Get a clear picture of the many-body Hilbert space of fermions and bosons:
  (Anti-)Symmetrized tensor product space.
  - n-body Hilbert space for identical particles $\mathcal{H}_n$ is a subspace of $(\mathcal{H}_1)^{\otimes n}$.
  - $\mathcal{H}_n$ is the image of the multi-linear (anti-)symmetrization mapping:
    $\mathcal{S}: \quad (\mathcal{H}_1)^{\otimes n} \mapsto \mathcal{H}_n$.
  - The (anti-)symmetrization mapping is defined on a tensor product basis as
    $\mathcal{S}:\ |\psi_1\rangle \dots |\psi_n\rangle \mapsto \frac{1}{\sqrt{n!}} \sum_{\sigma\in S_n} |\psi_{\sigma(1)}\rangle \dots |\psi_{\sigma(n)}\rangle \equiv |\psi_1, \dots, \psi_n\rangle$, for boson;
    $\mathcal{S}:\ |\psi_1\rangle \dots |\psi_n\rangle \mapsto \frac{1}{\sqrt{n!}} \sum_{\sigma\in S_n} (-1)^\sigma |\psi_{\sigma(1)}\rangle \dots |\psi_{\sigma(n)}\rangle \equiv |\psi_1, \dots, \psi_n\rangle$, for fermion.
  - NOTE: the above picture is rather inconvenient, and will not be used in practice.

- Be familiarized with the second quantization language:
  creation & annihilation operators, and their (anti-)commutation relations.
  Be able to use it to understand/formulate many-body Hamiltonians.

- Be familiarized with several simple('free particle') many-body wavefunctions:
  e.g. boson coherent states, fermion product states, BCS states.
  - They are the "vacuum" of certain single particle "annihilation" operators.

References:

J.J. Sakurai, *Modern Quantum Mechanics*, Chapter 6.

P.A.M. Dirac, *The Principle of Quantum Mechanics*, Chapter IX.

L.D. Landau, E.M. Lifschitz, *Quantum Mechanics: Non-relativistic Theory*, Chapter IX.

A. Altland, B.D. Simons, *Condensed Matter Field Theory*, Chapter 2.

I. THE FOCK SPACE

A. Trivia about the Permutation Group S_n

- A permutation $\sigma = \begin{pmatrix} 1 & 2 & \cdots & n \\ \sigma(1) & \sigma(2) & \cdots & \sigma(n) \end{pmatrix}$ means replacing 1 by $\sigma(1)$, 2 by $\sigma(2)$, $\cdots$, n by $\sigma(n)$, where $\sigma(1), \sigma(2), \cdots, \sigma(n)$ is a rearrangement of $1, 2, \cdots, n$.

- Product of permutations σ and μ (in one convention): $(\sigma \cdot \mu)(i) = \sigma(\mu(i))$.

- Transposition (i, j): exchange i and j while keeping the others fixed.

- Any permutation can be represented as a product of transpositions.
  In fact only transpositions of neighbors $(i, i+1)$ are needed.
  - Example: $\begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 1 & 4 & 2 \end{pmatrix} = (2,3)(3,4)(1,2) = (1,3)(2,3)(3,4) = \ldots$

- The parity of a permutation: parity of the number of transpositions.
  Even(Odd) permutation: product of even(odd) number of transpositions.

- The sign (signature) of a permutation $(-1)^\sigma$ [also denoted by $\mathrm{sgn}(\sigma)$]:
  $+1$ for even permutations; -1 for odd permutations.
  - An explicit formula: $(-1)^\sigma = \prod_{i<j} \mathrm{sgn}[\sigma(j) - \sigma(i)]$. Here $\mathrm{sgn}[x] = \begin{cases} +1, & x > 0; \\ -1, & x < 0. \end{cases}$
  - $(-1)^{\sigma \cdot \mu} = (-1)^\sigma \cdot (-1)^\mu$. Namely, (even perm.)$\cdot$(even perm.)=(even perm.), $\ldots$.

- The permutation group has only two 1-dimensional "representations":
  trivial representation: $R(\sigma) = 1$; and "alternating representation": $R(\sigma) = (-1)^\sigma$.

B. Identical Particle: Traditional Treatment using Wavefunctions

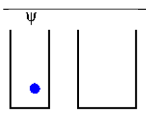
- The configuration of n identical(indistinguishable) particles
  $\boldsymbol{x} = (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n)$ should be equivalent to (all permutations of $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$).

- n-body state $\psi(\boldsymbol{x}) = \psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n)$ should be 'invariant' under permutations of $\boldsymbol{x}_i$.
  - The wavefunction may get complex phase, the density matrix should be the same.

- Assume: the n-body wavefunction is a one-dimensional representation of the permutation group S_n, then there are only two possibilities: bosons and fermions.
  - Being a 1D representation means, for a permutation $\sigma \in S_n$, $\psi(\boldsymbol{x}_{\sigma(1)}, \boldsymbol{x}_{\sigma(2)}, \ldots, \boldsymbol{x}_{\sigma(n)}) = R(\sigma) \cdot \psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n)$, where $R(\sigma)$ is a complex number of unit modulus, and $R(\sigma \cdot \mu) = R(\sigma) \cdot R(\mu)$.
  - Note that pairwise exchange(transposition) $\sigma_{i,j}$ $(\boldsymbol{x}_i \leftrightarrow \boldsymbol{x}_j)$ is its own inverse, $(\sigma_{i,j})^2 = \mathbb{1}$, then $[R(\sigma_{i,j})]^2 = 1$, namely $R(\sigma_{i,j}) = \pm 1$.
    - $\sigma_{i',j'} = \sigma_{i,i'}\sigma_{j,j'}\sigma_{i,j}\sigma_{i,i'}\sigma_{j,j'}$, therefore $R(\sigma_{i',j'}) = R(\sigma_{i,j})$.
  - Bosons: a pairwise exchange (any permutation) has no effect on the wavefunction. Trivial representation of permutation group.
  - Fermions: a pairwise exchange changes the sign of the wavefunction. Odd permutations(odd # of pair exchanges) changes the sign of the wavefunction. Alternating representation of permutation group.
  - In *two-dimensional space*, braiding group instead of permutation group should be considered. There are particles(anyons) beyond bosons and fermions. See *e.g.* C. Nayak *et al.*, *Rev. Mod. Phys.* **80**, 1083 (2008).

C. The Structure of Many-body Hilbert Space

- Fock space: the Hilbert space of identical particles with indefinite particle number, is the *direct sum* of 0-particle & 1-particle & … Hilbert spaces. $\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \ldots$.
  - generic states in Fock space: 'linear superpositions' of 0-particle state('vacuum'), and 1-particle state $\psi_{N=1}(\boldsymbol{r}_1)$, and 2-particle state $\psi_{N=2}(\boldsymbol{r}_1, \boldsymbol{r}_2)$, and ….
- 0-particle Hilbert space $\mathcal{H}_0$: Hilbert space containing only the "vacuum" state.
  - The "vacuum" state is usually denoted by $|\text{vac}\rangle$ or $|0\rangle$.
  - About the "vacuum": roughly speaking, it means that **no** particle (that we are considering) is in the coordinate space of 1-particle wavefunctions in $\mathcal{H}_1$.



Example: for this particle confined in the left well, the state is $|\psi\rangle_{\text{left}} \otimes |\text{vac}\rangle_{\text{right}}$

- 1-particle Hilbert space $\mathcal{H}_1$: linear space of 1-body wavefunctions, can be of finite or infinite dimension. Denote the 1-body states by *e.g.* $|\psi\rangle$.

- $n(\geq 2)$-particle Hilbert space $\mathcal{H}_n$: a *subspace* of the tensor product $(\mathcal{H}_1)^{\otimes n}$ $= \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1$, with (anti-)symmetrization between the factor $\mathcal{H}_1$s.

  (Anti-)Symmetrization is for identical particles so that they are indistinguishable.

- Consider the (anti-)symmetrization operation, which maps $\mathcal{H}_1^{\otimes n}$ to $\mathcal{H}_n$,
  $\mathcal{S}: \quad \mathcal{H}_1^{\otimes n} \mapsto \mathcal{H}_n, \quad |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle \mapsto |\psi_1, \psi_2, \cdots, \psi_n\rangle.$

  - $\mathcal{S}$ is multi-linear, namely linear with respect to each factor $|\psi_i\rangle$.
  - Permutations of ψ_i produce the same n-body state, up to an overall phase.
  - If ψ_i are orthonormal, $|\psi_1, \ldots, \psi_n\rangle$ is normalized (for both bosons and fermions).

- Bosons: permutations of ψ_i are trivial.

  - $\mathcal{S}: \ |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle \mapsto |\psi_1, \ldots, \psi_n\rangle \equiv \frac{1}{\sqrt{n!}} \sum_{\sigma \in S_n} |\psi_{\sigma(1)}\rangle \otimes \cdots \otimes |\psi_{\sigma(n)}\rangle$.
  - $|\psi_{\sigma(1)}, \cdots, \psi_{\sigma(n)}\rangle = |\psi_1, \cdots, \psi_n\rangle$, $\forall \sigma \in S_n$.

- Fermions: permutations of ψ_i produces the sign of permutation.

  - Exclusion principle: if $\psi_i = \psi_j$ $(i \neq j)$, fermion state $|\psi_1, \cdots, \psi_n\rangle = 0$. (by *W. Pauli*).
  - "Fermion exchange sign": $|\cdots \psi_i \cdots \psi_j \cdots\rangle = -|\cdots \psi_j \cdots \psi_i \cdots\rangle$.
    - "Proof": $0 = |\cdots (\psi_i + \psi_j) \cdots (\psi_i + \psi_j) \cdots\rangle$
      $= |\cdots \psi_i \cdots \psi_i \cdots\rangle + |\cdots \psi_j \cdots \psi_j \cdots\rangle + |\cdots \psi_i \cdots \psi_j \cdots\rangle + |\cdots \psi_j \cdots \psi_i \cdots\rangle$
      $= 0 + 0 + |\cdots \psi_i \cdots \psi_j \cdots\rangle + |\cdots \psi_j \cdots \psi_i \cdots\rangle$.
  - $\mathcal{S}: \ |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle \mapsto |\psi_1, \ldots, \psi_n\rangle \equiv \frac{1}{\sqrt{n!}} \sum_{\sigma \in S_n} (-1)^\sigma |\psi_{\sigma(1)}\rangle \otimes \cdots \otimes |\psi_{\sigma(n)}\rangle$
  - $|\psi_{\sigma(1)}, \cdots, \psi_{\sigma(n)}\rangle = (-1)^\sigma |\psi_1, \cdots \psi_n\rangle$, $\forall \sigma \in S_n$.

D. Basis of Many-body Hilbert Space

- The wavefunction is the expansion coefficient in the coordinate eigenstate basis.

  This time the coordinate basis are the tensor product states $|x_1\rangle \otimes \cdots \otimes |x_n\rangle$.

  The (un-normalized) wavefunction is $\psi(x_1, \cdots, x_n) = (|x_1\rangle \otimes \cdots \otimes |x_n\rangle, |\psi_1, \cdots, \psi_n\rangle)$.

- Bosons: $\psi(x_1,\cdots,x_n) = \frac{1}{\sqrt{n!}}\sum_{\sigma\in S_n}\langle x_1|\psi_{\sigma(1)}\rangle\cdots\langle x_n|\psi_{\sigma(n)}\rangle$
$= \frac{1}{\sqrt{n!}}\sum_{\sigma\in S_n}\psi_{\sigma(1)}(x_1)\cdots\psi_{\sigma(n)}(x_n) = \frac{1}{\sqrt{n!}}\mathrm{perm}[\psi_j(x_i)]$.
  - Permanent of a square matrix A_{ij}: $\mathrm{perm}[A] \equiv \sum_{\sigma\in S_n}\prod_i A_{i,\sigma(i)}$.
  - $\langle\phi_1,\ldots,\phi_n|\psi_1,\ldots,\psi_n\rangle = \mathrm{perm}[\langle\phi_i|\psi_j\rangle] = \sum_{\sigma\in S_n}\prod_i\langle\phi_i|\psi_{\sigma(i)}\rangle$. Exercise.
- Fermions: $\psi(x_1,\cdots,x_n) = \frac{1}{\sqrt{n!}}\sum_{\sigma\in S_n}(-1)^\sigma\langle x_1|\psi_{\sigma(1)}\rangle\cdots\langle x_n|\psi_{\sigma(n)}\rangle$
$= \frac{1}{\sqrt{n!}}\sum_{\sigma\in S_n}(-1)^\sigma\psi_{\sigma(1)}(x_1)\cdots\psi_{\sigma(n)}(x_n) = \frac{1}{\sqrt{n!}}\det[\psi_j(x_i)]$.
This is the Slater determinant.
  - Determinant of a square matrix A_{ij}: $\det[A] \equiv \sum_{\sigma\in S_n}(-1)^\sigma\prod_i A_{i,\sigma(i)}$.
  - $\langle\phi_1,\ldots,\phi_n|\psi_1,\ldots,\psi_n\rangle = \det[\langle\phi_i|\psi_j\rangle] = \sum_{\sigma\in S_n}(-1)^\sigma\prod_i\langle\phi_i|\psi_{\sigma(i)}\rangle$. Exercise.
- Suppose $\mathcal{H}_1$ has complete orthonormal basis $|e_i\rangle$. For simplicity, assume a m(finite)-dimensional $\mathcal{H}_1$ ($i = 1,\ldots,m$). The goal is to construct a basis for $\mathcal{H}_n$.
- Bosons: basis are $|e_{i_1},e_{i_2},\cdots,e_{i_n}\rangle$, for all $1 \le i_1 \le i_2 \le \cdots \le i_n \le m$.
  - These basis are orthogonal, but not normalized.
  - The number of basis (dimension of $\mathcal{H}_n$) is $\binom{m+n-1}{n} = \frac{(m+n-1)!}{n!(m-1)!}$.
- Fermions: basis are $|e_{i_1},e_{i_2},\cdots,e_{i_n}\rangle$, for all $1 \le i_1 < i_2 < \cdots < i_n \le m$.
  - Obviously, if $n > m$, there is no legitimate n-body state (exclusion principle).
  - These basis are orthonormal.
  - The number of basis (dimension of $\mathcal{H}_n$) is $\binom{m}{n} = \frac{m!}{n!(m-n)!}$.
- Occupation number representation:
denote the above basis $|e_{i_1},e_{i_2},\cdots,e_{i_n}\rangle$ as $|e_1^{n_1},e_2^{n_2},\cdots,e_m^{n_m}\rangle$,
where n_j is the number of appearance of e_j. Note that $n_1+n_2+\cdots n_m = n$.
The occupation basis $|n_1,n_2,\cdots,n_m\rangle$ is the state $|e_1^{n_1},e_2^{n_2},\cdots,e_m^{n_m}\rangle$ normalized:
$|n_1,n_2,\cdots,n_m\rangle = (n_1!)^{-1/2}(n_2!)^{-1/2}\cdots(n_m!)^{-1/2}\,|e_1^{n_1},e_2^{n_2},\cdots,e_m^{n_m}\rangle$.
  - For fermions, $n_j = 0$ or 1, the normalization factor is trivial.

II. SECOND QUANTIZATION

A. Creation and Annihilation Operators

- The goal is to define linear operators which creates(destroys) a particle of the 1-body state ψ, in the Fock space.
  - The creation operator $\hat{\psi}^\dagger$ maps $\mathcal{H}_n$ to $\mathcal{H}_{n+1}$.
    The annihilation operator $\hat{\psi}$ maps $\mathcal{H}_n$ to $\mathcal{H}_{n-1}$ (vanishes on "vacuum" $\mathcal{H}_0$).
- Creation operator: ("add a 1-body state as a new factor")
  $\hat{\psi}^\dagger : \quad \mathcal{H}_n \to \mathcal{H}_{n+1}, \quad |\psi_1, \cdots, \psi_n\rangle \mapsto |\psi, \psi_1, \cdots, \psi_n\rangle.$
  - In occupation basis (exercise: check these by definition):
    for bosons, $\hat{e}_i^\dagger|\cdots, n_i, \cdots\rangle = \sqrt{n_i + 1}|\cdots, (n_i + 1), \cdots\rangle$;
    for fermions, $\hat{e}_i^\dagger|\cdots, n_i = 0, \cdots\rangle = (-1)^{\sum_{j=1}^{i-1} n_j}|\cdots, n_i = 1, \cdots\rangle$.
- Annihilation operator: ("try to remove a 1-body state from each factor respectively")
  $\hat{\psi} : \quad \mathcal{H}_n \to \mathcal{H}_{n-1}, \quad |\psi_1, \cdots, \psi_n\rangle \mapsto \sum_{i=1}^n (\pm 1)^{i-1} \langle\psi|\psi_i\rangle \, |\psi_1, \cdots, \psi_{i-1}, \psi_{i+1}, \cdots, \psi_n\rangle,$
  where $+1$ is for bosons and -1 is for fermions.
  - In occupation basis (exercise: check these by definition):
    for bosons, $\hat{e}_i|\cdots, n_i, \cdots\rangle = \sqrt{n_i}|\cdots, (n_i - 1), \cdots\rangle$;
    for fermions, $\hat{e}_i|\cdots, n_i = 1, \cdots\rangle = (-1)^{\sum_{j=1}^{i-1} n_j}|\cdots, n_i = 0, \cdots\rangle$.
- Occupation basis $|n_1, \cdots, n_m\rangle = (n_1!)^{-1/2} \cdots (n_m!)^{-1/2} \, (\hat{e}_1^\dagger)^{n_1} \cdots (\hat{e}_m^\dagger)^{n_m} \, |0\rangle$.
- (Anti-)Commutation relations: Bosons: $[\hat{\psi}, \hat{\psi}^\dagger] = 1$. Fermions: $\{\hat{\psi}, \hat{\psi}^\dagger\} = 1$.
  And mode occupation number operator: $\hat{n}_\psi = \hat{\psi}^\dagger\hat{\psi}$, for normalized 1-particle state ψ,
  - $[\hat{n}_\psi, \hat{\psi}^\dagger] = \hat{\psi}^\dagger$, namely $\hat{\psi}^\dagger$ increases eigenvalue of $\hat{n}_\psi$ by 1.
    $[\hat{n}_\psi, \hat{\psi}] = -\hat{\psi}$, namely $\hat{\psi}$ decreases eigenvalue of $\hat{n}_\psi$ by 1.
    Exercise: check these statements for both bosons and fermions.
  - Eigenvalues of $\hat{n}_\psi$ are non-negative integers: $\hat{n}_\psi$ is hermition, positive semi-definite (because $\hat{\psi}^\dagger$ is indeed the hermitian conjugate of $\hat{\psi}$, see later)
  - Occupation basis $|n_1, \cdots, n_m\rangle$ are eigenstates of $\hat{n}_{e_i}$ with eigenvalue n_i.

- (Anti-)Commutation relations between annihilation/creation operators of different modes (exercise: check these by definition):
  Bosons: $[\hat{\psi}, \hat{\psi}'^\dagger] = \langle\psi|\psi'\rangle$, $[\hat{\psi}, \hat{\psi}'] = 0 = [\hat{\psi}^\dagger, \hat{\psi}'^\dagger]$.
  Fermions: $\{\hat{\psi}, \hat{\psi}'^\dagger\} = \langle\psi|\psi'\rangle$, $\{\hat{\psi}, \hat{\psi}'\} = 0 = \{\hat{\psi}^\dagger, \hat{\psi}'^\dagger\}$.

  - For the 1-body orthonormal basis e_i, corresponding operators satisfy:
    Bosons: $[\hat{e}_i, \hat{e}_j^\dagger] = \delta_{ij}$. Fermions: $\{\hat{e}_i, \hat{e}_j^\dagger\} = \delta_{ij}$.
  - For coordinate eigenstates $|x\rangle$, denote corresponding operators by $\widehat{\psi(x)}$ and $\widehat{\psi^\dagger(x)}$:
    Bosons: $[\widehat{\psi(x)}, \widehat{\psi^\dagger(x')}] = \delta(x - x')$. Fermions: $\{\widehat{\psi(x)}, \widehat{\psi^\dagger(x')}\} = \delta(x - x')$.
    NOTE: these are not related to some state ψ, symbols like ϕ may also be used.
  - (Anti-)Commutation relations of momentum eigenstate operators $\widehat{\psi(p)}$ & $\widehat{\psi^\dagger(p)}$ are similar.

- Basis change: $\hat{\psi}^\dagger = \sum_i \langle e_i|\psi\rangle\, \hat{e}_i^\dagger$, sum is over a complete orthonormal basis.
  In particular $\hat{\psi}^\dagger = \int \psi(x)\widehat{\psi^\dagger(x)}\, \mathrm{d}x$, where $\psi(x) = \langle x|\psi\rangle$ is the wavefunction.

  - If e_i and e_i' are two sets of complete orthonormal 1-body basis, then
    $\hat{e'}_i = \sum_j \langle e_i'|e_j\rangle \hat{e}_j$, or column vector $\hat{\boldsymbol{e}}' = U \cdot \hat{\boldsymbol{e}}$,
    where $U_{ij} = \langle e_i'|e_j\rangle$ is a unitary matrix.
  - Exercise: check the converse of the above statement.
    For orthonormal boson(fermion) basis $\hat{e}_i$ satisfying $[\hat{e}_i, \hat{e}_j^\dagger] = \delta_{ij}$ ($\{\hat{e}_i, \hat{e}_j^\dagger\} = \delta_{ij}$), the transformed operators $\hat{e'}_i = \sum_j U_{ij} \cdot \hat{e}_j$ satisfy the same form of commutation(anti-commutation) relations, $[\hat{e}_i', \hat{e}_j'^\dagger] = \delta_{ij}$ ($\{\hat{e}_i', \hat{e}_j'^\dagger\} = \delta_{ij}$), namely that $\hat{e'}_i$ also form orthonormal basis, if U is a unitary matrix.
  - (USEFUL) This can be used to "diagonalize" bilinear operators $\hat{M} = \sum_{i,j} \hat{e}_i^\dagger M_{ij} \hat{e}_j$ $= \hat{\boldsymbol{e}}^\dagger \cdot M \cdot \hat{\boldsymbol{e}} = \hat{\boldsymbol{e}}'^\dagger \cdot U \cdot M \cdot U^\dagger \cdot \hat{\boldsymbol{e}}'$. By choosing the unitary matrix $U_{ij} = \langle e_i'|e_j\rangle$, the matrix $U \cdot M \cdot U^\dagger$ may become diagonal with eigenvalues λ_i on the major diagonal. Then $\hat{M} = \sum_i \lambda_i \hat{e}_i'^\dagger \hat{e}_i' = \sum_i \lambda_i \hat{n}_i'$, and e_i' occupation basis are normalized eigenstates of $\hat{M}$ in the entire Fock space.

- "vacuum": $\hat{\psi}|0\rangle = 0$ for any "annihilation" operator $\hat{\psi}$,
  and $\langle 0|\hat{\psi}^\dagger = 0$ for any "creation" operator $\hat{\psi}^\dagger$.

1. *Creation and Annihilation Operators: Consistency Check*

- Check that $\hat\psi^\dagger$ is indeed $(\hat\psi)^\dagger$: show that
  $(\hat\psi^\dagger|\psi_1,\dots,\psi_{n-1}\rangle, |\phi_1,\dots,\phi_n\rangle) = (|\psi_1,\dots,\psi_{n-1}\rangle, \hat\psi|\phi_1,\dots,\phi_n\rangle)$,
  for any n-body state $|\phi_1,\dots,\phi_n\rangle$ and $(n-1)$-body state $|\psi_1,\dots,\psi_{n-1}\rangle$.

  - Bosons: (check Laplace expansion of permanent)
    $(\hat\psi^\dagger|\psi_1,\dots,\psi_{n-1}\rangle, |\phi_1,\dots,\phi_n\rangle) = \langle\psi,\psi_1,\dots,\psi_{n-1}|\phi_1,\dots,\phi_n\rangle$
    $= \sum_{\sigma\in S_n}\langle\psi|\phi_{\sigma(1)}\rangle\langle\psi_1|\phi_{\sigma(2)}\rangle\dots\langle\psi_{n-1}|\phi_{\sigma(n)}\rangle$.
    $(|\psi_1,\dots,\psi_{n-1}\rangle, \hat\psi|\phi_1,\dots,\phi_n\rangle) = \sum_{i=1}^n\langle\psi|\phi_i\rangle\langle\psi_1,\dots,\psi_{n-1}|\phi_1,\dots,\phi_n \text{ without } \phi_i\rangle$
    $= \sum_{i=1}^n\langle\psi|\phi_i\rangle\sum_{\text{permutation }\sigma'\text{ of }(1,\dots,\text{n, without i})}\langle\psi_1|\phi_{\sigma'(1)}\rangle\dots\langle\psi_{n-1}|\phi_{\sigma'(n-1)}\rangle$,
    $\sigma'(1),\dots,\sigma'(n-1)$ is a rearrangement of $n-1$ numbers $(1,\dots,n$, without $i)$,
    therefore the sequence $i,\sigma'(1),\dots,\sigma'(n-1)$ is a permutation σ of $1,\dots,n$,
    the two final results are summations over the same $n!$ terms.
  - Fermions: (check Laplace expansion of determinant). Exercise.

- Note that $\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger|0\rangle = |\psi_1,\cdots,\psi_n\rangle$, by definition of creation operators.

  - Action of creation operator $\hat\psi^\dagger$: $\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger|0\rangle \mapsto \hat\psi^\dagger\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger|0\rangle$,
    consistent with $\hat\psi^\dagger: \quad |\psi_1,\cdots,\psi_n\rangle \mapsto |\psi,\psi_1,\cdots,\psi_n\rangle$.
  - Action of annihilation operator $\hat\psi$:
    * Bosons: $\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger|0\rangle \mapsto \hat\psi\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger|0\rangle$
      $= [\hat\psi,\, \hat\psi_1^\dagger\cdots\hat\psi_n^\dagger]|0\rangle + \hat\psi_1^\dagger\cdots\hat\psi_n^\dagger\hat\psi|0\rangle = \sum_i\psi_1^\dagger\cdots[\hat\psi,\psi_i^\dagger]\cdots\psi_n^\dagger|0\rangle + 0$
      $= \sum_i\langle\psi|\psi_i\rangle\psi_1^\dagger\cdots\psi_{i-1}^\dagger\psi_{i+1}^\dagger\cdots\psi_n^\dagger|0\rangle$,
      consistent with the definition of $\hat\psi$ and commutation relation.
    * Fermions: $\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger|0\rangle \mapsto \hat\psi\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger|0\rangle$
      $= \sum_i(-1)^{i-1}\psi_1^\dagger\cdots\{\hat\psi,\psi_i^\dagger\}\cdots\psi_n^\dagger|0\rangle + (-1)^n\hat\psi_1^\dagger\cdots\hat\psi_n^\dagger\hat\psi|0\rangle$
      $= \sum_i(-1)^{i-1}\langle\psi|\psi_i\rangle\psi_1^\dagger\cdots\psi_{i-1}^\dagger\psi_{i+1}^\dagger\cdots\psi_n^\dagger|0\rangle$,
      consistent with the definition of $\hat\psi$ and anti-commutation relation.
  - Under coodinate basis: $\hat\psi^\dagger = \int\psi(x)\widehat{\psi^\dagger(x)}\,\mathrm{d}x$, $\hat\psi = \int\psi^*(x)\widehat{\psi(x)}\,\mathrm{d}x$.
    * Bosons: $[\hat\psi,\hat\psi'^\dagger] = \int\int\psi^*(x)\psi'(x')\,[\widehat{\psi(x)},\widehat{\psi^\dagger(x')}]\,\mathrm{d}x\mathrm{d}x'$
      $= \int\int\psi^*(x)\psi'(x')\,\delta(x-x')\,\mathrm{d}x\mathrm{d}x' = \int\psi^*(x)\psi'(x)\,\mathrm{d}x = \langle\psi|\psi'\rangle$.
      Anti-commutation relation of fermions is similar.

2. Creation and Annihilation Operators: Some Calculation Tricks

- For orthonormal basis of creation(annihilation) operators $\hat{e}_i^\dagger$ ($\hat{e}_i$), the commutator $[\hat{e}_i^\dagger \hat{e}_j, \hat{e}_k^\dagger] = \delta_{jk} \hat{e}_i^\dagger$. This is true for both bosons and fermions. Exercise: check this.
- By the above fact, $\hat{e}_i^\dagger \hat{e}_j \cdot \hat{e}_{i_1}^\dagger \dots \hat{e}_{i_n}^\dagger |\text{vac}\rangle =$ [sum of $\hat{e}_{i'_1}^\dagger \dots \hat{e}_{i'_n}^\dagger |\text{vac}\rangle$, where the sequence $(i'_1, \dots, i'_n)$ is $(i_1, \dots, i_n$ with one appearance of j replaced by $i)$].
  For example: $\hat{e}_1^\dagger \hat{e}_2 \cdot \hat{e}_1^\dagger \hat{e}_2^\dagger \hat{e}_2^\dagger \hat{e}_3^\dagger |\text{vac}\rangle = \hat{e}_1^\dagger \hat{e}_1^\dagger \hat{e}_2^\dagger \hat{e}_3^\dagger |\text{vac}\rangle + \hat{e}_1^\dagger \hat{e}_2^\dagger \hat{e}_1^\dagger \hat{e}_3^\dagger |\text{vac}\rangle$.

B. The Second Quantization

- The goal: use the creation & annihilation operators to simplify the presentations of operators for identical particles in Fock space.
- The rule of thumb: to get a many-body term (defined on the Fock space),
  replace the 1-body wavefunctions $\psi(x)$ [$\psi^*(x)$] in the expectation value formula for a product states by operator $\hat{\psi}(x)$ [$\widehat{\psi^\dagger(x)}$], remove the summations over particle indices. Some 'normal ordering' may be needed.
- Generic 1-body term $\hat{O}(x)$:
  - $\hat{O}(x)$ can be 'taking derivatives with respect to x' and 'multiplication by a function of x' and so on. Here x is the particle's coordinate.
  - For n identical particles with coordinates $x_1, \dots, x_n$, the corresponding many-body term in the 'first quantized' language is $\sum_{i=1}^n \hat{O}(x_i)$.
  - In a (anti-)symmetrized tensor product state $|\psi_1, \dots \psi_n\rangle$, the expectation value would be $\sum_{i=1}^n \int \psi_i^*(x_i)\, \hat{O}(x_i)\, \psi(x_i)\, \mathrm{d}x_i$.
  - The corresponding second quantized form is $\int \widehat{\psi^\dagger(x)}\, \hat{O}(x)\, \widehat{\psi(x)}\, \mathrm{d}x$.
- Example: 1-body kinetic energy term: $\sum_i \int \psi_i^*(x)(-\frac{\hbar^2 \partial_x^2}{2m})\psi_i(x)\, \mathrm{d}x$.
  Corresponding many-body term is $\int \widehat{\psi^\dagger(x)}(-\frac{\hbar^2 \partial_x^2}{2m})\widehat{\psi(x)}\, \mathrm{d}x = \int \widehat{\psi^\dagger(p)}(\frac{p^2}{2m})\widehat{\psi(p)}\, \mathrm{d}p$
- Example: 1-body potential term: $\sum_i \int V(x)\, \psi_i^*(x)\psi_i(x)\, \mathrm{d}x$.
  Corresponding many-body term is $\int V(x)\, \widehat{\psi^\dagger(x)}\widehat{\psi(x)}\, \mathrm{d}x$.
  Exercise: convert this into momentum eigenstate representation.

- Example: total particle number operator: $\hat{N} = \int \widehat{\psi^\dagger(x)}\widehat{\psi(x)}\,\mathrm{d}x$.
  It is difficult to write down the corresponding 'first quantized' form.

- Generic 2-body term $\hat{O}(x, x')$: x and x' are the two particles' coordinates.

  - For n identical particles with coordinates $x_1, \ldots, x_n$, the corresponding many-body term in the 'first quantized' language is $\frac{1}{2}\sum_{i,j,i\neq j}\hat{O}(x_i, x_j)$. Here the factor $\frac{1}{2}$ is to remove the double-counting of the same pair (x_i, x_j).
  - In a (anti-)symmetrized tensor product state $|\psi_1, \ldots \psi_n\rangle$, the expectation value would be $\frac{1}{2}\sum_{i,j,i\neq j}\int\int \psi_i^*(x_i)\psi_j^*(x_j)\,\hat{O}(x_i, x_j)\,\psi_j(x_j)\psi_i(x_i)\,\mathrm{d}x_i\mathrm{d}x_j$.
  - The corresponding second quantized form is
    $\frac{1}{2}\int\int \widehat{\psi^\dagger(x)}\widehat{\psi^\dagger(x')}\,\hat{O}(x, x')\,\widehat{\psi(x')}\widehat{\psi(x)}\,\mathrm{d}x\mathrm{d}x'$.

- Example: 2-body potential term: $(1/2)\sum_{i\neq j}\int V(x, x')\,\psi_i^*(x)\psi_i(x)\,\psi_j^*(x')\psi_j(x')\,\mathrm{d}x\mathrm{d}x'$.
  Corresponding many-body term is $\hat{V} = (1/2)\int V(x, x')\,\widehat{\psi^\dagger(x)}\widehat{\psi^\dagger(x')}\widehat{\psi(x')}\widehat{\psi(x)}\,\mathrm{d}x\mathrm{d}x$

  - Note the "normal ordering": put all creation operators in front of annihilation operators, be careful about the exchange sign in case of fermions.
  - Exercise: convert this into momentum eigenstate representation, in case that $V(x, x') = V(x - x')$ depends only on the distance of two particles.
  - In the 'first quantized' language, the 2-body potential term should be
    $\hat{V}: \quad \psi(x_1, \cdots, x_n) \mapsto (1/2)\sum_{i\neq j}V(x_i, x_j)\psi(x_1, \cdots, x_n)$.
  - Check: Assume the case of bosons.
    Many-body states can generically be expanded in terms of $|x_1, \cdots, x_n\rangle$ as $\int \psi(x_1, \cdots, x_n)|x_1, \cdots, x_n\rangle\,\mathrm{d}x_1\cdots\mathrm{d}x_n$. Apply the many-body term to coordinate basis state $|x_1, \cdots, x_n\rangle$. The result is
    $(1/2)\int V(x, x')\,\widehat{\psi^\dagger(x)}\hat{\psi}^\dagger(x')\sum_{i\neq j}\delta(x - x_i)\,\delta(x' - x_j)\,|x_i\&x_j \text{ removed}\rangle\,\mathrm{d}x\mathrm{d}x'$
    $= (1/2)\sum_{i\neq j}V(x_i, x_j)\,\hat{\psi}^\dagger(x_i)\hat{\psi}^\dagger(x_j)|x_i\&x_j \text{ removed}\rangle$
    $= (1/2)\sum_{i\neq j}V(x_i, x_j)\,|x_1, \cdots, x_n\rangle$.
    The above result shows that the action of $\hat{V}$ on many-body wavefunction $\psi(x_1, \cdots, x_n)$ is the same as the 'first quantized' description.
    Exercise: check the case of fermions, be careful about fermion exchange signs.

- Example: the Bose-Hubbard model.

$$\hat{H} = -t \sum_{<ij>} (\hat{b}_j^\dagger \hat{b}_i + h.c.) + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1),$$

where $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the occupation number operator, $h.c.$ means the Hermitian conjugate of the previous term. $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$ and all other commutators between them vanish.

  - On each site i of a lattice, there is one single-boson mode $\phi_i(\boldsymbol{x})$, and all ϕ_i form a complete orthonormal basis of 1-body Hilbert space. $\hat{b}_i^\dagger$ & $\hat{b}_i$ are the corresponding creation/annihilation operators.
  - The Hamiltonian consists of a kinetic energy term and an interaction term. The kinetic energy term makes a particle to 'hop' from site i to one of its neighbors j, with a matrix element $-t$. The interaction term creates repulsion energy U between each pair of particles on the same site.
  - Example: consider only two sites i & j, use the occupation number basis, the action of $\hat{H}$ on $|n_i = 3, n_j = 1\rangle$ is $\hat{H}\,|n_i = 3, n_j = 1\rangle =$
    $-t\,\sqrt{3}\,\sqrt{2}\,|n_i = 2, n_j = 2\rangle - t\,\sqrt{4}\,|n_i = 4, n_j = 0\rangle + 3\,U\,|n_i = 3, n_j = 1\rangle$.

III. SPECIAL MANY-BODY STATES

A. Fermion "Product" State (Fermi Sea)

- $|\psi_1, \cdots, \psi_n\rangle = \prod_{i=1}^n \hat{\psi}_i^\dagger\,|0\rangle$.
  Norm of this state is given by the Gram determinant $\sqrt{\det[\langle\psi_i|\psi_j\rangle]}$.
- If ψ_i are linearly dependent, this state vanishes.
- Linearly independent ψ_i span a n-dimensional 1-body Hilbert space. Given a complete orthonormal basis of this space c_i, then $|\psi_1, \cdots, \psi_n\rangle = \det[\langle c_i|\psi_j\rangle] \cdot |c_1, \cdots, c_n\rangle$,
  - Gram-Schmidt orthogonalization: the orthonormal basis can be constructed as
    $|c_1\rangle \propto |\psi_1\rangle$, e.g. $|c_1\rangle = \frac{|\psi_1\rangle}{\sqrt{\langle\psi_1|\psi_1\rangle}}$,
    $|c_2\rangle \propto |\psi_2\rangle - |c_1\rangle\langle c_1|\psi_2\rangle = |\psi_2\rangle - |\psi_1\rangle\frac{\langle\psi_1|\psi_2\rangle}{\langle\psi_1|\psi_1\rangle}$,
    $|c_3\rangle \propto |\psi_3\rangle - |c_1\rangle\langle c_1|\psi_3\rangle - |c_2\rangle\langle c_2|\psi_3\rangle$, ….

- If c_i $(i = 1, \cdots, m)$ form a complete orthonormal basis of 1-body Hilbert space, the total particle number $\hat{n} = \sum_i \hat{c}_i^\dagger \hat{c}_i$ is invariant under basis change. The state $|\psi_1, \cdots, \psi_n\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue n.
- The 'parent' Hamiltonian of this state: $\hat{H} = -\sum_{i=1}^{n} c_i^\dagger c_i + \sum_{i=n+1}^{m} c_i^\dagger c_i$. Namely the unique ground state of this Hamiltonian is this fermion product state.

1. *Particle-hole Transformation of Fermions*

- Particle-hole transformation of a single fermion mode: formally $\hat{c}_i \leftrightarrow \hat{c}_i^\dagger$, note that this preserves the anti-commutation relations.
  - This corresponds to a unitary transformation on the Fock space: $\hat{U} = (\hat{c}_i + \hat{c}_i^\dagger) \cdot (-1)^{\sum_{j\neq i} \hat{c}_j^\dagger \hat{c}_j}$.
    Exercise: check the following, $\hat{U}^\dagger \hat{U} = \mathbb{1}$, $\hat{U}\hat{c}_i\hat{U}^\dagger = \hat{c}_i^\dagger$, $\hat{U}\hat{c}_j\hat{U}^\dagger = \hat{c}_j$ for $j \neq i$.
  - The unitary transformation on occupation number basis is $|\cdots, n_i = 0, \cdots\rangle \leftrightarrow (-1)^{\sum_{j>i} n_j} |\cdots, n_i = 1, \cdots\rangle$.
    Note: the factor $(-1)^{\sum_{j>i} n_j}$ is to preserve the matrix elements of $\hat{\psi}_j \& \hat{\psi}_j^\dagger$ for $j > i$.
  - In particular, the new 'vacuum' is originally $|0, \cdots, n_i = 1, \cdots, 0\rangle$.
- Particle-hole transformation of all fermion modes: formally $\hat{c}_i \leftrightarrow \hat{c}_i^\dagger$ for all i.
  Exercise: what is the corresponding unitary transformation?
  what is the new 'vacuum'?
- By particle-hole transformation, the fermion product state $\hat{c}_1^\dagger \cdots \hat{c}_n^\dagger |0\rangle$ can be viewed as the 'vacuum' of $\hat{c'}_i = \begin{cases} c_i^\dagger, & 1 \le i \le n, \text{'hole' annihilation operators} \\ c_i, & n < i, \text{'particle' annihilation operators.} \end{cases}$

B. Fermion Pairing State (BCS State)

- Consider two orthonormal fermion modes c_1 & c_2, the pairing state is $|\lambda\rangle = (1 + |\lambda|^2)^{-1/2} \exp(\lambda\, \hat{c}_1^\dagger \hat{c}_2^\dagger)\, |0\rangle$, where $\lambda \in \mathbb{C}$ is a complex number.
  - This state is **not** an eigenstate of fermion number operator $\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2$.

– Bogoliubov transformation: define 'Bogoliubov quasiparticles',
$\hat\gamma_1 = u\hat c_1 + v\hat c_2^\dagger$, $\hat\gamma_2 = -v\hat c_1^\dagger + u\hat c_2$,
where $u = (1+|\lambda|^2)^{-1/2}$ and $v = -\lambda\,(1+|\lambda|^2)^{-1/2}$.
The pairing state is vanished by $\hat\gamma_{1,2}$, namely $\hat\gamma_{1,2}|\lambda\rangle = 0$.
Exercise: check this statement, and check that $\{\hat\gamma_i, \hat\gamma_j^\dagger\} = \delta_{ij}$.

– A 'parent' Hamiltonian is $\hat H = \hat\gamma_1^\dagger\hat\gamma_1 + \hat\gamma_2^\dagger\hat\gamma_2$. Exercise: rewrite this in terms of $\hat c$s.

- (Not required) Generic fermion pairing state $|\{f_{ij}\}\rangle \propto \exp(\frac{1}{2}\sum_{i,j} f_{ij}\hat c_i^\dagger \hat c_j^\dagger)|0\rangle$,
where $\hat c_i$ are some orthonormal basis, $f_{ij} = -f_{ji}$ are complex numbers.

– By a orthogonal transformation $\hat c_i^\dagger \to O_{ij}\hat{c'}_j^\dagger$, where O is an orthogonal matrix, the antisymmetric f matrix can be brought into a standard form

$$O^T \cdot f \cdot O = \begin{pmatrix} 0 & \lambda_1 & 0 & 0 & \cdots \\ -\lambda_1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \lambda_2 & \cdots \\ 0 & 0 & -\lambda_2 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

the state becomes $\propto \exp(\lambda_1 \hat{c'}_1^\dagger \hat{c'}_2^\dagger + \lambda_2 \hat{c'}_3^\dagger \hat{c'}_4^\dagger + \ldots)|0\rangle = e^{\lambda_1 \hat{c'}_1^\dagger \hat{c'}_2^\dagger} e^{\lambda_2 \hat{c'}_3^\dagger \hat{c'}_4^\dagger}\ldots|0\rangle$.
Bogoliubov transformations can then be defined on $\hat{c'}_{2i-1}$ & $\hat{c'}_{2i}$.

C. Boson Coherent State

- The coherent state from a single boson mode $\hat b$ is $|z\rangle = e^{-|z|^2/2}\, e^{z\hat b^\dagger}|0\rangle$,
where $z \in \mathbb{C}$ is a complex number.
Exercise: check the normalization of $|z\rangle$.

– This state is **not** an eigenstate of boson number $\hat b^\dagger \hat b$.

– (USEFUL) This state is an eigenstate of $\hat b$, $\hat b|z\rangle = z|z\rangle$.
Therefore the coherent state is vanished by $\hat b' = \hat b - z$.
Exercise: check this statement, and that $[\hat b', \hat b'^\dagger] = 1$.

– The 'parent' Hamiltonian is thus $\hat H = \hat b'^\dagger \hat b'$.

– Expectation value of 'normal ordered' polynomials of $\hat b^\dagger$ and $\hat b$ (all $\hat b^\dagger$s appear in front of $\hat b$s) in state $|z\rangle$ can be obtained by simply replacing $\hat b^\dagger$ by z^* and $\hat b$ by z.
Example: $\langle z|(\hat b^\dagger \hat b)^2|z\rangle = \langle z|(\hat b^\dagger\hat b^\dagger\hat b\hat b + \hat b^\dagger\hat b)|z\rangle = z^*z^*zz + z^*z = |z|^4 + |z|^2$.

D. Boson Pairing State

- Consider two orthonormal boson modes $\hat{b}_1$ & $\hat{b}_2$, the boson pairing state is $|\lambda\rangle = (1-|\lambda|^2)^{1/2}\exp(\lambda\,\hat{b}_1^\dagger\hat{b}_2^\dagger)\,|0\rangle$, where $\lambda\in\mathbb{C}$ is a complex number, and $|\lambda|<1$.
  Exercise: check the normalization of $|\lambda\rangle$.
  - This state is **not** an eigenstate of boson number $\hat{b}_1^\dagger\hat{b}_1+\hat{b}_2^\dagger\hat{b}_2$.
  - Bogoliubov transformation: define $\hat{\gamma}_1 = u\hat{b}_1 + v\hat{b}_2^\dagger$, $\hat{\gamma}_2 = u\hat{b}_2 + v\hat{b}_1^\dagger$,
    where $u=(1-|\lambda|^2)^{-1/2}$ and $v=-\lambda\,(1-|\lambda|^2)^{-1/2}$.
    Then $|\lambda\rangle$ is vanished by $\hat{\gamma}_{1,2}$, namely $\hat{\gamma}_{1,2}|\lambda\rangle=0$.
    Exercise: check this statement, and check that $[\hat{\gamma}_i,\hat{\gamma}_j^\dagger]=\delta_{ij}$.
  - A 'parent' Hamiltonian is $\hat{H}=\hat{\gamma}_1^\dagger\hat{\gamma}_1+\hat{\gamma}_2^\dagger\hat{\gamma}_2$. Exercise: rewrite this in terms of $\hat{b}$s.

E. Summary of These Special Many-body States

- All these special states are "free particle" states, they can be defined as the 'vacuum' of a complete set of single-particle "annihilation" operators.

Free particle state	complete set of "annihilation" operators
Fermion product state	(particle-hole transformed) fermion annihilation operators
Boson coherent state	boson annihilation operators shifted by constants
Boson(Fermion)pairing state	Bogoliubov quasi-particles (superposition of particles and 'holes')

- The Wick expansion: rough statement.
  Expectation value of a product of single-particle creation/annihilation operators in these states (except boson coherent states), can be expanded into a sum of products of pair expectation values, over all pair combinations with appropriate sign for fermions.

- The Wick expansion:
  Let $|0\rangle$ be the single-particle 'vacuum'. Let $\hat{A}_i$ $(i=1,\dots,2n)$ be a set of single-particle operators, namely linear combinations of annihilation and creation operators. Then $\langle 0|\hat{A}_1\hat{A}_2\cdots\hat{A}_{2n}|0\rangle$ is the Hafnian(Pfaffian) of matrix $\langle 0|\hat{A}_i\hat{A}_j|0\rangle$ for bosons(fermions).
  - Hafnian of $2n\times 2n$ symmetric matrix M_{ij} is
    $\mathrm{Hf}(M)=\frac{1}{n!}\sum_{\sigma\in S_{2n},\sigma(1)<\sigma(2),\sigma(3)<\sigma(4),\dots} M_{\sigma(1)\sigma(2)}M_{\sigma(3)\sigma(4)}\cdots M_{\sigma(2n-1)\sigma(2n)}$.

– Pfaffian of $2n \times 2n$ anti-symmetric matrix M_{ij} is
$\mathrm{Pf}(M) = \frac{1}{n!} \sum_{\sigma \in S_{2n}, \sigma(1)<\sigma(2), \sigma(3)<\sigma(4), \ldots} (-1)^{\sigma} M_{\sigma(1)\sigma(2)} M_{\sigma(3)\sigma(4)} \cdots M_{\sigma(2n-1)\sigma(2n)}$.

– NOTE: this is true only for such 'free particle' states $|0\rangle$.

– NOTE: the matrix $\langle 0|\hat{A}_i \hat{A}_j|0\rangle$ may not be symmetric or anti-symmetric. But the above definition for Hafnian/Pfaffian still works for the Wick expansion.

– Example: $\langle \hat{A}_1 \hat{A}_2 \hat{A}_3 \hat{A}_4 \rangle = \langle \hat{A}_1 \hat{A}_2 \rangle \langle \hat{A}_3 \hat{A}_4 \rangle + \langle \hat{A}_1 \hat{A}_4 \rangle \langle \hat{A}_2 \hat{A}_3 \rangle \pm \langle \hat{A}_1 \hat{A}_3 \rangle \langle \hat{A}_2 \hat{A}_4 \rangle$,
the $\pm$ sign is for boson or fermion cases respectively.

- The Wick expansion: sketch of a proof.

  Consider boson case first. Use mathematical induction.

  For the case of two operators, the Wick expansion is trivially true.

  Suppose the expansion is correct for product of $2n$ and less operators.

  Add two more operators, we just need to prove that
  $\langle \hat{A}_1 \cdots \hat{A}_{2n} \cdot \hat{A}_{2n+1} \hat{A}_{2n+2} \rangle = \langle \hat{A}_1 \cdots \hat{A}_{2n} \rangle \langle \hat{A}_{2n+1} \hat{A}_{2n+2} \rangle$
  $+ \sum_{i,j,i\neq j} \langle (\hat{A}_1 \cdots \hat{A}_{2n} \text{ without } \hat{A}_i, \hat{A}_j) \rangle \langle \hat{A}_i \hat{A}_{2n+1} \rangle \langle \hat{A}_j \hat{A}_{2n+2} \rangle$.
  Because of linearity, only need to consider four possible cases, with $(\hat{A}_{2n+1},\ \hat{A}_{2n+2}) =$
  (I) both annihilation operators $(\hat{\psi},\ \hat{\phi})$, this is trivially $0 = 0$;
  (II) both creation operators $(\hat{\psi}^\dagger,\ \hat{\phi}^\dagger)$, try to move A_{2n+1} and A_{2n+2} to the left side by commutation relations, $\langle \hat{A}_1 \cdots \hat{A}_{2n} \hat{A}_{2n+1} \hat{A}_{2n+2} \rangle$
  $= \langle \hat{A}_{2n+1} \cdot \hat{A}_1 \cdots \hat{A}_{2n} \cdot \hat{A}_{2n+2} \rangle + \langle [\hat{A}_1 \cdots \hat{A}_{2n}, \hat{A}_{2n+1}] \cdot \hat{A}_{2n+2} \rangle$
  $= 0 + \sum_i \langle (\hat{A}_1 \cdots \hat{A}_{2n} \text{ without } \hat{A}_i) [\hat{A}_i, \hat{A}_{2n+1}] \cdot \hat{A}_{2n+2} \rangle$
  (NOTE: $[\hat{A}_i, \hat{A}_{2n+1}]$ is a c-number)
  $= \sum_i \langle \hat{A}_{2n+2} \cdot (\hat{A}_1 \cdots \hat{A}_{2n} \text{ without } \hat{A}_i) \rangle \cdot [\hat{A}_i, \hat{A}_{2n+1}]$
  $+ \sum_i \langle [(\hat{A}_1 \cdots \hat{A}_{2n} \text{ without } \hat{A}_i), \hat{A}_{2n+2}] \rangle \cdot [\hat{A}_i, \hat{A}_{2n+1}]$
  $= 0 + \sum_i \sum_{j,j\neq i} \langle (\hat{A}_1 \cdots \hat{A}_{2n} \text{ without } \hat{A}_i, \hat{A}_j) \rangle \cdot [\hat{A}_i, \hat{A}_{2n+1}][\hat{A}_j, \hat{A}_{2n+2}]$.
  In this case, $[\hat{A}_i, \hat{A}_{2n+1}] = \langle \hat{A}_i \hat{A}_{2n+1} \rangle$, $[\hat{A}_j, \hat{A}_{2n+2}] = \langle \hat{A}_j \hat{A}_{2n+2} \rangle$, and $\langle \hat{A}_{2n+1} \hat{A}_{2n+2} \rangle = 0$.
  So this extends the Wick expansion to $2n + 2$ operator case.
  (III) $(\hat{\psi}^\dagger,\ \hat{\phi})$, and (IV) $(\hat{\psi},\ \hat{\phi}^\dagger)$ are left for exercise.
  Exercise: repeat the above reasoning for fermions.

Summary of Lecture #3: quantum dynamics

Goals and Requirements:

- Get a clear understanding about the Schrödinger $\{ \, \mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi,t\rangle = \hat{H}_{\mathrm{S}}(t)|\psi,t\rangle \, \}$
  and the Heisenberg $\{ \, \hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_{\mathrm{H}}(t) = \mathbb{i}\,[\hat{H}_{\mathrm{H}}(t), \hat{O}_{\mathrm{H}}(t)] \, \}$
  pictures about time evolution.

- Get some basic understanding about propagators (Green's functions):
  matrix element of time-evolution operator.

- Get some basic understanding about path integrals.

- Get some taste about geometric phase: Berry's phase.

- Get some basic understanding about gauge invariance in quantum mechanics.

- Optional references:
  J.J. Sakurai, *Modern Quantum Mechanics*, Chapter 2.
  P.A.M. Dirac, *The Principle of Quantum Mechanics*, Chapter V.
  R.P. Feynman, A.R. Hibbs, *Quantum Mechanics and Path Integral*, Chapter 2.
  A. Altland, B.D. Simons, *Condensed Matter Field Theory*, Chapter 3.
  M.E. Peskin, D.V. Schroeder, *An Introduction to Quantum Field Theory*, Section 9.1

- Note: for simplicity I will frequently assume the space is one-dimensional,
  generalization to higher spatial dimensions should be obvious in most cases.

I. TIME EVOLUTION

A. Unitary Time Evolution

- The basic assumption of quantum dynamics:
  time evolution of a *closed* system is unitary.
  - State at t is related to state at t_0 by a unitary operator $\hat{U}(t, t_0)$:
    $|\psi, t\rangle = \hat{U}(t, t_0)|\psi, t_0\rangle$, $\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0) = \mathbb{1}$.
  - $\hat{U}(t, t_1) \cdot \hat{U}(t_1, t_0) = \hat{U}(t, t_0)$, and $\hat{U}(t_0, t_0) = \mathbb{1}$.
  - The time evolution is usually 'continuous', and reversible, $\hat{U}^\dagger(t, t_0) = [\hat{U}(t, t_0)]^{-1}$.
- The infinitesimal time evolution: $\hat{U}(t_0 + \mathrm{d}t, t_0) = \mathbb{1} - \frac{\mathbb{i}}{\hbar}\hat{H}(t_0)\,\mathrm{d}t + O(\mathrm{d}t^2)$.
  The Hamiltonian $\hat{H}(t_0) = \mathbb{i}\hbar\,\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0)\Big|_{t=t_0} = \mathbb{i}\hbar\,\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) \cdot \hat{U}^\dagger(t, t_0)\Big|_{t=t_0}$.
  - $\hat{H}(t) = \mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) \cdot \hat{U}^\dagger(t, t_0)$, independent of the choice of t_0:
    $\mathbb{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0') \cdot \hat{U}^\dagger(t, t_0') = \mathbb{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0)\hat{U}(t_0, t_0') \cdot [\hat{U}(t, t_0)\hat{U}(t_0, t_0')]^\dagger$
    $= \mathbb{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0)\hat{U}(t_0, t_0') \cdot \hat{U}^\dagger(t_0, t_0')\hat{U}^\dagger(t, t_0) = \mathbb{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) \cdot \hat{U}^\dagger(t, t_0)$.
  - $\hat{H}$ is Hermitian:
    $\hat{H}^\dagger = -\mathbb{i}\hbar\hat{U}(t, t_0)\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}^\dagger(t, t_0) = -\mathbb{i}\hbar\{\frac{\mathrm{d}}{\mathrm{d}t}[\hat{U}(t, t_0) \cdot \hat{U}^\dagger(t, t_0)] - \frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) \cdot \hat{U}^\dagger(t, t_0)\}$
    $= -\mathbb{i}\hbar\{\frac{\mathrm{d}}{\mathrm{d}t}(\mathbb{1}) - \frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) \cdot \hat{U}^\dagger(t, t_0)\} = \mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) \cdot \hat{U}^\dagger(t, t_0) = \hat{H}$

B. The Schrödinger Equation and The Schrödinger Picture

- From the definition of Hamiltonian, we have the
  Schrödinger equation for the time evolution operator: $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) = \hat{H}(t) \cdot \hat{U}(t, t_0)$.
- This translates into the
  Schrödinger equation for the quantum state: $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi, t\rangle = \hat{H}(t)|\psi, t\rangle$,
  and the Schrödinger equation for the 'bra': $-\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi, t| = \langle\psi, t|\hat{H}(t)$.
- Explicit form of the time evolution operator in terms of $\hat{H}$:
  - If $\hat{H}$ is independent of t, $\hat{U}(t, t_0) = \exp[-\mathbb{i}(t - t_0)\hat{H}/\hbar]$. (IMPORTANT)
    Conversely, if $\hat{U}(t, t_0)$ depends only on $(t - t_0)$, then $\hat{H}$ is independent of time.

  - In general, $\hat{U}(t,t_0) = \mathcal{T}(\exp[-\frac{\mathbb{i}}{\hbar}\int_{t'=t_0}^{t}\hat{H}(t')\mathrm{d}t'])$, where $\mathcal{T}$ means time-ordering.
    * Time-ordering for bosonic $\hat{A}$ & $\hat{B}$, $\mathcal{T}[\hat{A}(t)\hat{B}(t')] = \begin{cases} \hat{A}(t)\hat{B}(t'), & t > t', \\ \hat{B}(t')\hat{A}(t), & t' > t. \end{cases}$
  - This is equivalent to the Dyson series,
    $\hat{U}(t,t_0) = \mathbb{1} + \frac{-\mathbb{i}}{\hbar}\int_{t_1=t_0}^{t}\hat{H}(t_1)\mathrm{d}t_1 + (\frac{-\mathbb{i}}{\hbar})^2\int_{t_2=t_0}^{t}\int_{t_1=t_0}^{t_2}\hat{H}(t_2)\hat{H}(t_1)\mathrm{d}t_2\mathrm{d}t_1 + \cdots$.

- Stationary states: eigenstates of $\hat{H}$, $|\hat{H}=E,t\rangle = e^{-\mathbb{i}E(t-t_0)}|\hat{H}=E,t_0\rangle$.
  Expectation value of any operator does not change over time (stationary).
  Density matrix does not change over time.

- This is the Schrödinger picture (subscript $_\mathrm{S}$ hereafter):
  time evolution is implemented on the states.

C. The Heisenberg picture

- The Heisenberg picture (subscript $_\mathrm{H}$ hereafter):
  time evolution is encoded in operators, while the states have no evolution.

- Consider the time evolution of matrix elements of an operator $\hat{O}_\mathrm{S}$:
  $\langle\phi,t|\hat{O}_\mathrm{S}|\psi,t\rangle = \langle\phi,t_0=0|\hat{U}^\dagger(t)\hat{O}_\mathrm{S}\hat{U}(t)|\psi,t_0=0\rangle$.

- Define the time-dependent operator $\hat{O}_\mathrm{H}(t)$ in the Heisenberg picture:
  (IMPORTANT) $\hat{O}_\mathrm{H}(t) = \hat{U}^\dagger(t)\hat{O}_\mathrm{S}\hat{U}(t)$.
  The time-dependent matrix element is simply $\langle\phi|\hat{O}_\mathrm{H}(t)|\psi\rangle$,
  where the states ϕ & ψ do not evolve over time in Heisenberg picture.

- The Heisenberg equation of motion: $\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_\mathrm{H}(t) = \mathbb{i}\,[\hat{H}_\mathrm{H}(t),\hat{O}_\mathrm{H}(t)]$.
  NOTE: the Hamiltonian $\hat{H}_\mathrm{H}(t)$ here is also in the Heisenberg picture, $\hat{H}_\mathrm{H}(t) = \mathbb{i}\hbar\,\hat{U}^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t) = \hat{U}^\dagger(t)\hat{H}_\mathrm{S}(t)\hat{U}(t)$.
  - Proof: use $\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t) = -\mathbb{i}\hat{U}(t)\cdot\mathbb{i}\hbar\hat{U}^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t) = -\mathbb{i}\hat{U}(t)\cdot\hat{H}_\mathrm{H}(t)$, and
    $\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}^\dagger(t) = \hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}^\dagger(t)\cdot\hat{U}(t)\hat{U}^\dagger(t) = -\hbar\hat{U}^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)\cdot\hat{U}^\dagger(t) = \mathbb{i}\hat{H}_\mathrm{H}(t)\cdot\hat{U}^\dagger(t)$.
    Then $\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_\mathrm{H}(t) = \hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}^\dagger(t)\cdot\hat{O}_\mathrm{S}\cdot\hat{U}(t) + \hat{U}^\dagger(t)\cdot\hat{O}_\mathrm{S}\cdot\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)$
    $= \mathbb{i}\hat{H}_\mathrm{H}(t)\cdot\hat{U}^\dagger(t)\cdot\hat{O}_\mathrm{S}\cdot\hat{U}(t) - \mathbb{i}\hat{U}^\dagger(t)\cdot\hat{O}_\mathrm{S}\cdot\hat{U}(t)\cdot\hat{H}_\mathrm{H}(t) = \mathbb{i}\,[\hat{H}_\mathrm{H}(t),\hat{O}_\mathrm{H}(t)]$.
  - If $\hat{H}_\mathrm{S}(t)$ is independent of time, then $\hat{H}$ commutes with $\hat{U}(t)$, and $\hat{H}_\mathrm{H} = \hat{H}_\mathrm{S}$.

D. Some Applications

- The Schrödinger picture: quantum Liouville equation,
  time evolution of density matrix: $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = [\hat{H}_{\mathrm{S}}(t), \hat{\rho}(t)]$.
- Consider time-independent $\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}})$.
  - The Schrödinger picture: continuity equation, $\frac{\mathrm{d}}{\mathrm{d}t}[\rho(\boldsymbol{x},t)] + \nabla\cdot\boldsymbol{J}(\boldsymbol{x},t) = 0$,
    where the probability density $\rho(\boldsymbol{x},t) = \psi^*(\boldsymbol{x},t)\psi(\boldsymbol{x},t) = \langle x|\hat{\rho}(t)|x\rangle$,
    probability current $\boldsymbol{J}(\boldsymbol{x},t) = \mathrm{Re}[\psi^*(\boldsymbol{x},t)\frac{-\mathbb{i}\hbar\partial_{\boldsymbol{x}}}{m}\psi(\boldsymbol{x},t)]$.
  - The Heisenberg picture: Ehrenfest theorem:
    the equation of motion of position $\hat{\boldsymbol{x}}$ and momentum $\hat{\boldsymbol{p}}$ are (subscript $_{\mathrm{H}}$ omitted)
    $\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{x}}(t) = \frac{\mathbb{i}}{\hbar}[\hat{H}, \hat{\boldsymbol{x}}(t)] = \hat{\boldsymbol{p}}/m$,
    $\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{p}}(t) = \frac{\mathbb{i}}{\hbar}[\hat{H}, \hat{\boldsymbol{p}}(t)] = \mathbb{i}[V(\hat{\boldsymbol{x}}), \hat{\boldsymbol{p}}] = -\frac{\partial}{\partial\boldsymbol{x}}V(\boldsymbol{x})$.
    Combine them, $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\hat{\boldsymbol{x}}(t) = -\frac{\partial}{\partial\boldsymbol{x}}V(\boldsymbol{x})$, or equivalently, $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{\boldsymbol{x}}\rangle = -\langle\frac{\partial}{\partial\boldsymbol{x}}V(\boldsymbol{x})\rangle$,
    which looks like the classical equation of motion.
- 1D harmonic oscillator: time-independent $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2)$,
  where $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{\mathbb{i}\hat{p}}{m\omega})$, $[\hat{a}, \hat{a}^\dagger] = 1$. $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$, $\hat{p} = -\mathbb{i}\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^\dagger)$.
  Normalized ground state $|0\rangle$ ($\hat{a}|0\rangle = 0$), and excited states $|n\rangle \equiv \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle$, energy eigenvalues $E_n = \hbar\omega\cdot(n + \frac{1}{2})$.
  - Equation of motion: $\frac{\mathrm{d}}{\mathrm{d}t}\hat{a}(t) = \frac{\mathbb{i}}{\hbar}[\hat{H}, \hat{a}(t)] = -\mathbb{i}\omega\,\hat{a}(t)$. Then
    $\hat{a}(t) = e^{-\mathbb{i}\omega t}\,\hat{a}(0)$, $\hat{a}^\dagger(t) = e^{\mathbb{i}\omega t}\,\hat{a}^\dagger(0)$.
  - Solution to the equation of motion of $\hat{x}$ and $\hat{p}$: ellipse on $\langle x\rangle$-$\langle p\rangle$ plane,
    $\hat{x}(t) = \cos(\omega t)\,\hat{x}(0) + \frac{1}{m\omega}\sin(\omega t)\,\hat{p}(0)$,
    $\hat{p}(t) = -m\omega\sin(\omega t)\,\hat{x}(0) + \cos(\omega t)\,\hat{p}(0)$.
  - Example: $t = 0$ state is coherent state, $|\psi(0)\rangle = e^{-|z|^2/2}e^{z\hat{a}^\dagger}|0\rangle$, with $\langle\hat{a}(0)\rangle = z$.
    Then $\langle\hat{x}(0)\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}(z)$, $\langle\hat{p}(0)\rangle = \sqrt{2\hbar m\omega}\,\mathrm{Im}(z)$.
    The expectation value of $\hat{x}$ at time t is $\langle\hat{x}(t)\rangle = \cos(\omega t)\langle\hat{x}(0)\rangle + \frac{\sin(\omega t)}{m\omega}\langle\hat{p}(0)\rangle$
    $= \sqrt{\frac{2\hbar}{m\omega}}\mathrm{Re}(ze^{-\mathbb{i}\omega t})$. You do not need to solve $|\psi(t)\rangle = e^{-\frac{\mathbb{i}}{\hbar}\hat{H}\cdot t}|\psi(0)\rangle$.
  - The coherent state satisfies the minimal uncertainty relation for $\hat{x}$ and $\hat{p}$:
    $\langle\hat{x}^2\rangle - (\langle\hat{x}\rangle)^2 = \frac{\hbar}{2m\omega}$, $\langle\hat{p}^2\rangle - (\langle\hat{p}\rangle)^2 = \frac{\hbar m\omega}{2}$, so $\langle(\Delta\hat{x})^2\rangle\,\langle(\Delta\hat{p})^2\rangle = \frac{\hbar^2}{4} = \frac{1}{4}|\langle[\hat{x}, \hat{p}]\rangle|^2$.
    Exercise: check the proof of uncertainty relation to see why.

- Landau level: time-independent $\hat{H} = \frac{1}{2m}\hat{\boldsymbol{P}}^2 = \frac{1}{2m}[\hat{\boldsymbol{p}} - q\boldsymbol{A}(\boldsymbol{r})]^2$,
charge-q particle in xy-plane under uniform magnetic field $\boldsymbol{B} = B\boldsymbol{e}_z$ along z ($B > 0$), $\boldsymbol{r} = (x, y)$, $\hat{\boldsymbol{p}} = -\mathbb{i}(\frac{\partial}{\partial x}, \frac{\partial}{\partial y})$, $\boldsymbol{A}$ is vector potential with $\nabla\times\boldsymbol{A} = \boldsymbol{B}$ or $\frac{\partial}{\partial x}A_y - \frac{\partial}{\partial y}A_x = B$.

  - Note: $[\hat{r}_a, \hat{r}_b] = 0$, $[\hat{r}_a, \hat{P}_b] = \mathbb{i}\hbar\delta_{ab}$,
  $[\hat{P}_a, \hat{P}_b] = [\hat{p}_a - qA_a, \hat{p}_b - qA_b] = \mathbb{i}\hbar q\,(\partial_a A_b - \partial_b A_a) = \mathbb{i}\hbar q \sum_c \epsilon_{abc}B_c$.
  - Equation of motion: $\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{r}} = \frac{\mathbb{i}}{\hbar}[\hat{H}, \hat{\boldsymbol{r}}] = \frac{1}{m}\hat{\boldsymbol{P}}$,
  $\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{P}} = \frac{\mathbb{i}}{\hbar}[\hat{H}, \hat{\boldsymbol{P}}] = \frac{q}{2m}(\hat{\boldsymbol{P}}\times\boldsymbol{B} - \boldsymbol{B}\times\hat{\boldsymbol{P}})$, for uniform $\boldsymbol{B}$, $\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{P}} = \frac{q}{m}\hat{\boldsymbol{P}}\times\boldsymbol{B}$.
  Combine these, $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\hat{\boldsymbol{r}}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{r}}(t)\times q\boldsymbol{B}$, Lorentz force & cyclotron motion.
  - Define $\hat{b} = \sqrt{\frac{1}{2\hbar qB}}(\hat{P}_x + \mathbb{i}\hat{P}_y)$, then $[\hat{b}, \hat{b}^\dagger] = 1$, and $\hat{H} = \hbar\omega_c(\hat{b}^\dagger\hat{b} + 1/2)$.
  $\omega_c = qB/m$ is the cyclotron frequency, energy levels are $E_n = \hbar\omega_c\cdot(n + 1/2)$ for non-negative integer n. Exercise: check these statements.
  - Guiding center coordinates: $\hat{\boldsymbol{R}} = (\hat{X}, \hat{Y}) = \hat{\boldsymbol{r}} - \frac{\boldsymbol{e}_z}{qB}\times\hat{\boldsymbol{P}} = (\hat{x} + \frac{\hat{P}_y}{qB}, \hat{y} - \frac{\hat{P}_x}{qB})$.
  $\hat{\boldsymbol{R}}$ is conserved: $\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{R}}(t) = \mathbb{i}[\hat{H}, \hat{\boldsymbol{R}}] = 0$.
  NOTE: $[\hat{X}, \hat{Y}] = -\frac{\mathbb{i}}{qB} \neq 0$, indicates degeneracy of Landau level.
  Exercise: $e^{\mathbb{i}\hat{X}}$ commutes with $\hat{H}$, but changes eigenvalue of $\hat{Y}$ by $-1/qB$.

- The adiabatic theorem: roughly speaking, if a system starts at (one of) the instantaneous ground state(s), and the Hamiltonian changes *slowly* with time, then the system will remain to be (one of) the instantaneous ground state(s) at later times.

  - Sketch of a proof (for non-degenerate case):
  Denote the instantaneous eigenstates of $\hat{H}_S(t)$ by $|\psi_n(t)\rangle$, and corresponding eigenvalues by $E_n(t)$, where $n = 0, 1, 2, \ldots$, and $E_0(t) < E_1(t) < E_2(t) < \ldots$.
  Suppose $|\psi, t\rangle$ satisfies $\mathbb{i}\hbar\frac{\partial}{\partial t}|\psi, t\rangle = \hat{H}_S(t)|\psi, t\rangle$, and $|\psi, t = 0\rangle = |\psi_0(t = 0)\rangle$.
  Expand $|\psi, t\rangle$, $|\psi, t\rangle = \sum_n c_n(t)e^{-\mathbb{i}\theta_n(t)}|\psi_n(t)\rangle$, where $\theta_n(t) \equiv \frac{1}{\hbar}\int_0^t E_n(t)\mathrm{d}t$. The Schrödinger equation becomes differential equations for coefficients $c_n(t)$,
  $\frac{\partial}{\partial t}c_n(t) = -\sum_m \langle\psi_n(t)|(\frac{\partial}{\partial t}|\psi_m(t)\rangle)\cdot e^{\mathbb{i}\theta_n(t) - \mathbb{i}\theta_m(t)}\cdot c_m(t)$, and $c_0(t = 0) = 1$, $c_{n\neq 0}(t = 0) = 0$. Take t-derivative on $\langle\psi_n(t)|\psi_m(t)\rangle = \delta_{mn}$ and $\langle\psi_n(t)|\hat{H}_S(t)|\psi_m(t)\rangle = \delta_{mn}E_n(t)$, we have $\langle\psi_n(t)|(\frac{\partial}{\partial t}|\psi_m(t)\rangle) = \frac{1}{E_m(t) - E_n(t)}\cdot\langle\psi_n(t)|\frac{\partial\hat{H}_S(t)}{\partial t}|\psi_m(t)\rangle$ for $m \neq n$. So if the magnitude of $\left[\frac{1}{E_0(t) - E_n(t)}\cdot\langle\psi_n(t)|\frac{\partial\hat{H}_S(t)}{\partial t}|\psi_0(t)\rangle\cdot(\text{time duration})\right]$ is small, the final $c_{n\neq 0}(t)$ will be small, the system will approximately remain to be the instantaneous ground state (up to an overall phase).

II. PROPAGATOR AND PATH INTEGRAL

A. Brief Review of Gaussian Integrals

- One dimensional case: $\int_{-\infty}^{\infty} e^{-x^2/2a}\,\mathrm{d}x = \sqrt{2\pi\, a}$.
  - $\langle x^2 \rangle = \frac{\int x^2\, e^{-x^2/2a}\,\mathrm{d}x}{\int e^{-x^2/2a}\,\mathrm{d}x} = a$.
  - $\langle x^{2n} \rangle = \frac{\int x^{2n}\, e^{-x^2/2a}\,\mathrm{d}x}{\int e^{-x^2/2a}\,\mathrm{d}x} = a^n \cdot (2n-1)!!$, satisfies the 'Wick expansion' [$(2n-1)!! = (2n-1)(2n-3)\cdots(1)$ ways of pairing up xs].
  - $\int_{-\infty}^{\infty} e^{-x^2/2a+yx}\,\mathrm{d}x = \sqrt{2\pi\, a}\cdot e^{ay^2/2}$.
- Higher dimensional Gaussian integral: $\int \exp(-\frac{\boldsymbol{x}\cdot\boldsymbol{A}^{-1}\cdot\boldsymbol{x}}{2})\,\mathrm{d}^m\boldsymbol{x} = (2\pi)^{m/2}\sqrt{\det \boldsymbol{A}}$, where $\boldsymbol{x} = (x_i)$ is m-component real vector, $\boldsymbol{A} = (A_{ij})$ is $m\times m$ real symmetric positive-definite matrix, the integral is over all components of $\boldsymbol{x}$ from $-\infty$ to $+\infty$.
  - $\langle x_i x_j \rangle = \frac{\int x_i x_j\, \exp(-\boldsymbol{x}\cdot\boldsymbol{A}^{-1}\cdot\boldsymbol{x}/2)\,\mathrm{d}^m\boldsymbol{x}}{\int \exp(-\boldsymbol{x}\cdot\boldsymbol{A}^{-1}\cdot\boldsymbol{x}/2)\,\mathrm{d}^m\boldsymbol{x}} = A_{ij}$.
  - 'Wick expansion': all possible ways of pairing up xs,
    example, $\langle x_i x_j x_k x_\ell \rangle = A_{ij}A_{k\ell} + A_{ik}A_{j\ell} + A_{i\ell}A_{jk}$.
  - $\int \exp(-\boldsymbol{x}\cdot\boldsymbol{A}^{-1}\cdot\boldsymbol{x}/2 + \boldsymbol{y}\cdot\boldsymbol{x})\,\mathrm{d}^m\boldsymbol{x} = (2\pi)^{m/2}\sqrt{\det \boldsymbol{A}}\cdot\exp(\boldsymbol{y}\cdot\boldsymbol{A}\cdot\boldsymbol{y}/2)$.
- Complex Gaussian integral: $\int e^{-z^* z/a}\,\mathrm{d}^2 z = \pi a$,
  where $\mathrm{d}^2 z = \mathrm{dRe}z\,\mathrm{dIm}z$, and the integral is over $\mathrm{Re}z$ and $\mathrm{Im}z$ from $-\infty$ to $+\infty$.
  - $\langle z\, z^* \rangle = \frac{\int z\, z^*\, e^{-z^* z/a}\,\mathrm{d}^2 z}{\int e^{-z^* z/a}\,\mathrm{d}^2 z} = a$.
  - $\langle z^n\,(z^*)^m \rangle = 0$ if $n \neq m$. Consider $z \to e^{\mathrm{i}\theta} z$.
  - $\langle z^n\,(z^*)^n \rangle = a^n \cdot n!$ ('Wick expansion': $n!$ ways of pairing up z^* and z).
  - $\int e^{-z^* z/a + y^* z + z^* y}\,\mathrm{d}^2 z = \pi a\, e^{a y^* y}$.
- Higher dimensional complex Gaussian integral: $\int \exp(-\boldsymbol{z}^*\cdot\boldsymbol{A}^{-1}\cdot\boldsymbol{z})\,\mathrm{d}^{2m}\boldsymbol{z} = \pi^m\,\det(\boldsymbol{A})$, where $\boldsymbol{z} = (z_i)$ is m-component complex vector, $\boldsymbol{A} = (A_{ij})$ is a $m\times m$ Hermitian positive-definite matrix.
  - $\langle z_i z_j^* \rangle = A_{ij}$.
  - Non-vanishing 'correlators' must contain the same number of z^* and z.

- 'Wick expansion': all possible ways of pairing up z^* and z,
  example, $\langle z_i z_j z_k^* z_\ell^* \rangle = A_{ik}A_{j\ell} + A_{i\ell}A_{jk}$.
- $\int \exp(-\boldsymbol{z}^* \cdot \boldsymbol{A}^{-1} \cdot \boldsymbol{z} + \boldsymbol{y}^* \cdot \boldsymbol{z} + \boldsymbol{z}^* \cdot \boldsymbol{y})\, \mathrm{d}^{2m}\boldsymbol{z} = \pi^m \det(\boldsymbol{A}) \exp(\boldsymbol{y}^* \cdot \boldsymbol{A} \cdot \boldsymbol{y})$.

B. Propagator

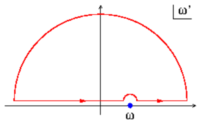
- The propagator is the time-evolution operator represented in coordinate basis: $K(x', t; x, t_0) = \langle x'|\hat{U}(t, t_0)|x\rangle$, then $K(x', t; x, t) = \delta(x' - x)$.
  - By definition, $\psi(x', t) = \int K(x', t; x, t_0)\psi(x, t_0)\, \mathrm{d}x$.
  - It is the *transition probability amplitude* for the particle (the system) to start at x at time t_0 and end up at x' at time t.
- Customarily, when $t < t_0$, $K(x', t; x, t_0) \equiv 0$, then K is the Green's function satisfying $[H' - \mathbb{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}]K(x', t; x, t_0) = -\mathbb{i}\hbar\delta(x' - x)\delta(t - t_0)$, where H' is the Hamiltonian acting on x'.
- For time-independent $\hat{H}$ with energy eigenstates $|E\rangle$,
  $K(x', t; x, t_0) = \sum_E e^{-\mathbb{i}E\,(t-t_0)/\hbar}\langle x'|E\rangle\langle E|x\rangle$, for $t > t_0$.
  - For $\hat{H} = \frac{\hat{p}^2}{2m}$,
    $K(x', t; x, t_0) = \int \frac{\mathrm{d}p}{\hbar} e^{-\frac{\mathbb{i}}{\hbar}\frac{p^2}{2m}(t-t_0)} \frac{1}{2\pi} e^{\frac{\mathbb{i}}{\hbar}p\,(x'-x)} = \sqrt{\frac{m}{2\pi\hbar(t-t_0)\mathbb{i}}} \exp[\frac{\mathbb{i}m\,(x'-x)^2}{2\hbar(t-t_0)}]$.
    Exercise: draw qualitatively the shape of real/imaginary part of K.
- Trace of time-evolution operator $G(t, t_0) = \mathrm{Tr}[\hat{U}(t, t_0)] = \int K(x, t; x, t_0)\, \mathrm{d}x$.
  For time-independent $\hat{H}$ with eigenvalues E_i, $G(t) = \sum_i \exp[-\mathbb{i}E\,t/\hbar]$, for $t > 0$, similar to finite temperature partition function (with β replaced by $\mathbb{i}t/\hbar$).

1. *Brief Notes on Causal Functions*

- The propagator and $G(t)$ are "causal functions": nonzero only for *later* ($t > 0$) times.
- You especially experimentalists will frequently encounter/measure such functions (response functions): perturb the system and measure the response at *later* times.

- Consider the Fourier transform $\tilde{G}(\omega) = -\mathbb{i} \int G(t)\, e^{\mathbb{i}\omega t}\, \mathrm{d}t$.
  Because $G(t<0)=0$, $\tilde{G}(\omega' + \mathbb{i}\omega'')$ is non-singular(analytic) for $\omega''>0$ for all real ω', and tends to zero fast enough at infinity with $\omega''>0$.

- Kramer-Kronig relation (Hilbert transform): for such functions $\tilde{G}(\omega)$,
  $\mathrm{Re}\tilde{G}(\omega) = \frac{1}{\pi}\mathsf{P}\int_{-\infty}^{+\infty} \frac{\mathrm{Im}\tilde{G}(\omega')}{\omega'-\omega}\,\mathrm{d}\omega'$, $\mathrm{Im}\tilde{G}(\omega) = -\frac{1}{\pi}\mathsf{P}\int_{-\infty}^{+\infty} \frac{\mathrm{Re}\tilde{G}(\omega')}{\omega'-\omega}\,\mathrm{d}\omega'$.
  Or equivalently, $\mathbb{i}\pi\,\tilde{G}(\omega) = \mathsf{P}\int_{-\infty}^{+\infty} \frac{\tilde{G}(\omega')}{\omega'-\omega}\,\mathrm{d}\omega'$.
  Here P means Cauchy principal value.
  For a proof, consider the integral of $\frac{\tilde{G}(\omega')}{\omega'-\omega}$ over ω' contour on the right.



- Measurements usually observe the imaginary part (dissipation, absorption, *etc.*) of the response functions. Kramer-Kronig can be used to get the real part.

- Example: $G(t>0) = e^{-\mathbb{i}Et}$, then $\tilde{G}(\omega) = \frac{1}{\omega - E} - \mathbb{i}\,\pi\,\delta(\omega - E)$.
  The imaginary part (poles) can be used to identify the energy spectrum.

C. Reminder about Classical Mechanics

- The *Lagrangian* for dynamical system is $L(q,\dot{q}) = T - V$ (kinetic − potential energy), which is a function of generalized coordinate q and generalized velocity $\dot{q} = \frac{\mathrm{d}}{\mathrm{d}t}q$.

- Dynamics follows the principle of least action: classical trajectory 'minimizes' the *action*, $S = \int L(q,\dot{q})\,\mathrm{d}t$, among all trajectories with the same boundary condition.

- Euler-Lagrange equation: $\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0$, from $\delta S = 0$.

- The *Hamiltonian* is $H(p,q) = p\dot{q} - L(q,\dot{q})$, the Legendre transformation of Lagrangian, where the generalized momentum $p = \frac{\partial L}{\partial \dot{q}}$, and $\dot{q}$ should be solved in terms of p and q.

- The Hamilton's equation: $\dot{p} = -\frac{\partial H}{\partial q}$ and $\dot{q} = +\frac{\partial H}{\partial p}$.

- Poisson bracket: $\{A,B\} = \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q}$.
  Corresponds to quantum commutator $-\frac{\mathbb{i}}{\hbar}[\hat{A},\hat{B}]$ of corresponding observables.

- Equation of motion: $\frac{\mathrm{d}}{\mathrm{d}t}A(p,q) = -\{H,A\}$.
  Corresponds to the Heisenberg equation of motion, $\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}(t) = \frac{\mathbb{i}}{\hbar}[\hat{H},\hat{A}]$.

- Hamilton's principal function: $S(q_f, t_f; q_i, t_i) = \int_{t_i}^{t_f} L(q, \dot{q})\,\mathrm{d}t$, with $q(t_i) = q_i$ & $q(t_f) = q_f$, integrated over a classical trajectory. $\frac{\partial S}{\partial q_f} = p(t = t_f)$, $\frac{\partial S}{\partial t_f} = -H(t = t_f)$.
- Hamilton-Jacobi equation: $\frac{\partial S}{\partial t_f} + H(\frac{\partial S}{\partial q_f}, q_f) = 0$.

D. Path Integral in Quantum Mechanics

- The goal: try to describe the quantum dynamics from a 'classical' point of view, as particle moving in coordinate space (or coordinate-momentum phase space). Then quantum interference between paths must be considered.
- Path integral version #1:
  $K(x', x, t) = \int \mathcal{D}[x(\tau)]\ \exp[\frac{\mathrm{i}}{\hbar} \int_0^t L(x(\tau), \dot{x}(\tau))\,\mathrm{d}\tau] = \int \mathcal{D}[x]\ \exp[\frac{\mathrm{i}}{\hbar} S]$.
  - $\int \mathcal{D}[x(\tau)]$: *functional integral* over all *path* $x(\tau)$ with $x(0) = x$ and $x(t) = x'$. The measure of paths is very difficult to define.
  - $L(x, \dot{x})$: the Lagrangian.
    $\dot{x} = \frac{\mathrm{d}}{\mathrm{d}\tau} x$: the 'velocity' on the path $x(\tau)$.
    S: the action of path $x(\tau)$, $S[x(\tau)] \equiv \int_0^t L(x(\tau), \dot{x}(\tau))\,\mathrm{d}\tau$.
- Path integral version #2:
  $K(x', x, t) = \int \mathcal{D}[x(\tau)]\mathcal{D}[p(\tau)]\ \exp[\frac{\mathrm{i}}{\hbar} \int_0^t [p\dot{x} - H(p, x)]\,\mathrm{d}\tau$.
  - $\int \mathcal{D}[p(\tau)]$: integral over all path in momentum space, with proper measure. Path of p has no boundary condition.
  - $H(p, x)$: classical Hamiltonian.
- An example: time-independent $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$. Propagator $K(x', x, t) = \langle x'|e^{-\frac{\mathrm{i}}{\hbar} t\hat{H}}|x\rangle$.
  - Divide this propagation over time t into N steps, each of time $\epsilon = t/N$, $K(x', x, t) = \langle x'|(e^{-\frac{\mathrm{i}}{\hbar}\epsilon\hat{H}})^N|x\rangle$, insert $N-1$ resolution of identities. $K(x', x, t) = \int \mathrm{d}x_{N-1} \cdots \int \mathrm{d}x_2 \int \mathrm{d}x_1\ \langle x'|e^{-\frac{\mathrm{i}}{\hbar}\epsilon\hat{H}}|x_{N-1}\rangle \cdots \langle x_2|e^{-\frac{\mathrm{i}}{\hbar}\epsilon\hat{H}}|x_1\rangle\langle x_1|e^{-\frac{\mathrm{i}}{\hbar}\epsilon\hat{H}}|x\rangle$.
  - Approximation (Trotter-Suzuki): $e^{-\frac{\mathrm{i}}{\hbar}\epsilon\hat{H}} = e^{-\frac{\mathrm{i}}{\hbar}\epsilon\frac{\hat{p}^2}{2m}} e^{-\frac{\mathrm{i}}{\hbar}\epsilon V(x)} + O(\epsilon^2)$.
    $\langle x_{i+1}|e^{-\frac{\mathrm{i}}{\hbar}\epsilon\hat{H}}|x_i\rangle \approx \langle x_{i+1}|e^{-\frac{\mathrm{i}}{\hbar}\epsilon\frac{\hat{p}^2}{2m}}|x_i\rangle\, e^{-\frac{\mathrm{i}}{\hbar}\epsilon V(x_i)} = \sqrt{\frac{m}{2\pi\hbar\epsilon\mathrm{i}}} e^{\frac{\mathrm{i}}{\hbar}\epsilon\,[\frac{m}{2}(\frac{x_{i+1}-x_i}{\epsilon})^2 - V(x_i)]}$.

- $K(x', x, t) \approx \int \mathrm{d}x_{N-1} \cdots \mathrm{d}x_1 \, (\frac{m}{2\pi\hbar\epsilon\mathbb{i}})^{\frac{N}{2}} \, \exp(\frac{\mathbb{i}}{\hbar} \sum_{i=0}^{N-1} \epsilon \, [\frac{m}{2}(\frac{x_{i+1}-x_i}{\epsilon})^2 - V(x_i)])$,
  where $x_0 = x$ & $x_N = x'$. The integral is over the discretized path
  $x_0(\tau = 0) = x, x_1(\tau = \epsilon), \cdots, x_N(\tau = N\epsilon = t) = x'$.
- Take $N \to \infty$ ($\epsilon \to 0$) limit, sum in the exponent ($\sum_{i=0}^{N-1} \epsilon$) becomes integral $\int_0^t \mathrm{d}\tau$, then $K(x', x, t) = \int \mathcal{D}[x(\tau)] \, \exp(\frac{\mathbb{i}}{\hbar} \int_0^t [\frac{m\dot{x}^2}{2} - V(x)]\mathrm{d}\tau)$
  $= \int \mathcal{D}[x(\tau)] \, \exp(\frac{\mathbb{i}}{\hbar} \int_0^t L(x, \dot{x}) \, \mathrm{d}\tau)$.
  * NOTE: there is an ugly normalization factor $(\frac{m}{2\pi\hbar\epsilon\mathbb{i}})^{\frac{N}{2}}$ hidden in $\mathcal{D}[x(\tau)]$.

- The example again: $\hat{H} = \frac{\hat{p}^2}{2m} + V(x) = T(\hat{p}) + V(x)$.
  $K(x', x, t) = \langle x'| e^{-\frac{\mathbb{i}}{\hbar} t\hat{H}} |x\rangle = \langle x'| (e^{-\frac{\mathbb{i}}{\hbar}\epsilon\hat{H}})^N |x\rangle$.
  - Trotter-Suzuki: $e^{-\frac{\mathbb{i}}{\hbar}\epsilon\hat{H}} = e^{-\frac{\mathbb{i}}{\hbar}\epsilon T(\hat{p})} e^{-\frac{\mathbb{i}}{\hbar}\epsilon V(x)} + O(\epsilon^2)$.
  - Insert $N-1$ resolution of identity in terms of x eigenstates,
    and N resolution of identity in terms of $\hat{p}$ eigenstates,
    $K(x', x, t) = \int \hbar^{-N} \mathrm{d}p_{N-1} \cdots \mathrm{d}p_0 \, \mathrm{d}x_{N-1} \cdots \mathrm{d}x_1$
    $\times \langle x_N| e^{-\frac{\mathbb{i}}{\hbar}\epsilon T(\hat{p})} |p_{N-1}\rangle \langle p_{N-1}| e^{-\frac{\mathbb{i}}{\hbar}\epsilon V(x)} |x_{N-1}\rangle \cdots \langle x_1| e^{-\frac{\mathbb{i}}{\hbar}\epsilon T(\hat{p})} |p_0\rangle \langle p_0| e^{-\frac{\mathbb{i}}{\hbar}\epsilon V(x)} |x_0\rangle$
    $= \int \hbar^{-N} \mathrm{d}p_{N-1} \cdots \mathrm{d}p_0 \, \mathrm{d}x_{N-1} \cdots \mathrm{d}x_1 \, \exp\{-\frac{\mathbb{i}}{\hbar} \sum_{i=0}^{N-1} \epsilon \, [T(p_i) + V(x_i)]\}$
    $\times \langle x_N|p_{N-1}\rangle \langle p_{N-1}|x_{N-1}\rangle \cdots \langle x_1|p_0\rangle \langle p_0|x_0\rangle$
    $= \int \hbar^{-N} \mathrm{d}p_{N-1} \cdots \mathrm{d}p_0 \, \mathrm{d}x_{N-1} \cdots \mathrm{d}x_1 \, (2\pi)^{-N}$
    $\times \exp\{\frac{\mathbb{i}}{\hbar} \sum_{i=0}^{N-1} \epsilon \, [p_i(\frac{x_{i+1}-x_i}{\epsilon}) - T(p_i) - V(x_i)]\}$
  - In the $N \to \infty$ limit, $K(x', x, t) = \int \mathcal{D}[x]\mathcal{D}[p] \, \exp(\frac{\mathbb{i}}{\hbar} \int_0^t [p\dot{x} - H(p, x)] \, \mathrm{d}\tau)$.
    * The measure of paths $\mathcal{D}[x]\mathcal{D}[p]$ contains the $(2\pi\hbar)^{-N}$ normalization factor.
  - If the Hamiltonian contains terms like $\hat{p}\hat{x}$ or $\hat{x}\hat{p}$, special care is needed.
    See *e.g.* Peskin&Schroeder, Section 9.1.

E. Equivalence of Path Integral to the Schrödinger Equation

- The example: $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$.

- Consider $K(x', x, t+\epsilon)$, add one last step ($x_{N+1} = x'$) to the path integral.
  $K(x', x, t+\epsilon) = \int \mathrm{d}x_N \, \langle x'| e^{-\frac{\mathbb{i}}{\hbar}\epsilon\hat{H}} |x_N\rangle \, K(x_N, x, t)$
  $\approx \int \mathrm{d}x_N \sqrt{\frac{m}{2\pi\hbar\epsilon\mathbb{i}}} \, e^{\frac{\mathbb{i}}{\hbar}\epsilon \, [\frac{m}{2}(\frac{x'-x_N}{\epsilon})^2 - V(x_N)]} \, K(x_N, x, t)$.

- Expand $K(x_N, x, t)$ around $x_N \sim x'$, $K(x', x, t+\epsilon)$
  $\approx \int \mathrm{d}x_N \sqrt{\frac{m}{2\pi\hbar\epsilon\mathbb{i}}} e^{\frac{\mathbb{i}}{\hbar}\epsilon[\frac{m}{2}(\frac{x'-x_N}{\epsilon})^2 - V(x_N)]} \left[1 + (x_N - x')\frac{\partial}{\partial x'} + \frac{(x_N-x')^2}{2}\frac{\partial^2}{\partial x'^2} + \cdots\right] K(x', x, t)$.

- Do the Gaussian integral, keep terms up to $O(\epsilon)$,
  $K(x', x, t+\epsilon) \approx [1 + \frac{\mathbb{i}}{\hbar}\frac{\epsilon}{2m}\frac{\partial^2}{\partial x'^2} - \frac{\mathbb{i}}{\hbar}\epsilon V(x') + O(\epsilon^2)]K(x', x, t)$.

- Finally, taking limit of $\epsilon \to 0$,
  $\frac{\partial}{\partial t}K(x', x, t) = -\frac{\mathbb{i}}{\hbar}[-\frac{1}{2m}\frac{\partial^2}{\partial x'^2} + V(x')]K(x', x, t) = -\frac{\mathbb{i}}{\hbar}\hat{H}'K(x', x, t)$,
  which is the Schrödinger equation for propagator.

F. Stationary Phase Approximation

- For $\int e^{\mathbb{i}k\,f(x)}\,\mathrm{d}x$ with large k, most contribution comes from x_s where f is 'stationary' $[f'(x_s) = 0]$, where the integrand has no rapid oscillation. Expand f around x_s, $f(x) \approx f(x_s) + \frac{1}{2}f''(x_s)\,(x - x_s)^2$, do the Gaussian integral, sum over all stationary x_s,
  $\int e^{\mathbb{i}k\,f(x)}\,\mathrm{d}x \approx \sum_{x_s}\sqrt{\frac{2\pi\mathbb{i}}{k\,f''(x_s)}}e^{\mathbb{i}k\,f(x_s)}$.

- For n-dimensional integral, $\int e^{\mathbb{i}k\,f(\boldsymbol{x})}\,\mathrm{d}^n\boldsymbol{x}$, where $\boldsymbol{x} = (x_i)$ is n-component vector, expand f around stationary point $\boldsymbol{x}_s$, $f(\boldsymbol{x}) \approx f(\boldsymbol{x}_s) + \frac{1}{2}\frac{\partial^2 f(\boldsymbol{x}_s)}{\partial x_i \partial x_j}(\boldsymbol{x} - \boldsymbol{x}_s)_i(\boldsymbol{x} - \boldsymbol{x}_s)_j$,
  do the Gaussian integral, sum over all stationary points $\boldsymbol{x}_s$,
  $\int e^{\mathbb{i}k\,f(\boldsymbol{x})}\,\mathrm{d}^n\boldsymbol{x} \approx \sum_{\boldsymbol{x}_s}(\frac{2\pi\mathbb{i}}{k})^{n/2}\left(\det\frac{\partial^2 f(\boldsymbol{x}_s)}{\partial x_i \partial x_j}\right)^{-1/2} e^{\mathbb{i}k\,f(\boldsymbol{x}_s)}$.

- In path integral formulation of quantum mechanics, the large number k is $1/\hbar$.
  The stationary phase approximation is the semi-classical approximation ($\hbar \to 0$).
  - The stationary phase condition for $\int \mathcal{D}[x]\,e^{\frac{\mathbb{i}}{\hbar}S}$ is
    $\frac{\delta S}{\delta x} = 0$, or the classical equation of motion (Euler-Lagrange equation).
  - (Not required) van Vleck formula: (see *e.g.* Prof. Littlejohn's lecture notes #9)
    $K(x', x, t) = \int \mathcal{D}[x]\,e^{\frac{\mathbb{i}}{\hbar}S} \approx \sum \frac{1}{\sqrt{2\pi\hbar\mathbb{i}}}(\frac{\partial^2 S}{\partial x'\partial x})^{1/2}\exp[\frac{\mathbb{i}}{\hbar}S(x', x, t)]$,
    the sum is over all classical trajectories from x to x' in time t.

III. GEOMETRIC PHASE

- Consider an adiabatic periodic evolution of a Hamiltonian $\hat{H}(t)$ with $\hat{H}(T) = \hat{H}(0)$. Suppose the Hamiltonian always has a unique ground state $|E_0(t)\rangle$ of energy $E_0(t)$.

After the periodic evolution, what is the phase acquired by the ground state?

- The phase factor is $\langle E_0(0)|\hat{U}(T)|E_0(0)\rangle$, where $U(T) = \mathcal{T}(\exp[-\frac{\mathbb{i}}{\hbar}\int_{t'=0}^{T}\hat{H}(t')\mathrm{d}t'])$.
  - Note that $|E_0(t)\rangle$ is not a "trajectory" of time evolution, t here is just a parameter of these states. $\hat{U}(t)|E_0(0)\rangle$ is not *exactly* $|E_0(t)\rangle$, but by the adiabatic theorem they will only differ by a complex phase.
- Divide T into N intervals of $\epsilon = T/N$, define $t_n = n\epsilon$. Then up to $O(\epsilon^2)$ error, $\langle E_0(0)|\hat{U}(T)|E_0(0)\rangle \approx \langle E_0(0)|e^{-\frac{\mathbb{i}}{\hbar}\epsilon\hat{H}(t_{N-1})}|E_0(t_{N-1})\rangle\cdots\langle E_0(t_1)|e^{-\frac{\mathbb{i}}{\hbar}\epsilon\hat{H}(t_0)}|E_0(0)\rangle$ $\approx e^{-\frac{\mathbb{i}}{\hbar}\epsilon\sum_{i=0}^{N-1}E(t_i)}\langle E_0(0)|E_0(t_{N-1})\rangle\cdots\langle E_0(t_1)|E_0(0)\rangle$.
- With $\epsilon\to 0$ ($N\to\infty$) limit, the first factor becomes $e^{-\frac{\mathbb{i}}{\hbar}\int_0^T E(t)\mathrm{d}t}$, which is the expected *dynamic* phase acquired from time-evolution.
- The second factor is $\langle E_0(0)|E_0(t_{N-1})\rangle\cdots\langle E_0(t_n)|E_0(t_{n-1}\rangle\cdots\langle E_0(t_1)|E_0(0)\rangle$.
  IF $|E_0(0)\rangle = |E_0(t_N = T)\rangle$, this is $\prod_{n=1}^{N}\langle E_0(t_n)|E_0(t_{n-1})\rangle$
  $\approx \prod_{n=1}^{N}[1-\epsilon\langle E_0(t_n)|\,(\frac{\partial}{\partial t_n}|E_0(t_n)\rangle)] \approx \exp[\sum_{n=1}^{N}\epsilon\,\mathbb{i}A_t(t_n)] \approx \exp[\mathbb{i}\int_0^T A_t(\tau)\mathrm{d}\tau]$,
  where $A_t(t) = \mathbb{i}\langle E_0(t)|\,(\frac{\partial}{\partial t}|E_0(t)\rangle)$.
- The Berry's phase: $\int A_t(t)\mathrm{d}t$, where t parametrizes a *periodic* evolution $|\psi(t)\rangle$, the Berry connection (with respect to t) is $A_t = \mathbb{i}\langle\psi(t)|(\frac{\partial}{\partial t}|\psi(t)\rangle)$.
  - Periodicity requirement: $\psi(t_{\text{final}}) = \psi(t_{\text{initial}})$.
    Otherwise $\int A_t(t)\mathrm{d}t$ is not the total Berry's phase accumulated.
  - Here t is just a parameter describing the path in the Hilbert space.
    $|\psi(t)\rangle$ is not a "trajectory" of time-evolution, $|\psi(t)\rangle$ is not *exactly* $\hat{U}(t, t_{\text{initial}})|\psi(t_{\text{initial}})\rangle$.
- NOTE: The Berry's phase does not depend on the speed of evolution,
  it only depends on the closed path (geometry) in Hilbert space.
  - Consider another evolution parametrized by $u = f(t)$, then
    $A_u = \mathbb{i}\langle\psi|(\frac{\partial}{\partial u}|\psi\rangle) = (f')^{-1}\cdot\mathbb{i}\langle\psi|(\frac{\partial}{\partial t}|\psi\rangle) = (f')^{-1}A_t$,
    the Berry's phase $\int A_u(u)\mathrm{d}u = \int(f')^{-1}A_t\cdot f'\mathrm{d}t = \int A_t\mathrm{d}t$.
- The Berry's phase does not depend on $\hbar$.

- 'Gauge transformation' of the Berry connection:
  add (t-dependent) complex phases to the wavefunctions $|\psi(t)\rangle \to e^{\mathbb{i}\theta(t)}|\psi(t)\rangle$,
  note that $\theta(T) - \theta(0) \equiv 0 \mod 2\pi$ for periodicity.
  - The Berry connection becomes,
    $A_t \to \mathbb{i}\,\langle\psi(t)|e^{-\mathbb{i}\theta(t)}\frac{\partial}{\partial t}\left(e^{\mathbb{i}\theta(t)}|\psi(t)\rangle\right) = A_t - \frac{\mathrm{d}\theta}{\mathrm{d}t}$.
  - The Berry's phase becomes $\int A_t \mathrm{d}t \to \int A_t \mathrm{d}t - \int \frac{\mathrm{d}\theta}{\mathrm{d}t}\mathrm{d}t = \int A_t \mathrm{d}t - [\theta(T) - \theta(0)] = \int A_t \mathrm{d}t \mod 2\pi$.
- Example: spin-1/2 under a Zeeman field rotating in xy-plane.
  - $\hat{H}(\phi) = -(g\mu_B B/2)(\cos\phi\cdot\sigma_x + \sin\phi\cdot\sigma_y) = -(g\mu_B B/2)\begin{pmatrix} 0 & e^{-\mathbb{i}\phi} \\ e^{\mathbb{i}\phi} & 0 \end{pmatrix}$.
  - The ground state is $(\sqrt{1/2},\ \sqrt{1/2}e^{\mathbb{i}\phi})^T$, periodic with ϕ from 0 to 2π.
  - The Berry connection $A_\phi = \mathbb{i}(\sqrt{1/2},\ \sqrt{1/2}e^{-\mathbb{i}\phi})\cdot(0, \mathbb{i}\sqrt{1/2}e^{\mathbb{i}\phi})^T = -(1/2)$.
  - The Berry's phase is $\int_0^{2\pi} A_\phi \mathrm{d}\phi = \pi$.
    The state acquires an additional minus sign after this periodic evolution.
  - Another choice of eigenvector $(\sqrt{1/2}e^{-\mathbb{i}\phi/2},\ \sqrt{1/2}e^{\mathbb{i}\phi/2})^T$ is not good for computing Berry's phase (not explicitly periodic for ϕ from 0 to 2π).

IV. GAUGE INVARIANCE AND ELECTROMAGNETIC FIELD

- Consider non-relativistic particle described by normalized wavefunction $\psi(\boldsymbol{r}, t)$.
  - The Schrödinger equation is $[\frac{-\hbar^2}{2m}\partial_{\boldsymbol{r}}^2 + V(\boldsymbol{r})]\psi = \mathbb{i}\hbar\partial_t\psi$.
  - The probability density is $\rho(\boldsymbol{r}, t) = |\psi|^2$.
  - The probability current density is $\boldsymbol{J}(\boldsymbol{r}, t) = \mathrm{Re}[\psi^*\frac{\hat{\boldsymbol{p}}}{m}\psi] = -\mathbb{i}\frac{\hbar}{2m}(\psi^*\partial_{\boldsymbol{r}}\psi - \psi\partial_{\boldsymbol{r}}\psi^*)$.
  - The continuity equation for probability is $\frac{\mathrm{d}}{\mathrm{d}t}[\rho(\boldsymbol{r}, t)] + \nabla_{\boldsymbol{r}}\cdot\boldsymbol{J}(\boldsymbol{r}, t) = 0$
- Adding a global phase factor $\psi \to e^{\mathbb{i}\theta}\psi$ with real θ independent of $\boldsymbol{r}$ and t will not change the above results.

- If θ depends on $\boldsymbol{r}$,t, then $\partial_t\psi \to e^{\mathbb{i}\theta}\partial_t\psi + (\mathbb{i}\partial_t\theta)e^{\mathbb{i}\theta}\psi$, $\partial_{\boldsymbol{r}}\psi \to e^{\mathbb{i}\theta}\partial_{\boldsymbol{r}}\psi + (\mathbb{i}\partial_{\boldsymbol{r}}\theta)e^{\mathbb{i}\theta}\psi$, $\rho \to \rho$, $\boldsymbol{J} \to \boldsymbol{J} + \frac{\hbar}{m}(\partial_{\boldsymbol{r}}\theta)\rho$. It seems that the Schrödinger equation is not preserved, the probability current density changes, and the continuity equation is violated.

- To make the theory formally "gauge invariant" under arbitrary $\psi \to e^{\mathbb{i}\theta}\psi$, we need to absorb the $\partial_t\theta$ and $\partial_{\boldsymbol{r}}\theta$ terms into the transformation of a "gauge field".

  – Define a 4-component space-time-dependent real-valued "gauge field" $(a_0, \boldsymbol{a})$. Define the canonical momentum $\hat{\boldsymbol{P}} = \hat{\boldsymbol{p}} - \hbar\boldsymbol{a}$.

  – Demand the gauge transform to be: $\psi \to e^{\mathbb{i}\theta}\psi$, $\boldsymbol{a} \to \boldsymbol{a} + \partial_{\boldsymbol{r}}\theta$, $a_0 \to a_0 + \partial_t\theta$. Then it is easy to see that $\hat{\boldsymbol{P}}\psi \to e^{\mathbb{i}\theta}\hat{\boldsymbol{P}}\psi$.

  – Modify the Schrödinger equation as $[\frac{\hat{\boldsymbol{P}}^2}{2m} + V(\boldsymbol{r})]\psi = \hbar(\mathbb{i}\partial_t + a_0)\psi$.
  This will be invariant under the above gauge transformation.

  – Modify the definition of probability current density as $\boldsymbol{J}(\boldsymbol{r}, t) = \mathrm{Re}[\psi^*\frac{\hat{\boldsymbol{P}}}{m}\psi] = -\mathbb{i}\frac{\hbar}{2m}(\psi^*\partial_{\boldsymbol{r}}\psi - \psi\partial_{\boldsymbol{r}}\psi^*) - \frac{\hbar}{m}\boldsymbol{a}\rho$. This is invariant under the gauge transformation. So continuity equation is preserved.

- For particle with electric charge q, the above "gauge field" is the electromagnetic 4-potential, $(a_0, \boldsymbol{a}) = \frac{q}{\hbar}(-\phi, \boldsymbol{A})$, (under SI units), where ϕ is the electrostatic potential (electric field $\boldsymbol{E} = -\nabla\phi - \partial_t\boldsymbol{A}$), $\boldsymbol{A}$ is the vector potential (magnetic field $\boldsymbol{B} = \nabla\times\boldsymbol{A}$). The gauge transformation of wavefunction is related to the gauge transformation of electromagnetic 4-potential.

Summary of Lecture #4: symmetry in quantum mechanics

Goals and Requirements:

- Get a clear picture of the role of symmetry in quantum mechanics.
  - Generators of continuous symmetry group are conserved observables.
  - For a Hamiltonian with certain symmetry, the degenerate energy levels(states) form a *linear representation* of the symmetry group.
  - Symmetry group elements are represented by (anti-)unitary operators.
- Be familiarized with the analysis of symmetry of a system, and its application in *conservation laws* & *selection rules.*
  - Be familiarized with certain discrete symmetries of condensed matter systems: discrete translations, point groups.
- NOTE: natural unit $\hbar = 1$, and the Einstein convention of implicit summation of repeated indices, are sometimes used.
- Optional references:
  J.J. Sakurai, *Modern Quantum Mechanics*, Chapter 4.
  L.D. Landau, E.M. Lifschitz, *Quantum Mechanics: Non-relativistic Theory*, Chapter XII.
  Reference for space group:
  International Tables for Crystallography, Volume A, Springer, 2005.

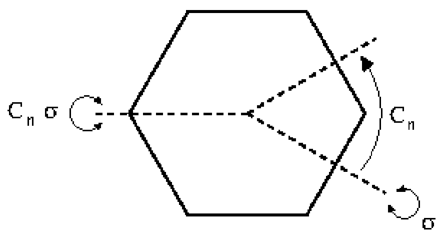
I. BASICS OF GROUP THEORY

A. Defining a Group

- Group: a set G with a binary multiplication $\circ:\ G \times G \mapsto G$ defined, satisfying,
  - Associativity: $f \circ (g \circ h) = (f \circ g) \circ h$. The $\circ$ will be omitted hereafter.
  - Existence of identity: there is a (unique) $\mathbf{1} \in G$ so that(s.t.) $\mathbf{1}\, g = g\, \mathbf{1} = g$.
  - Existence of inverse: for any $g \in G$, there is a $g^{-1} \in G$ s.t. $g^{-1}\, g = g\, g^{-1} = \mathbf{1}$.
- Group multiplication table: all results of the binary multiplication $\circ$.
  NOTE: need to check if this table satisfies the above defining properties.

	$\cdot$	h	$\cdot$
$\cdot$	$\cdot$	$\cdot$	$\cdot$
g	$\cdot$	gh	$\cdot$
$\cdot$	$\cdot$	$\cdot$	$\cdot$

- Free presentation of group: $\{\text{generators} \,|\, \text{defining relations}\}$, *roughly* it is all sequences of generators (free group) "modulo" the defining relations.
  - Free group: $\sim$ all sequences of generators (& their inverses), group multiplication is just concatenation of sequences. It is usually non-Abelian.
    - Example: the free group generated by x, y contains $\{\mathbf{1}, x, y, x^{-1}, y^{-1}, x^2 \equiv xx, xy, xy^{-1}, x^{-2} \equiv x^{-1}x^{-1}, x^{-1}y, x^{-1}y{-}1, yx, y^2, yx^{-1}, \ldots\}$, and $x \circ y = xy$, $y \circ x = yx$, $\ldots$, $yx \circ x^{-1}y = yxx^{-1}y = yy \equiv y^2$, $\ldots$.
  - Example: the cyclic group $\mathbb{Z}_3$: $\{x \,|\, x^3 = \mathbf{1}\}$ means all $x^{(n \mod 3)}$, or $\{\mathbf{1}, x, x^2\}$.
  - Example: 2D dihedral group D_n, $\{C_n, \sigma \,|\, C_n^n = \sigma^2 = (C_n\sigma)^2 = \mathbf{1}\}$,
    it is the symmetry of the regular n-sided polygon in 2D space,
    the last relation is $C_n^{-1}\sigma = \sigma C_n$, by this all sequence $C_n^{p_1}\sigma^{q_1}C_n^{p_2}\cdots$
    can be converted to $C_n^p\sigma^q$, then by the first two relations,
    the $2n$ elements are $C_n^{(p \mod n)}\sigma^{(q \mod 2)}$:
    $\{\mathbf{1}, C_n, C_n^2, \cdots, C_n^{n-1}, \sigma, C_n\sigma, \cdots, C_n^{n-1}\sigma\}$,
    multiplication rule is
    $C_n^m \cdot C_n^{m'} = C_n^{m+m'}, \quad C_n^m\sigma \cdot C_n^{m'} = C_n^{m-m'}\sigma,$
    $C_n^m \cdot C_n^{m'}\sigma = C_n^{m+m'}\sigma, \quad C_n^m\sigma \cdot C_n^{m'}\sigma = C_n^{m-m'},$
    where $m \pm m'$ should be understood with implicit modulo n.



B. Concepts and Terminology

- order of group $|G|$: 'number' of group elements.
- order of an element $|g|$: minimal integer n s.t. $g^n = \mathbf{1}$ (or ∞ if n does not exist).
- Abelian group: $gh = hg$ for all $g, h \in G$. (non-Abelian: not Abelian)
- subgroup $H \leq G$: a subset $H \subseteq G$ which is also a group under multiplication $\circ$.
- left(right) coset $gH(Hg)$: set of elements of the form gh (hg) for all h in subgroup H.
- normal subgroup $H \trianglelefteq G$: a subgroup H satisfying $gH = Hg$ for all g.
- quotient group G/H: the group of cosets for normal subgroup H of G.
- conjugacy class: f and h are conjugate if there is g s.t. $gfg^{-1} = h$.
  All elements conjugate to f form the conjugacy class of f.
  - Elements in one conjugacy class have the same order: $(gfg^{-1})^n = gf^ng^{-1}$.
- direct product of groups $G \times H$: the set of (g, h) with $g \in G$ & $h \in H$, and $(g, h) \circ (g', h') = (gg', hh')$, usually the element (g, h) is denoted just as gh.

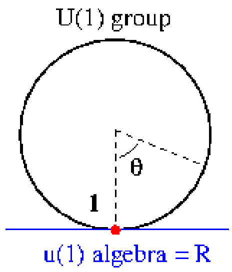
C. Examples of Groups

- Useful examples of abstract groups:
  - group of integer, real, complex numbers, $\mathbb{Z}$, $\mathbb{R}$, $\mathbb{C}$: Abelian,
    group multiplication is just number addition, group identity is number 0.
  - cyclic group $\mathbb{Z}_n$: Abelian, $\{\mathbf{1}, g, g^2, \cdots, g^{n-1}\}$, with $g^n = \mathbf{1}$; or the group of integers modulo n.
  - symmetric group Sym$X$: generically non-Abelian, all permutation actions on elements of the set X. If $X = \{1, \cdots, n\}$, this is the permutation group S_n.
- G is isomorphic to a subgroup of the permutation group Sym$G$. - *Cayley's Theorem.*
  Left(Right) multiplication of a group element just permutes all group elements.
  Each row(column) of the multiplication table is a permutation of group elements.
  $\sum_{g\in G} F(g) = \sum_{g\in G} F(gh) = \sum_{g\in G} F(hg)$, for any 'function' F, and fixed $h \in G$.

- Groups of $n \times n$ real or complex non-singular matrices: generically non-Abelian. Group multiplication is the matrix multiplication. Group identity is the identity matrix.
  - general non-singular matrices $\mathrm{GL}(n, \mathbb{R})$, $\mathrm{GL}(n, \mathbb{C})$,
  - real orthogonal matrices $\mathrm{O}(n, \mathbb{R})$ [usually just $\mathrm{O}(n)$], $O^T O = \mathbb{1}$ for $O \in \mathrm{O}(n)$,
  - unitary matrices $\mathrm{U}(n, \mathbb{C})$ [usually just $\mathrm{U}(n)$], $U^\dagger U = \mathbb{1}$ for $U \in \mathrm{U}(n)$,
  - "special" verions: $\mathrm{SL}(n, \mathbb{R})$, $\mathrm{SL}(n, \mathbb{C})$, $\mathrm{SO}(n)$, $\mathrm{SU}(n)$. Determinants are unity. All of these are Lie groups.

D. Lie Groups and Lie Algebra

- Lie group: the group elements form a differentiable manifold,
  - group U(1) :
    $\{e^{\mathbb{i}\theta}\}$ with real $\theta \mod 2\pi$ has the geometry of a circle.



  - group $\mathrm{U}(1) \times \mathrm{U}(1)$: $\{(e^{\mathbb{i}\theta}, e^{\mathbb{i}\phi})\}$ with real $\theta, \phi \mod 2\pi$, is a torus.
  - group SU(2) : $\{\begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix}\}$, $u, v \in \mathbb{C}$, is 3-sphere S^3, $(\mathrm{Re}u)^2 + (\mathrm{Im}u)^2 + (\mathrm{Re}v)^2 + (\mathrm{Im}v)^2 = 1$.

- Lie algebra LG: *roughly speaking*, the linear space tangent to Lie group manifold G at identity $\mathbf{1}$, spanned by 'derivatives' of Lie group elements, $-\mathbb{i}\frac{\partial}{\partial(\text{real parameter})} g|_{g=\mathbf{1}}$.
  - Example: SU(2) group $\{\exp(\mathbb{i}\theta \boldsymbol{n} \cdot \boldsymbol{\sigma})\}$ with real θ and unit vector $\boldsymbol{n}$, the Lie algebra $\mathfrak{su}(2)$ is the linear space spanned by $\sigma_{1,2,3}$: suppose $\theta\boldsymbol{n}$ depends on parameter t, and $\theta\boldsymbol{n}|_{t=0} = \mathbf{0}$ [so $\exp(\mathbb{i}\theta\boldsymbol{n} \cdot \boldsymbol{\sigma})|_{t=0} = \mathbb{1}_{2\times 2}$], then "$-\mathbb{i}\frac{\partial}{\partial(\text{real parameter})} g|_{g=\mathbf{1}}$" $= [\frac{\mathrm{d}}{\mathrm{d}t}(\theta\boldsymbol{n})]_{t=0} \cdot \boldsymbol{\sigma}$, which can be any real-coefficient linear combinations of $\sigma_{1,2,3}$.
  - For connected Lie group, any element g is formally an exponential $g = \exp(\mathbb{i}tX)$, where X is a basis vector in Lie algebra, t is a real number (may not be unique).
    * $X = -\mathbb{i}\, g^{-1}\frac{\mathrm{d}}{\mathrm{d}t} g$.
    * *E.g.* $\mathrm{U}(1) \times \mathrm{U}(1)$ element $(e^{\mathbb{i}\theta}, e^{2\mathbb{i}\theta}) = \exp[\mathbb{i}\sqrt{5}\theta\,(\frac{1}{\sqrt{5}}, \frac{2}{\sqrt{5}})]$, where $(\frac{1}{\sqrt{5}}, \frac{2}{\sqrt{5}})$ is a basis vector in the Abelian Lie algebra $\mathfrak{u}(1) \times \mathfrak{u}(1) \sim \mathbb{R}^2$.

    * There are disconnected Lie groups, *e.g.*, orthogonal group $\mathrm{O}(n)$. The two kinds of orthogonal matrices with $\det O = \pm 1$ are disconnected.

  - Commutator of two elements $\mathbb{i}[X, Y]$ is also an element of Lie algebra: $\mathbb{i}[X, Y] \equiv \frac{\partial}{\partial s}\left[-\mathbb{i}\frac{\partial}{\partial t}(e^{\mathbb{i}tX}e^{\mathbb{i}sY}e^{-\mathbb{i}tX}e^{-\mathbb{i}sY})\right]_{t=0}\Big|_{s=0}$. The $\left[\ldots\right]_{t=0}$ term is an element of Lie algebra, by the above definition, and it depends on real parameter s.

II. BASICS OF GROUP REPRESENTATION THEORY

A. Basic Concepts of Group Representation

- Linear representation of group G on linear space V: homomorphism R from G to $\mathrm{GL}(V)$, $R(g)$ is a linear transformation on V satisfying $R(g)R(h) = R(gh)$.
  - usually consider (n-dimensional) complex linear space [(n-dim'l) Hilbert space], the linear representation is a matrix representation, $R(g) \in \mathrm{GL}(n, \mathbb{C})$.
  - $R(\mathbf{1}) = \mathbb{1}$, $R(g^{-1}) = R(g)^{-1}$
  - $A \cdot R(g) \cdot A^{-1}$ is also a representation, for constant nonsingular A.
  - there is always the *trivial representation* $R(g) = \mathbb{1}$ for all g.
  - if all $R(g)$ are unitary, this is a unitary representation. NOTE: we will only deal with unitary representations here.

- Adjoint representation of Lie groups: the representation space is the Lie algebra LG, the representation $R(g)$ satisfies $g \cdot \boldsymbol{x} \cdot g^{-1} = \boldsymbol{x} \circ R(g)$, for $g \in G$ and $\boldsymbol{x} \in \mathrm{L}G$.
  - $g \cdot \boldsymbol{x} \cdot g^{-1}$ is defined as another Lie algebra element $-\mathbb{i}\frac{\mathrm{d}}{\mathrm{d}t}(g \cdot e^{\mathbb{i}t\boldsymbol{x}} \cdot g^{-1})\big|_{t=0}$.
  - $\boldsymbol{x} \circ R(g)$ means the vector $\boldsymbol{x}$ transformed by linear transformation $R(g)$. If $\boldsymbol{e}_i$ is a basis of Lie algebra, $\boldsymbol{x} = \sum_i \boldsymbol{e}_i x_i$, then $\boldsymbol{x} \circ R(g) = \sum_{i,j} \boldsymbol{e}_j [R(g)]_{ji} x_i$.
  - Example: $e^{\mathbb{i}\frac{\theta}{2}\boldsymbol{n}\cdot\boldsymbol{\sigma}} \in \mathrm{SU}(2)$ is represented by $\mathrm{SO}(3)$ matrix $[R(e^{\mathbb{i}\frac{\theta}{2}\boldsymbol{n}\cdot\boldsymbol{\sigma}})]_{ij} = \cos\theta\, \delta_{ij} + (1-\cos\theta) n_i n_j - \sin\theta\, \epsilon_{ijk} n_k$, namely, $e^{\mathbb{i}\frac{\theta}{2}\boldsymbol{n}\cdot\boldsymbol{\sigma}} \cdot \sigma_i \cdot e^{-\mathbb{i}\frac{\theta}{2}\boldsymbol{n}\cdot\boldsymbol{\sigma}} = \sum_j \sigma_j \cdot [R(e^{\mathbb{i}\frac{\theta}{2}\boldsymbol{n}\cdot\boldsymbol{\sigma}})]_{ji}$.

- Direct sum $\oplus$ & tensor product $\otimes$ of representations: similar to quantum operators and matrices.

- Reducible representations:
  a representation that all $R(g)$ can be *simultaneously* block-diagonalized, namely a subspace of representation space V is invariant under action of G.

- Irreducible representations (irrep.): representations that are not reducible. reducible representation can be decomposed into a direct sum of irreps.

B. Orthogonality Theorem

- *Orthogonality theorem*:
  for two "inequivalent" unitary irreps. $\sum_{g\in G} R(g)^*_{ij} R'(g)_{i'j'} = 0$;
  for the same unitary irrep. $\sum_{g\in G} R(g)^*_{ij} R(g)_{i'j'} = \frac{|G|}{\dim R}\delta_{ii'}\delta_{jj'}$.

  - If $R'(g) = A\cdot R(g)\cdot A^{-1}$, they are "equivalent"; otherwise they are "inequivalent".
  - If $R'(g) = A\cdot R(g)\cdot A^{-1}$ then $\sum_{g\in G} R(g)^*_{ij} R'(g)_{i'j'} = \frac{|G|}{\dim R}(A)_{ii'}(A^{-1})_{jj'}$.
  - For compact Lie group, $\sum_g F(g)$ should be replace by the integral $\int F(g)\mathrm{d}\mu(g)$, where $\mathrm{d}\mu(g)$ is the "Haar measure", satisfying $\int F(g)\mathrm{d}\mu(g) = \int F(gh)\mathrm{d}\mu(g) = \int F(hg)\mathrm{d}\mu(g)$, for any function F and fixed $h\in G$. $|G|$ should be replaced by the 'volume' of the group, $\int \mathrm{d}\mu(g)$.
  - Example: U(1) group $g = e^{\mathbb{i}\theta} = x + \mathbb{i}y$, $\mathrm{d}\mu(g) \propto \mathrm{d}\theta = \delta(\sqrt{x^2+y^2}-1)\mathrm{d}x\mathrm{d}y$.
    1D irreps. are $R_n(g) = e^{\mathbb{i}n\theta}$, then $\int R_n(g)^* R_m(g)\mathrm{d}\mu(g) = \frac{2\pi}{1}\delta_{n,m}$.
  - Example: SU(2) group $g = a_0\sigma_0 - \mathbb{i}\sum_{i=1}^3 a_i\sigma_i$, $\mathrm{d}\mu(g) \propto \delta(\sqrt{\sum a_i^2}-1)\prod_{i=0}^4 \mathrm{d}a_i$.

- Character: $\chi_R(g) = \mathrm{Tr}R(g)$. Here Tr is the matrix trace.

  - $\chi_R(g)$ is invariant under similarity transformation of representation.
    $R'(g) = A\cdot R(g)\cdot A^{-1}$ for all g with constant A, then $\chi_{R'}(g) = \chi_R(g)$.
  - Elements of the same conjugacy class have the same character,
    $\chi(hgh^{-1}) = \mathrm{Tr}[R(hgh^{-1}] = \mathrm{Tr}[R(h)R(g)R(h^{-1})] = \mathrm{Tr}[R(h)^{-1}R(h)R(g)] = \chi(g)$.
  - $\chi_{R\oplus R'}(g) = \chi_R(g) + \chi_{R'}(g)$, $\chi_{R\otimes R'}(g) = \chi_R(g)\cdot\chi_{R'}(g)$.
  - Example: SU(2),
    fundamental representation $R(g) = \exp(\mathbb{i}\frac{\theta}{2}\boldsymbol{n}\cdot\boldsymbol{\sigma})$, $\chi_{S=\frac{1}{2}}(g) = 2\cos\frac{\theta}{2}$;
    adjoint representation (previous page), $\chi_{S=1}(g) = 1 + 2\cos\theta$.

- *Orthogonality of characters*:
  for two inequivalent unitary irreps. $\sum_{g\in G}\chi_R(g)^*\,\chi_{R'}(g)=0$;
  for two equivalent unitary irreps. $\sum_{g\in G}\chi_R(g)^*\,\chi_R(g)=|G|$.
  - Example: SU(2) group, $g=a_0\sigma_0-\mathbb{i}\sum_{i=1}^3 a_i\sigma_i$ (fundamental rep.), $\mathrm{d}\mu(g)\propto\delta(\sqrt{\sum a_i^2}-1)\prod_{i=0}^4\mathrm{d}a_i$, volume of group is $\int\mathrm{d}\mu(g)=2\pi^2$.
    For the examples on previous page, $\chi_{S=\frac{1}{2}}(g)=2a_0$, $\chi_{S=1}(g)=4a_0^2-1$.
    then $\int|\chi_{S=\frac{1}{2}}(g)|^2\mathrm{d}\,\mu(g)=\int|\chi_{S=1}(g)|^2\,\mathrm{d}\mu(g)=2\pi^2$,
    and $\int\,\chi_{S=\frac{1}{2}}(g)^*\,\chi_{S=1}(g)\,\mathrm{d}\mu(g)=0$.
    Exercise: check these results, use 4D polar coordinates.
  - This relation generalizes Fourier series [U(1) group].

- For finite group, (number of inequivalent irreps) = (number of conjugacy classes); and (sum of squares of irrep. dimensions) = (the order of the group); and (dimension of irrep.) divides (the order of the group).
  - Abelian group of order n: n conjugacy classes, n inequivalent 1-dim'l irreps.
  - S_3 group: three classes, identity $\{()\}$, transpositions $\{(12),(13),(23)\}$, cyclic permutations $\{(123),(132)\}$, three irreps. $|S_3|=6=1^2+1^2+2^2$:
    trivial irrep.: $\{1,1,1,1,1,1\}$; alternating irrep.: $\{1,-1,-1,-1,1,1\}$;
    2dim'l irrep.: $\{\sigma_0,\sigma_3,\frac{-\sigma_3+\sqrt{3}\sigma_1}{2},\frac{-\sigma_3-\sqrt{3}\sigma_1}{2},\frac{-\sigma_0+\mathbb{i}\sqrt{3}\sigma_2}{2},\frac{-\sigma_0-\mathbb{i}\sqrt{3}\sigma_2}{2}\}$

- Character table:

	size & representative of conjugacy classes
name of irrep. #1	characters
name of irrep. #2	characters
$\vdots$	$\ddots$

  Example: D_4 group: conjugacy classes $\{\mathbf{1}\}$, $\{C_4,C_4^3\}$, $\{C_4^2\}$, $\{\sigma,C_4^2\sigma\}$, $\{C_4\sigma,C_4^3\sigma\}$, generators $C_4:\ (x,\,y)\to(-y,\,x)$, and $\sigma:\ (x,\,y)\to(x,\,-y)$

D_4 (C_{4v})	$\mathbf{1}$	$2C_4$	C_4^2	2σ	$2C_4\sigma$	irrep. basis in space of homogeneous functions
Γ_1 (A_1)	1	1	1	1	1	$1,\ x^2+y^2,\ \ldots$
Γ_2 (A_2)	1	1	1	-1	-1	$xy(x^2-y^2)$
Γ_3 (B_1)	1	-1	1	1	-1	x^2-y^2
Γ_4 (B_2)	1	-1	1	-1	1	xy
Γ_5 (E)	2	0	-2	0	0	(x,y)

- Projection operator:
  given a possibly reducible representation R of group G, and the characters of one irrep. $\chi_{R'}$, it is possible to build an irrep. R' within the representation space of R.
  - Denote the orthonormal basis of representation R by $|e_i\rangle$, $i = 1, \ldots, \dim(R)$. The action of group element g on the basis is $\hat{g}|e_i\rangle = \sum_j |e_j\rangle R(g)_{ji}$.
  - Build new basis $|\tilde{e}_i\rangle = \sum_{g\in G} \hat{g}|e_i\rangle \cdot \chi^*_{R'}(g) = \sum_{g\in G} \sum_j |e_j\rangle R(g)_{ji}\chi^*_{R'}(g)$.
    These are usually not linearly independent and not orthonormal.
  - If R contains irrep. R', then $|\tilde{e}_i\rangle$ will span a finite dimensional space (not all $|\tilde{e}_i\rangle$ are zero), then the group G is represented on this subspace as (several copies of) the irrep. R'.

III. CONSERVATION LAW AND DEGENERACY

A. Symmetry as Unitary Operator: 1-Particle Hilbert Space

- Think of a symmetry group G acting on the coordinate space,
  e.g. spatial translations/rotations/reflections. Such symmetries $\boldsymbol{x} \to g\boldsymbol{x}$ induce unitary transformations (normalization depends on convention) $|\boldsymbol{x}\rangle \to |g\boldsymbol{x}\rangle$.
  - $|\psi\rangle = \int \psi(\boldsymbol{x})|\boldsymbol{x}\rangle\, \mathrm{d}\boldsymbol{x} \to |g\psi\rangle = \int \psi(\boldsymbol{x})|g\boldsymbol{x}\rangle\, \mathrm{d}\boldsymbol{x} = \int \psi(g^{-1}\boldsymbol{x})|x\rangle\, J^{-1}\mathrm{d}\boldsymbol{x}$, so the wavefunction $(g\psi)(\boldsymbol{x}) = J^{-1}\psi(g^{-1}\boldsymbol{x})$, where $J = |\det \frac{\partial(g\boldsymbol{x})_j}{\partial x_i}|$ is the Jacobian.
  - Assume $J = 1$ hereafter, no need to worry about normalization.
  - Associativity: we write $|hg\psi\rangle$ with no ambiguity, because
    $(h(g\psi))(\boldsymbol{x}) = (g\psi)(h^{-1}\boldsymbol{x}) = \psi(g^{-1}h^{-1}\boldsymbol{x}) = \psi((hg)^{-1}\boldsymbol{x}) = ((hg)\psi)(\boldsymbol{x})$.
  - Given a complete orthonormal basis $|e_i\rangle$, $|g\, e_i\rangle$ are also orthonormal basis.
    g induces a unitary transformation $\hat{g} = \sum_i |g\, e_i\rangle\langle e_i|$, $|g\, e_i\rangle = \hat{g}|e_i\rangle$.
  - $\hat{g}$ has a unitary matrix representation, $(\hat{g})_{ij} = \langle e_i|g\, e_j\rangle$.
    Note: $|g\, e_j\rangle = \sum_i |e_i\rangle\, (\hat{g})_{ij}$ in this convention, and $(\widehat{hg})_{ij} = \sum_k (\hat{h})_{ik}(\hat{g})_{kj}$, from $|hg\, e_j\rangle \overset{g}{=\!=} \sum_k |h\, e_k\rangle(\hat{g})_{kj} \overset{h}{=\!=} \sum_i \sum_k |e_i\rangle(\hat{h})_{ik}(\hat{g})_{kj}$.
  - Basis change induces similarity transformation of the representation:

$\langle e_i|g\,e_j\rangle = \sum_{i',j'}\langle e_i|e'_{i'}\rangle\langle e'_{i'}|g\,e'_{j'}\rangle\langle g\,e'_{j'}|g\,e_j\rangle = \sum_{i',j'}\langle e_i|e'_{i'}\rangle\langle e'_{i'}|g\,e'_{j'}\rangle\langle e'_{j'}|e_j\rangle$ for unitary symmetry g.

- Some symmetries act on internal degrees of freedom, *e.g.* spin.

B. Symmetry as Unitary Operator: Fock space

- Implicit assumption: the vacuum is invariant under symmetry. Be careful about this!
- Symmetry operation $\hat{g}$ defined on single particle Hilbert space induces symmetry operation on Fock space, as the tensor product $\hat{g}\otimes\hat{g}\otimes\cdots\otimes\hat{g}$ restricted in the the (anit-)symmetrized many-body Hilbert space. *E.g.*: Homework #2, Problem 2.
- A more concise way is to consider the symmetry operations on the annihilation/creation operators, which generates the Fock space.
- The rule of thumb: $\hat{\psi}$ transforms as $\langle\psi|$, $\hat{\psi}^\dagger$ transforms as $|\psi\rangle$.
  - For complete orthonormal 1-particle basis e_i: $\widehat{ge_j} = g^*_{ij}\hat{e}_i$, $\widehat{ge_j}^\dagger = \hat{e}_i{}^\dagger g_{ij}$.
    Treating $\hat{e}_i(\hat{e}_i{}^\dagger)$ as a column(row) vector $\hat{\boldsymbol{e}}(\hat{\boldsymbol{e}}^\dagger)$, this can be written as vector-matrix products, $\widehat{g\boldsymbol{e}} = g^\dagger\cdot\hat{\boldsymbol{e}}$, $\widehat{g\boldsymbol{e}}^\dagger = \hat{\boldsymbol{e}}^\dagger\cdot g$.
  - The argument for this relation: $|0\rangle$ is invarient, $|ge_j\rangle = |e_i\rangle\, g_{ij}$, the corresponding creation operators must be $\widehat{ge_j}^\dagger = \hat{e}_i{}^\dagger g_{ij}$.
- The operator of total particle number (both bosons and fermions) $\hat{\boldsymbol{e}}^\dagger\cdot\hat{\boldsymbol{e}} = \sum_i \hat{e}_i{}^\dagger\hat{e}_i$ is invariant under symmetry transformation.
- For fermions, the total product $\prod_i \hat{e}_i{}^\dagger$ is invariant (up to a phase) under symmetry transformation, $\prod_i \widehat{ge_i}^\dagger = \det(\hat{g})\prod_i \hat{e}_i{}^\dagger$.

C. Symmetry as Unitary Operator: Action on Operators

- Similar to the Heisenberg picture of time evolution, we can transfer the symmetry operation on states to operations on operators: $\hat{O}\xrightarrow{g}\widehat{gO}$.

- Convention #1: like the Heisenberg picture of time evolution, let the symmetry acts only on the operator, with matrix element being the same as that of transforming only states, $\langle g\psi|\hat{O}|g\phi\rangle = \langle\psi|\widehat{gO}|\phi\rangle$, then $\widehat{gO} = \hat{g}^{-1}\hat{O}\hat{g}$.

- Convention #2: demand the matrix element to be invariant under symmetry operation, $\langle g\psi|\widehat{gO}|g\phi\rangle = \langle\psi|\hat{O}|\phi\rangle$, then $\widehat{gO} = \hat{g}\hat{O}\hat{g}^{-1}$. This is more commonly used.

- A set of linear operators $\hat{O}_i$ can also form a linear representation $R(g)$ of the group, $\widehat{gO_i} = \sum_j \widehat{O_j}\, R(g)_{ji}$.
  - Example: angular momentum operators $\hat{L}_{x,y,z}$ form the adjoint representation of SO(3) (spatial rotation).

D. Symmetry Generators as Conserved Observables

- Noether's theorem: continuous symmetries correspond to conserved quantities,
  for classical system described by the action $S = \int L(q,\dot{q},t)\,\mathrm{d}t$,
  if the action is invariant under 'translation' $q(t) \to q(t) + \epsilon f(t)$ for infinitesimal ϵ,
  then 'momentum' $P = \frac{\partial L}{\partial \dot{q}} \cdot f$ is conserved, $\frac{\mathrm{d}}{\mathrm{d}t}P = 0$;
  if the action is invariant under translation in time $t \to t + \epsilon$ (L is in independent of t),
  then the Hamiltonian $H = \frac{\partial L}{\partial \dot{q}}\dot{q} - L$ is conserved, $\frac{\mathrm{d}}{\mathrm{d}t}H = 0$.

- Symmetry of a quantum system: the Hamiltonian is invariant under the action of g, $\langle g\phi|\hat{H}|g\psi\rangle = \langle\phi|\hat{H}|\psi\rangle$ for all states ϕ, ψ, namely $\hat{g}^\dagger \cdot \hat{H} \cdot \hat{g} = \hat{H}$,
  or $[\hat{H}, \hat{g}] = 0$ for unitary symmetry.

- In quantum mechanics,
  generators of continuous unitary symmetry corresponds to conserved observables.
  - For generator X (element of Lie algebra), the corresponding observable is
    $\widehat{X} = -\mathbb{i}\widehat{e^{\mathbb{i}\theta X}}^{-1} \cdot \frac{\mathrm{d}}{\mathrm{d}\theta}\widehat{e^{\mathbb{i}\theta X}}$ (this is independent of the value of θ where $\frac{\mathrm{d}}{\mathrm{d}\theta}$ is taken).
  - $\hat{X}$ is Hermitian, and $\frac{\mathrm{d}}{\mathrm{d}t}\hat{X} = \mathbb{i}[\hat{H}, \hat{X}] = 0$.
    Proof: consider $\widehat{e^{\mathbb{i}\theta X}}^\dagger \cdot \hat{H} \cdot \widehat{e^{\mathbb{i}\theta X}} = \widehat{e^{\mathbb{i}\theta X}}^{-1} \cdot \hat{H} \cdot \widehat{e^{\mathbb{i}\theta X}} = \hat{H}$, take $\frac{\mathrm{d}}{\mathrm{d}\theta}$ at $\theta = 0$, and use the fact that $\hat{X} = -\mathbb{i}\frac{\mathrm{d}}{\mathrm{d}\theta}\widehat{e^{\mathbb{i}\theta X}}|_{\theta=0} = -\mathbb{i}\frac{\mathrm{d}}{\mathrm{d}\theta}\widehat{e^{\mathbb{i}\theta X}} \cdot \widehat{e^{\mathbb{i}\theta X}}^{-1}|_{\theta=0} = \mathbb{i}\widehat{e^{\mathbb{i}\theta X}} \cdot \frac{\mathrm{d}}{\mathrm{d}\theta}[\widehat{e^{\mathbb{i}\theta X}}^{-1}]|_{\theta=0} = \mathbb{i}\frac{\mathrm{d}}{\mathrm{d}\theta}[\widehat{e^{\mathbb{i}\theta X}}^{-1}]|_{\theta=0}$

- Symmetry quantum number carried by an operator $\hat{O}$:
  operator $\hat{O}$ carries quantum number λ of the symmetry generator $\hat{X}$ if $[\hat{X}, \hat{O}] = \lambda \hat{O}$.
  - Operators invariant under a continuous symmetry should commute with the symmetry generators (carry vanishing quantum number).
  - Example: $\hat{H} = \hbar\omega\,(\hat{b}^\dagger \hat{b} + 1/2)$, and $[\hat{H}, \hat{b}] = -\hbar\omega \hat{b}$, so the 'energy' ($\hat{H}$ quantum number) of $\hat{b}$ is $(-\hbar\omega)$.

E. Symmetry and Level Degeneracy

- A symmetry g satisfies $[\hat{H}, \hat{g}] = 0$, therefore g does not change energy eigenvalue.
  Degenerate energy eigenstates form a representation space of the symmetry group.
  Representation of g is block diagonalized in energy eigenbasis.
- Nondegenerate energy eigenstates are one-dimensional representations
  (the state may only change phase under action of symmetry).
- Existence of non-commuting symmetry generators,
  $\hat{X}$ and $\hat{Y}$ with $[\hat{H}, \hat{X}] = [\hat{H}, \hat{Y}] = 0$ and $[\hat{X}, \hat{Y}] \neq 0$,
  usually implies degeneracy of energy levels.
  - If $[\hat{X}, \hat{Y}] = \mathbb{i} z$ is a non-zero c-number, there must be degeneracy. Unitary operator $e^{\mathbb{i}\hat{X}}$ changes eigenvalue of $\hat{Y}$ by z. See Landau level example of Lecture #3.
  - If $[\hat{X}, \hat{Y}]$ is not a c-number, there may be a non-degenerate energy level,
    IF the state is vanished by commutators of all order, $0 = [\hat{X}, \hat{Y}]|E\rangle = [\hat{X}, [\hat{X}, \hat{Y}]]|E\rangle = [\hat{Y}, [\hat{X}, \hat{Y}]]|E\rangle = \ldots$.
    Example: ground state of electron in hydrogen atom (ignore spin) with angular momentum $L = 0$, take $\hat{X} = \hat{L}_x$ & $\hat{Y} = \hat{L}_y$.
- Usually label the degenerate levels by the representation of symmetry they belong to.
  E.g. with spatial translation, label the states by momentum $|\boldsymbol{p}\rangle$;
  with spatial rotation, label the states by angular momentum $|L, L_z\rangle$, *etc.*

F. Examples: Translation

- Continuous translation in 1D open space: $T_a: \ x \to x + a$, for all $a \in \mathbb{R}$.
  They form an Abelian group, $T_a T_{a'} = T_{a+a'}$, which is isomorphic to $\mathbb{R}$.
  - The related unitary operator is $\hat{T}_a = \int |x+a\rangle\langle x|\,\mathrm{d}x$.
  - Use momentum basis, this is simply $\hat{T}_a = \exp(-\mathbb{i}a\,\hat{p}/\hbar)$.
    * $\hat{T}_a = \int |p\rangle\langle p|x+a\rangle\langle x|p'\rangle\langle p'|\mathrm{d}p\mathrm{d}p'\mathrm{d}x = \int \frac{e^{(-\mathbb{i}p\,(x+a)+\mathbb{i}p'\,x)/\hbar}}{2\pi\hbar}|p\rangle\langle p'|\,\mathrm{d}p\mathrm{d}p'\mathrm{d}x$
      $= \int \delta(p-p')e^{-\mathbb{i}p\,a/\hbar}|p\rangle\langle p'|\,\mathrm{d}p\mathrm{d}p' = \int e^{-\mathbb{i}p\,a/\hbar}|p\rangle\langle p|\,\mathrm{d}p = \exp(-\mathbb{i}a\,\hat{p}/\hbar)$, where $\hat{p} = \int p|p\rangle\langle p|\,\mathrm{d}p$ is the momentum operator.
    * Exercise: use $\hat{p} = -\mathbb{i}\frac{\partial}{\partial x}$, check that $\exp(-a\frac{\partial}{\partial x})\psi(x) = \psi(T_a^{-1}x) = \psi(x-a)$.
  - The 1D Lie algebra is spanned by the single generator, the momentum $\hat{p}$, which is conserved in translation-invariant systems, *e.g.* $\hat{H} = \hat{p}^2/2m$.
  - The momenum eigenstates $|p\rangle$ are 1D irreps. of this translation group, with the representation matrix (and character) $e^{-\mathbb{i}ap/\hbar}$.

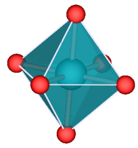
G. Example: Discrete Translation

- Discrete translation (lattice translation): define $T: \ x \to x + a$ for a constant $a \neq 0$, the discrete translation group is the cyclic group generated by T, $\{T^n\}$ for all $n \in \mathbb{Z}$.
  - The unitary operator is still $\hat{T} = \exp(-\mathbb{i}a\,\hat{p}/\hbar)$.
  - There is no associated Lie algebra and conserved observables.
  - Unitary irreps are 1D, $\hat{T} = e^{\mathbb{i}\theta}$ with real $\theta \mod 2\pi$.
  - Momentum eigenstates $|p + \frac{2\pi\hbar}{a}n\rangle$ for $n \in \mathbb{Z}$ belong to the same 1D irrep. $e^{-\mathbb{i}ap/\hbar}$
  - *Bloch's theorem*: for system with the above translation symmetry, $[\hat{H}, \hat{T}] = 0$, The m-th energy eigenstate of irrep $\hat{T} = e^{-\mathbb{i}ap/\hbar}$ is a superposition of $|p + nG\hbar\rangle$, $|E_m, p\rangle = \sum_n u_{mn}|p + nG\hbar\rangle$, with $n \in \mathbb{Z}$ and $G = \frac{2\pi}{a}$ (the reciprocal lattice vector). The wavefunction is thus $\langle x|E_m, p\rangle = \sum_n u_{mn}e^{2\pi\mathbb{i}n\frac{x}{a}}\,e^{\mathbb{i}xp/\hbar} = u_m(x)\,e^{\mathbb{i}xp/\hbar}$, the "Bloch function" $u_m(x) = \sum_n u_{mn}e^{2\pi\mathbb{i}n\,(x/a)}$ is periodic, $u_m(x+a) = u_m(x)$.

– The Bloch function $u_m(x)$ (or Fourier coefficients u_{mn}), and
the "crystal momentum" p in first Brillouin zone ($-\pi/a \leq \frac{p}{\hbar} < \pi/a$ in this case),
define the eigenstates(Bloch waves).

H. Examples: Point Group O_h

- In many materials there are the following oxygen octahedron structure:
one cation surrounded by six oxygens (or other anions),
the symmetry of the central atom is reduced
from continuous rotation to discrete rotation+reflections.
The point group (transformations leaving the central point invariant) is O_h.
The energy levels of electron orbitals on central cation
are classified by irreducible representations of O_h.



- Character table of O_h:

	E	$8C_3$	$6C_2'$	$6C_4$	$3C_2$	I	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	basis of rep.	
A_{1g}	1	1	1	1	1	1	1	1	1	1	$1, \quad r^2$	s-orbital
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
E_g	2	-1	0	0	2	2	0	-1	2	0	$(3z^2 - r^2, \sqrt{3}(x^2 - y^2))$	some d-orbitals
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1		
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1	(yz, zx, xy)	some d-orbitals
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1	xyz	one f-orbital
E_u	2	-1	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z), $(x, y, z)r^2$ (x^3, y^3, z^3)	p-orbitals, some f-orbitals
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1	$(x(y^2 - z^2), y(z^2 - x^2), z(x^2 - y^2))$	some f-orbitals

Some group elements of O_h: action results of the (x, y, z) point.

E	$8C_3$	$6C_2'$	$6C_4$	$3C_2$	I	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
$\begin{pmatrix}x\\y\\z\end{pmatrix}$	$\begin{pmatrix}y\\z\\x\end{pmatrix}$	$\begin{pmatrix}y\\x\\-z\end{pmatrix}$	$\begin{pmatrix}-y\\x\\z\end{pmatrix}$	$\begin{pmatrix}-x\\-y\\z\end{pmatrix}$	$\begin{pmatrix}-x\\-y\\-z\end{pmatrix}$	$\begin{pmatrix}y\\-x\\-z\end{pmatrix}$	$\begin{pmatrix}-y\\-z\\-x\end{pmatrix}$	$\begin{pmatrix}x\\y\\-z\end{pmatrix}$	$\begin{pmatrix}-y\\-x\\z\end{pmatrix}$

IV. SELECTION RULE

A. Symmetry Constraints on Matrix Elements

- In general we want to consider the matrix element $(f_k)_{ij} = \langle \phi_i | \hat{f}_k | \psi_j \rangle$,
  where $i(j)$ indicates that $\phi_i(\psi_j)$ is one of the degenerate energy levels of irrep. $R_\phi(R_\psi)$,
  and k means that $\hat{f}_k$ belongs to a set of operators forming irrep. R_f,
  then these matrix elements shall form a tensor product representation $R_f \otimes R_\phi^* \otimes R_\psi$.
  - $\widehat{f_k}$ form a representation, in the sense that $\hat{g}\widehat{f_k}\hat{g}^{-1} = \widehat{f_{k'}} R_f(g)_{k'k}$.
  - R_ϕ^* is the conjugate representation of R_ϕ, $R_\phi^*(g) = [R_\phi(g)]^*$.
    $\langle g\phi_i | = \langle \phi_i | \hat{g}^\dagger = R_\phi^*(g)_{i'i} \langle \phi_{i'} |$.
  - $(f_k)_{ij}$ form a tensor representation in the sense that
    $(f_k)_{ij} = \langle \phi_i | \hat{f}_k | \psi_j \rangle = \langle \phi_i | \hat{g}^{-1} \hat{g} \hat{f}_k \hat{g}^{-1} \hat{g} | \psi_j \rangle = R_\phi^*(g)_{i'i} R_f(g)_{k'k} R_\psi(g)_{j'j} \langle \phi_{i'} | \hat{f}_{k'} | \psi_{j'} \rangle =$
    $R_f(g)_{k'k} R_\phi^*(g)_{i'i} R_\psi(g)_{j'j} \, (f_{k'})_{i'j'}$.
  - Sum over g, by the orthogonality theorem, we have the ...

- Selection rule: the matrix element $(f_k)_{ij} = \langle \phi_i | \hat{f}_k | \psi_j \rangle$ will vanish
  if the tensor representation $R_f \otimes R_\phi^* \otimes R_\psi$, after decomposed into direct sum of irreps.,
  does not contain *trivial representation*.
  - Special case: if R_f, R_ϕ, R_ψ are all 1-dim'l irrep., then $R_f \otimes R_\phi^* \otimes R_\psi$ is also a 1-dim'l irrep., then $\langle \phi | \hat{f} | \psi \rangle$ will vanish if $R_f \otimes R_\phi^* \otimes R_\psi$ is not the trivial irrep.
  - Special case: if R_f is the trivial irrep. (there is only one $\hat{f}$, and it is invariant under the group actions), and if R_ϕ and R_ψ are both irrep., then
    (i) $\langle \phi_i | \hat{f} | \psi_j \rangle$ will vanish if R_ϕ and R_ψ are "inequivalent" irrep.;
    (ii) if $R_\phi = R_\psi$ (exactly same matrices), then $\langle \phi_i | \hat{f} | \psi_j \rangle = \delta_{ij} \cdot \frac{1}{\dim R_\phi} \sum_{i'} \langle \phi_{i'} | \hat{f} | \psi_{i'} \rangle$.

B. Examples: Selection Rule

- Parity selection rule (or usually "optical selection rule"):
  consider group $\{\mathbf{1}, I\}$ generated by spatial inversion I with $I^2 = \mathbf{1}$,
  it has only two irreps.: trivial (even) $\{1, 1\}$ and odd representation $\{1, -1\}$.

- States & operators are classified into "parity odd" (usually subscript $_\mathrm{u}$) and "parity even" (usually subscript $_\mathrm{g}$) classes.
- Atomic orbitals of even(odd) angular momentum are parity even(odd).
- The matrix element is nonzero only for $\langle\psi_\mathrm{g}|\hat{O}_\mathrm{g}|\psi'_\mathrm{g}\rangle$, $\langle\psi_\mathrm{g}|\hat{O}_\mathrm{u}|\psi_\mathrm{u}\rangle$, $\langle\psi_\mathrm{u}|\hat{O}_\mathrm{g}|\psi'_\mathrm{u}\rangle$, $\langle\psi_\mathrm{u}|\hat{O}_\mathrm{u}|\psi_\mathrm{g}\rangle$. Here $\hat{I}|\psi_g\rangle = +|\psi_g\rangle$, $\hat{I}|\psi_u\rangle = -|\psi_u\rangle$, $\hat{I}\hat{O}_g\hat{I}^\dagger = +\hat{O}_g$, $\hat{I}\hat{O}_u\hat{I}^\dagger = -\hat{O}_u$, ... (Check the special cases under the "selection rule")
- The optical transition (absorption/emission of one photon) probability amplitude is proportional to $\langle\psi_\mathrm{final}|\boldsymbol{E}\cdot\hat{\boldsymbol{r}}|\psi_\mathrm{initial}\rangle$ (under lowest order of perturbation theory), where $\boldsymbol{E}$ is the external electric field, the electric dipole operator $\hat{\boldsymbol{r}}$ is parity odd ($I:\ \boldsymbol{r}\to-\boldsymbol{r}$), so initial and final states should have opposite parity.
- Pseudo-vector: vectors that are even under inversion,
  e.g. the angular momentum operator $\boldsymbol{L} = \boldsymbol{r}\times\boldsymbol{p}$, the magnetic moment $\boldsymbol{M}$.
- Pseudo-scalar: scalars that are odd under inversion,
  e.g. inner product of a pseudo-vector and a vector is a pseudo-scalar.

- Raman selection rule: absorb a photon of polarization $\boldsymbol{E}_\mathrm{in}$ and emit a photon of polarization $\boldsymbol{E}_\mathrm{out}$, the relevant matrix element is $\langle\mathrm{final}|(\boldsymbol{E}_\mathrm{out}\cdot\boldsymbol{r})(\boldsymbol{E}_\mathrm{in}\cdot\boldsymbol{r})|\mathrm{initial}\rangle$.
  - If the system have C_{4v} symmetry (2D D_4 symmetry, character table on page 7), the initial state is of trivial representation A_1 (*e.g.* s-orbital), $\boldsymbol{E}_\mathrm{in,out}$ are along x, y directions respectively, then the final state must have the symmetry of function xy, or B_2 representation (*e.g.* d_{xy} orbital).

C. Examples: Symmetry-allowed Hamiltonian

- In many cases you know the symmetry of your system, but don't know the exact Hamiltonian. The goal is to write down a Hamiltonian consistent with the symmetry.
  - The general rule: find out representation $\hat{g}$ of all symmetry generators, and demand that $\hat{g}^{-1}\hat{H}\hat{g} = \hat{H}$.
  - For continuous symmetry, $\hat{H}$ should commute with all symmetry generators, or carry vanishing symmetry quantum number.

- Example: translation symmetry, momentum conservation.

  If the system has continuous translation symmetry, then for each monomial of operators in $\hat{H}$, the sum of "momentum quantum numbers" of the factors must be zero, *e.g.* $\widehat{\psi(p)}^\dagger\widehat{\psi(p)}$, $\widehat{\psi(-p)}\widehat{\psi(p)}$, $\widehat{\psi(p_1)}^\dagger\widehat{\psi(p_2)}^\dagger\widehat{\psi(p_3)}\widehat{\psi(p_4)}\delta(p_1+p_2-p_3-p_4)$.

  Here $\widehat{\psi(p)}^\dagger$ is the creation operator for momentum eigenstate $|p\rangle$, and carries "momentum quantum number" p (will change total momentum of the system by p); the annihilation operator $\widehat{\psi(p)}$ carries "momentum quantum number" $-p$.

- Example: particle number conservation $U(1)$ symmetry.

  $\hat{e}_i^\dagger$ are creation operators for orthonormal modes (bosons or fermions). The total particle number operator, $\hat{N} \equiv \sum_i \hat{e}_i^\dagger \hat{e}_i$, generates a $U(1)$ group, $\widehat{g(\theta)} = e^{-\mathbb{i}\theta\hat{N}}$, for real θ mod 2π. From $[\hat{N}, \hat{e}_i^\dagger] = +\hat{e}_i^\dagger$, the creation operators carry "particle number quantum number" $+1$ (the annihilation operators carry "particle number quantum number" -1). Then if $\hat{H}$ has "particle number conservation symmetry", namely $\widehat{g(\theta)}\hat{H}\widehat{g(\theta)}^\dagger$ for any θ, or equivalently $[\hat{H}, \hat{N}] = 0$, each term in $\hat{H}$ must have the same number of creation operators and annihilation operators, *e.g.* $\hat{e}_i^\dagger\hat{e}_j$, $\hat{e}_i^\dagger\hat{e}_j^\dagger\hat{e}_k\hat{e}_\ell$.

- Example: point group symmetry on free particle Hamiltonian $\hat{H} = \int \hat{\boldsymbol{\psi}}_{\boldsymbol{k}}^\dagger \cdot H(\boldsymbol{k}) \cdot \hat{\boldsymbol{\psi}}_{\boldsymbol{k}}\, \mathrm{d}\boldsymbol{k}$, where $\hat{\boldsymbol{\psi}}_{\boldsymbol{k}}$ is a column vector of annihilation operators, $H(\boldsymbol{k})$ is a matrix.

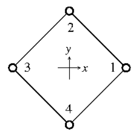
  Under g: $\hat{\boldsymbol{\psi}}_{\boldsymbol{k}} \xrightarrow{g} R(g)\cdot\hat{\boldsymbol{\psi}}_{g\boldsymbol{k}}$, $\quad \hat{H} \xrightarrow{g} \int \hat{\boldsymbol{\psi}}_{g\boldsymbol{k}}^\dagger \cdot R(g)^{-1}\cdot H(\boldsymbol{k})\cdot R(g)\cdot \hat{\boldsymbol{\psi}}_{g\boldsymbol{k}}\,\mathrm{d}\boldsymbol{k}$, then $H(g\boldsymbol{k}) = R(g)^{-1}\cdot H(\boldsymbol{k})\cdot R(g)$.

  - C_{4v} symmetry generated by $C_4:\ (x,y)\to(-y,x)$, and $\sigma_v:\ (x,y)\to(x,-y)$, consider the case $\hat{\boldsymbol{\psi}}^\dagger$ =(creation operators for p_x, p_y orbitals),
    then $R(C_4) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathbb{i}\sigma_y$, $R(\sigma_v) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z$,
    so $\sigma_y H(k_x,k_y)\sigma_y = H(-k_y,k_x)$, $\quad \sigma_z H(k_x,k_y)\sigma_z = H(k_x,-k_y)$,
    let 2×2 matrix $H(\boldsymbol{k}) = \sum_{i=0}^3 h_i(\boldsymbol{k})\sigma_i$, the real functions $h_i(\boldsymbol{k})$ must satisfy
    $h_0(k_x,k_y) = h_0(-k_y,k_x) = h_0(k_x,-k_y) \sim A_1$ irrep.,
    $h_1(k_x,k_y) = -h_1(-k_y,k_x) = -h_1(k_x,-k_y) \sim B_2$ irrep.,
    $h_2(k_x,k_y) = h_2(-k_y,k_x) = -h_2(k_x,-k_y) \sim A_2$ irrep.,
    $h_3(k_x,k_y) = -h_3(-k_y,k_x) = h_3(k_x,-k_y) \sim B_1$ irrep.,
    this constrains the form of H matrix up to $O(k^2)$ around $k=(0,0)$ as
    $H(k_x,k_y) = (c_0 + c_1\boldsymbol{k}^2)\sigma_0 + c_2\cdot k_xk_y\cdot\sigma_x + c_3\cdot(k_x^2-k_y^2)\cdot\sigma_z$, with real constant cs.

D. Examples: Symmetry-assisted Diagonalization of Hamiltonian

- Given a Hamiltonian, first analyze its symmetry, then divide the Hilbert space into smaller subspaces of different irreps of symmetry group.

- Example: Bose-Hubbard model on a 4-site square,
  $\hat{H} = -t\,(\hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_3 + \hat{b}_3^\dagger \hat{b}_4 + \hat{b}_4^\dagger \hat{b}_1 + h.c.) + \frac{U}{2}\sum_{i=1}^{4} \hat{n}_i(\hat{n}_i - 1)$,
  solve the eigenstates of two bosons (10-dimensional Hilbert space).



  - The apparent symmetry is C_{4v} (2D D_4, character table on p.7). Generated by
    $C_4: \quad \hat{b}_1 \mapsto \hat{b}_2,\ \hat{b}_2 \mapsto \hat{b}_3,\ \hat{b}_3 \mapsto \hat{b}_4,\ \hat{b}_4 \mapsto \hat{b}_1$; and
    $\sigma: \quad \hat{b}_1 \mapsto \hat{b}_1,\ \hat{b}_2 \mapsto \hat{b}_4,\ \hat{b}_3 \mapsto \hat{b}_3,\ \hat{b}_4 \mapsto \hat{b}_2$.

  - The basis of creation operators can be chosen as (use projection operator):
    $\widehat{A_1}^\dagger : \frac{1}{2}\sum_i \hat{b}_i^\dagger,\ \ \widehat{B_1}^\dagger : \frac{1}{2}(\hat{b}_1^\dagger - \hat{b}_2^\dagger + \hat{b}_3^\dagger - \hat{b}_4^\dagger),\ \ \widehat{E_{x,y}}^\dagger : \frac{1}{\sqrt{2}}(\hat{b}_1^\dagger - \hat{b}_3^\dagger)\ \&\ \frac{1}{\sqrt{2}}(\hat{b}_2^\dagger - \hat{b}_4^\dagger)$
    They correspond to single boson eigenstates of $\hat{H}$.
    Action of C_4: $\widehat{A_1}^\dagger \mapsto \widehat{A_1}^\dagger \cdot (1)$, $\widehat{B_1}^\dagger \mapsto \widehat{B_1}^\dagger \cdot (-1)$, $(\widehat{E_x}^\dagger, \widehat{E_y}^\dagger) \mapsto (\widehat{E_x}^\dagger, \widehat{E_y}^\dagger) \cdot \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.
    Action of σ: $\widehat{A_1}^\dagger \mapsto \widehat{A_1}^\dagger \cdot (1)$, $\widehat{B_1}^\dagger \mapsto \widehat{B_1}^\dagger \cdot (1)$, $(\widehat{E_x}^\dagger, \widehat{E_y}^\dagger) \mapsto (\widehat{E_x}^\dagger, \widehat{E_y}^\dagger) \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

  - The procedures of applying the "projection operator" are summarized in the following tables,

g	$\mathbf{1}$	C_4	C_4^3	C_4^2	σ	$C_4^2\sigma$	$C_4\sigma$	$C_4^3\sigma$
$\widehat{gb_1^\dagger}$	$\hat{b}_1^\dagger$	$\hat{b}_2^\dagger$	$\hat{b}_4^\dagger$	$\hat{b}_3^\dagger$	$\hat{b}_1^\dagger$	$\hat{b}_3^\dagger$	$\hat{b}_2^\dagger$	$\hat{b}_4^\dagger$
$\widehat{gb_2^\dagger}$	$\hat{b}_2^\dagger$	$\hat{b}_3^\dagger$	$\hat{b}_1^\dagger$	$\hat{b}_4^\dagger$	$\hat{b}_4^\dagger$	$\hat{b}_2^\dagger$	$\hat{b}_1^\dagger$	$\hat{b}_3^\dagger$
$\widehat{gb_3^\dagger}$	$\hat{b}_3^\dagger$	$\hat{b}_4^\dagger$	$\hat{b}_2^\dagger$	$\hat{b}_1^\dagger$	$\hat{b}_3^\dagger$	$\hat{b}_1^\dagger$	$\hat{b}_4^\dagger$	$\hat{b}_2^\dagger$
$\widehat{gb_4^\dagger}$	$\hat{b}_4^\dagger$	$\hat{b}_1^\dagger$	$\hat{b}_3^\dagger$	$\hat{b}_2^\dagger$	$\hat{b}_2^\dagger$	$\hat{b}_4^\dagger$	$\hat{b}_3^\dagger$	$\hat{b}_1^\dagger$
$\chi_{A_1}(g)$	1	1	1	1	1	1	1	1
$\chi_{A_2}(g)$	1	1	1	1	-1	-1	-1	-1
$\chi_{B_1}(g)$	1	-1	-1	1	1	1	-1	-1
$\chi_{B_2}(g)$	1	-1	-1	1	-1	-1	1	1
$\chi_E(g)$	2	0	0	-2	0	0	0	0

$\sum_g \chi_R^*(g)\widehat{g b_i^\dagger}$	$R=A_1$	$R=A_2$	$R=B_1$	$R=B_2$	$R=E$
$i=1$	$2(\hat{b}_1^\dagger+\hat{b}_2^\dagger+\hat{b}_3^\dagger+\hat{b}_4^\dagger)$	0	$2(\hat{b}_1^\dagger-\hat{b}_2^\dagger+\hat{b}_3^\dagger-\hat{b}_4^\dagger)$	0	$2(\hat{b}_1^\dagger-\hat{b}_3^\dagger)$
$i=2$	$2(\hat{b}_2^\dagger+\hat{b}_3^\dagger+\hat{b}_4^\dagger+\hat{b}_1^\dagger)$	0	$2(\hat{b}_2^\dagger-\hat{b}_3^\dagger+\hat{b}_4^\dagger-\hat{b}_1^\dagger)$	0	$2(\hat{b}_2^\dagger-\hat{b}_4^\dagger)$
$i=3$	$2(\hat{b}_3^\dagger+\hat{b}_4^\dagger+\hat{b}_1^\dagger+\hat{b}_2^\dagger)$	0	$2(\hat{b}_3^\dagger-\hat{b}_4^\dagger+\hat{b}_1^\dagger-\hat{b}_2^\dagger)$	0	$2(\hat{b}_3^\dagger-\hat{b}_1^\dagger)$
$i=4$	$2(\hat{b}_4^\dagger+\hat{b}_1^\dagger+\hat{b}_2^\dagger+\hat{b}_3^\dagger)$	0	$2(\hat{b}_4^\dagger-\hat{b}_1^\dagger+\hat{b}_2^\dagger-\hat{b}_3^\dagger)$	0	$2(\hat{b}_4^\dagger-\hat{b}_2^\dagger)$

– Two boson states: symmetrized tensor product (use symbol $\odot$) representations, these states are classified into irreps as
$A_1^{(2)}$: $A_1\odot A_1$: $\frac{1}{\sqrt{2}}(\widehat{A_1}^\dagger)^2|0\rangle$; $B_1\odot B_1$: $\frac{1}{\sqrt{2}}(\widehat{B_1}^\dagger)^2|0\rangle$; $E\odot E$: $\frac{1}{2}[(\widehat{E_x}^\dagger)^2+(\widehat{E_y}^\dagger)^2]|0\rangle$,
$B_1^{(2)}$: $A_1\odot B_1$: $\widehat{A_1}^\dagger\widehat{B_1}^\dagger|0\rangle$; $E\odot E$: $\frac{1}{2}[(\widehat{E_x}^\dagger)^2-(\widehat{E_y}^\dagger)^2]|0\rangle$,
$B_2^{(2)}$: $E\odot E$: $\frac{1}{2}(\widehat{E_x}^\dagger\widehat{E_y}^\dagger+\widehat{E_y}^\dagger\widehat{E_x}^\dagger)|0\rangle=\widehat{E_x}^\dagger\widehat{E_y}^\dagger|0\rangle$,
$E^{(2)}$: $A_1\odot E$: $(\widehat{A_1}^\dagger\widehat{E_x}^\dagger|0\rangle,\widehat{A_1}^\dagger\widehat{E_y}^\dagger|0\rangle)$; $B_1\odot E$: $(\widehat{B_1}^\dagger\widehat{E_x}^\dagger|0\rangle,-\widehat{B_1}^\dagger\widehat{E_y}^\dagger|0\rangle)$.
The 10×10 problem is reduced(block-diagonalized) to
A_1 irreps: 3×3, B_1 irreps: 2×2, B_2 irreps: 1×1, and E irreps: 2×2 (!).

– Note that $E\otimes E=A_1\oplus A_2\oplus B_1\oplus B_2$, however the A_2 irrep here is anti-symmetric with respect to the two factors and does not appear in boson system.

– Why E representation sub-problem is 2×2 instead of 4×4?
Note that (A_1E_x, A_1E_y) and $(B_1E_x,-B_1E_y)$ are exactly the same 2-dim'l representation, with exactly the same representation matrices,
$C_4\to\begin{pmatrix}0&-1\\1&0\end{pmatrix}$, $\sigma\to\begin{pmatrix}1&0\\0&-1\end{pmatrix}$.
By symmetry (check the special cases under the "selection rule")
$\langle A_1E_x|\hat{H}|B_1E_x\rangle=\langle A_1E_y|\hat{H}|-B_1E_y\rangle=\langle B_1E_x|\hat{H}|A_1E_x\rangle^*=\langle -B_1E_y|\hat{H}|A_1E_y\rangle^*$,
$\langle A_1E_x|\hat{H}|A_1E_x\rangle=\langle A_1E_y|\hat{H}|A_1E_y\rangle$, $\langle B_1E_x|\hat{H}|B_1E_x\rangle=\langle -B_1E_y|\hat{H}|-B_1E_y\rangle$, and other matrix elements are zero. The 4×4 matrix is two copies of the same 2×2 matrix, $\begin{pmatrix}\langle A_1E_x|\hat{H}|A_1E_x\rangle, & \langle A_1E_x|\hat{H}|B_1E_x\rangle\\ \langle B_1E_x|\hat{H}|A_1E_x\rangle, & \langle B_1E_x|\hat{H}|B_1E_x\rangle\end{pmatrix}$
$=\begin{pmatrix}\langle A_1E_y|\hat{H}|A_1E_y\rangle, & \langle A_1E_y|\hat{H}|-B_1E_y\rangle\\ \langle -B_1E_y|\hat{H}|A_1E_y\rangle, & \langle -B_1E_y|\hat{H}|-B_1E_y\rangle\end{pmatrix}$

– Hamiltonian is $\hat{H}=-2t\,\widehat{A_1}^\dagger\widehat{A_1}+2t\,\widehat{B_1}^\dagger\widehat{B_1}+\frac{U}{2}\sum_i\hat{n}_i(\hat{n}_i-1)$.

– The matrix elements between $A_1^{(2)}$ states are
$\hat{H}|A_1^{(2)}:A_1\odot A_1\rangle=-4t|A_1^{(2)}:A_1\odot A_1\rangle+U\sum_i\frac{1}{4\sqrt{2}}(\hat{b}_i^\dagger)^2|0\rangle$

$= -4t|A_1^{(2)} : A_1 \odot A_1\rangle + U(\frac{1}{4}|A_1^{(2)} : A_1 \odot A_1\rangle + \frac{1}{4}|A_1^{(2)} : B_1 \odot B_1\rangle + \frac{\sqrt{2}}{4}|A_1^{(2)} : E \odot E\rangle)$;
$\hat{H}|A_1^{(2)} : B_1 \odot B_1\rangle = +4t|A_1^{(2)} : B_1 \odot B_1\rangle + U\sum_i \frac{1}{4\sqrt{2}}(\hat{b}_i^\dagger)^2|0\rangle$
$= +4t|A_1^{(2)} : B_1 \odot B_1\rangle + U(\frac{1}{4}|A_1^{(2)} : A_1 \odot A_1\rangle + \frac{1}{4}|A_1^{(2)} : B_1 \odot B_1\rangle + \frac{\sqrt{2}}{4}|A_1^{(2)} : E \odot E\rangle)$;
$\hat{H}|A_1^{(2)} : E \odot E\rangle = U\sum_i \frac{1}{4}(\hat{b}_i^\dagger)^2|0\rangle$
$= U(\frac{\sqrt{2}}{4}|A_1^{(2)} : A_1 \odot A_1\rangle + \frac{\sqrt{2}}{4}|A_1^{(2)} : B_1 \odot B_1\rangle + \frac{1}{2}|A_1^{(2)} : E \odot E\rangle)$.
So the Hamiltonian in the $A_1^{(2)}$ subspace is $\begin{pmatrix} -4t + \frac{U}{4} & \frac{U}{4} & \frac{\sqrt{2}U}{4} \\ \frac{U}{4} & 4t + \frac{U}{4} & \frac{\sqrt{2}U}{4} \\ \frac{\sqrt{2}U}{4} & \frac{\sqrt{2}U}{4} & \frac{U}{2} \end{pmatrix}$.

- The matrix elements between $B_1^{(2)}$ states are
  $\hat{H}|B_1^{(2)} : A_1 \odot B_1\rangle = U\sum_i \frac{1}{4}(-1)^{i-1}(\hat{b}_i^\dagger)^2|0\rangle$
  $= U(\frac{1}{2}|B_1^{(2)} : A_1 \odot B_1\rangle + \frac{1}{2}|B_1^{(2)} : E \odot E\rangle)$;
  $\hat{H}|B_1^{(2)} : E \odot E\rangle = U\sum_i \frac{1}{4}(-1)^{i-1}(\hat{b}_i^\dagger)^2|0\rangle$
  $= U(\frac{1}{2}|B_1^{(2)} : A_1 \odot B_1\rangle + \frac{1}{2}|B_1^{(2)} : E \odot E\rangle)$.
  So the Hamiltonian in the $B_1^{(2)}$ subspace is $\begin{pmatrix} \frac{U}{2} & \frac{U}{2} \\ \frac{U}{2} & \frac{U}{2} \end{pmatrix}$.
- The matrix elements between $B_2^{(2)}$ states are
  $\hat{H}|B_2^{(2)} : E \odot E\rangle = 0$.
- The matrix elements between $E^{(2)}$ states are
  $\hat{H}|E^{(2)} : A_1 \odot E_x\rangle = -2t\,|E^{(2)} : A_1 \odot E_x\rangle + U \cdot \frac{1}{2\sqrt{2}}[(\hat{b}_1^\dagger)^2 - (\hat{b}_3^\dagger)^2]|0\rangle$
  $= -2t\,|E^{(2)} : A_1 \odot E_x\rangle + U(\frac{1}{2}|E^{(2)} : A_1 \odot E_x\rangle + \frac{1}{2}|E^{(2)} : B_1 \odot E_x\rangle)$;
  $\hat{H}|E^{(2)} : B_1 \odot E_x\rangle = +2t\,|E^{(2)} : B_1 \odot E_x\rangle + U \cdot \frac{1}{2\sqrt{2}}[(\hat{b}_1^\dagger)^2 - (\hat{b}_3^\dagger)^2]|0\rangle$
  $= +2t\,|E^{(2)} : B_1 \odot E_x\rangle + U(\frac{1}{2}|E^{(2)} : A_1 \odot E_x\rangle + \frac{1}{2}|E^{(2)} : B_1 \odot E_x\rangle)$.
  So the Hamiltonian in the $E^{(2)}$ subspace is two copies of $\begin{pmatrix} -2t + \frac{U}{2} & \frac{U}{2} \\ \frac{U}{2} & 2t + \frac{U}{2} \end{pmatrix}$.

Summary of Lecture #5: angular momentum and spin

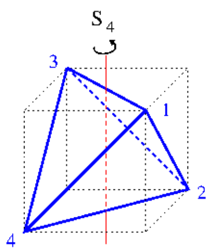
Goals and Requirements:

- Get some understanding of the SO(3) and SU(2) group, their representations, and their relations.
  - Finite dimensional irreducible representations of SU(2) are labeled by half-integer 'angular momentum' j. Integer j representations are irreducible representations of SO(3).
  - Roughly speaking SU(2) is twice as large as SO(3), SO(3) $\simeq$ SU(2)/$\mathbb{Z}_2$.
- Be familiarized with orbital angular momentum and spin, and basic calculations involving them.
  - Be familiarized with ladder operators and calculations involving them.
  - Basic tools for computation of g-factors and similar quantities.
- Get a clear understanding of time-reversal symmetry $\hat{\mathcal{T}}$, especially its effect on spin.
  - Time-reversal symmetry is anti-unitary, namely a unitary operator times the complex conjugation operator.
  - For half-odd-integer spin, $\hat{\mathcal{T}}^2 = -1$. Such system with time-reversal symmetry must have two-fold level degeneracy (Kramers theorem).
- Optional references:
  J.J. Sakurai, *Modern Quantum Mechanics*, Chapter 4.
  Landau & Lifschitz, *Quantum Mechanics: Non-relativistic Theory*, Chapter IV & VIII.
  A. Auerbach, *Interacting Electrons and Quantum Magnetism*, Chapter 7.
- NOTE: Einstein convention for implicit summation over repeated indices is frequently used.
- ★ indicates advanced topics (NOT required).

I. SU(2) AND SO(3) GROUPS

A. Defining SO(3) Group

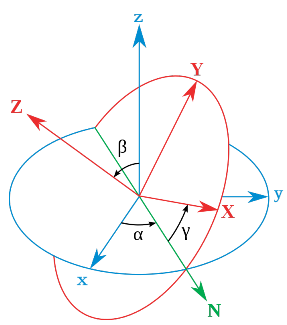
- SO(3) group: the group of proper rotations in 3-dimensional space, $\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \overleftrightarrow{R} \bullet \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, with $\overleftrightarrow{R}^T \bullet \overleftrightarrow{R} = \overleftrightarrow{1}$ and $\det(\overleftrightarrow{R}) = 1$. The notation $\overleftrightarrow{R}$ means it is a 3×3 matrix. The symbol $\bullet$ means multiplication between 3-component vector and 3×3 matrix, or multiplication between 3×3 matrices.
  - improper rotation (rotary reflection): those with $\det(\overleftrightarrow{R}) = -1$. Improper rotations are a proper rotation followed by inversion.

    Example: S_4 point group symmetry (do not confuse with permutation group). The tetrahedron has no 4-fold axis, but the 4-fold improper rotation $S_4 = I \cdot C_4^{-1}$ (clockwise 4-fold rotation C_4^{-1} followed by an inversion I about the center) is its symmetry (vertices transform as $1 \to 2 \to 3 \to 4 \to 1$).
  - (Proper + improper rotations) form O(3) group.

- Some facts about SO(3) group:
  - Any $SO(3)$ rotation is a rotation of some angle θ around some axis $\boldsymbol{n}$ (3D unit vector), denoted by $\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)$ hereafter. $[\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)]^{-1} = \overleftrightarrow{R}_{\boldsymbol{n}}(-\theta)$.
  - $\overleftrightarrow{R}_{\boldsymbol{n}}(\theta) = \overleftrightarrow{R}_{-\boldsymbol{n}}(-\theta)$, two-fold redundancy for representing SO(3) by $\boldsymbol{n}$ and θ.
  - $\overleftrightarrow{R'} \bullet \overleftrightarrow{R}_{\boldsymbol{n}}(\theta) \bullet \overleftrightarrow{R'}^{-1} = \overleftrightarrow{R}_{\overleftrightarrow{R'}\bullet\boldsymbol{n}}(\theta)$: R'^{-1} followed by rotation around $\boldsymbol{n}$ axis of angle θ then followed by R', is equivalent to a rotation around $\overleftrightarrow{R'} \bullet \boldsymbol{n}$ axis of angle θ.
  - $[\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)]_{i,j} = n_i n_j + \cos\theta \cdot (\delta_{i,j} - n_i n_j) - \sin\theta \cdot \sum_c \epsilon_{ijk} n_k$, here $i, j, k = x, y, z$.

- Parametrizing SO(3) group: Euler angles.
  any SO(3) rotation can be represented as $\overleftrightarrow{R}_z(\alpha) \bullet \overleftrightarrow{R}_y(\beta) \bullet \overleftrightarrow{R}_z(\gamma)$, with three Euler angles $\alpha \in [0, 2\pi)$, $\beta \in [0, \pi)$, $\gamma \in [0, 2\pi)$.



– Rotations around principal axis are explicitly,
$$\overleftrightarrow{R}_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \overleftrightarrow{R}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}, \overleftrightarrow{R}_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}.$$

– Representing group multiplication, Haar measure (volume element of group space), *et cetera*, are not convenient in terms of Euler angles, or $\boldsymbol{n}$ and θ.

B. Defining SU(2) Group

- SU(2) group: the group of 2×2 special unitary matrices, $U^\dagger \cdot U = \mathbb{1}$, and $\det(U) = 1$.
  - U(2) group: no unity determinant condition. Any U(2) matrix $\tilde{U}$ is of the form of $\tilde{U} = e^{\mathbb{i}\theta} U$ with $U \in \mathrm{SU}(2)$, with $\theta = \mathrm{Arg}(\det \tilde{U})/2$.

- Parametrizing SU(2) group: $U = \begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix}$, with $|u|^2 + |v|^2 = 1$,

  the two complex number u, v give a faithful(1-to-1) parametrization of SU(2).

- Quaternion representation of SU(2): $U = a_0\sigma_0 - \mathbb{i}(a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3) = a_0\sigma_0 - \mathbb{i}\boldsymbol{a}\cdot\boldsymbol{\sigma}$, with 4 real numbers $(a_0, a_1, a_2, a_3) = (a_0, \boldsymbol{a})$ with $\sum_i a_i^2 = a_0^2 + \boldsymbol{a}^2 = 1$.
  - Relation to u, v: $a_0 = \mathrm{Re}(u)$, $a_3 = -\mathrm{Im}(u)$, $a_1 = -\mathrm{Im}(v)$, $a_2 = -\mathrm{Re}(v)$.
  - Quaternion: numbers of the form $a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$, represented as $(a_0, \boldsymbol{a})$, where $\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -1$.
    * Note the three "square roots of (-1)" $\mathbf{i}, \mathbf{j}, \mathbf{k}$ anti-commute, $\mathbf{ij} = -\mathbf{ji} = \mathbf{k}$, $\mathbf{jk} = -\mathbf{kj} = \mathbf{i}$, $\mathbf{ki} = -\mathbf{ik} = \mathbf{j}$.
    * $\mathbf{i}, \mathbf{j}, \mathbf{k}$ can be represented by $(-\mathbb{i}\sigma_{1,2,3})$. Exercise: check this.
  - SU(2) group multiplication becomes quaternion number multiplication, and looks like a rotation of 4-component vectors by a $SO(4)$ matrix,
  $$(a_0, \boldsymbol{a}) \circ (b_0, \boldsymbol{b}) \equiv (a_0 b_0 - \boldsymbol{a}\cdot\boldsymbol{b}, a_0\boldsymbol{b} + b_0\boldsymbol{a} + \boldsymbol{a}\times\boldsymbol{b}) = (a_0, a_1, a_2, a_3) \begin{pmatrix} b_0 & b_1 & b_2 & b_3 \\ -b_1 & b_0 & -b_3 & b_2 \\ -b_2 & b_3 & b_0 & -b_1 \\ -b_3 & -b_2 & b_1 & b_0 \end{pmatrix}.$$
  - $\exp(-\mathbb{i}\frac{\theta}{2}\boldsymbol{n}\bullet\boldsymbol{\sigma})$ is represented by $(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}\cdot\boldsymbol{n})$, for unit vector $\boldsymbol{n}$ and real θ.
  - SU(2) manifold is 3-sphere S^3: points $\vec{a}$ in 4D Euclidean space with $|\vec{a}| = 1$. Group multiplications are rotations of S^3 in 4D space.

C. Defining SO(3) and SU(2) Groups

- Relation between SU(2) (quaternion) and SO(3):
  the adjoint representation of SU(2) element $e^{-\mathrm{i}\frac{\theta}{2}\boldsymbol{n}\bullet\boldsymbol{\sigma}}$ is the 3×3 rotation matrix $\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)$.
  $e^{-\mathrm{i}\frac{\theta}{2}\boldsymbol{n}\bullet\boldsymbol{\sigma}}\cdot(\boldsymbol{\sigma}\bullet\boldsymbol{A})\cdot e^{\mathrm{i}\frac{\theta}{2}\boldsymbol{n}\bullet\boldsymbol{\sigma}} = \boldsymbol{\sigma}\bullet\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)\bullet\boldsymbol{A}$. Or $e^{-\mathrm{i}\frac{\theta}{2}\boldsymbol{n}\bullet\boldsymbol{\sigma}}\cdot\sigma_a\cdot e^{\mathrm{i}\frac{\theta}{2}\boldsymbol{n}\bullet\boldsymbol{\sigma}} = \sum_b \sigma_b\cdot[\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)]_{ba}$.
  - NOTE the two-to-one nature of this mapping from SU(2) to SO(3):
    $\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)$ is a quadratic function of quaternion (a_i), so (a_i) and $(-a_i)$, or SU(2) matrices U and $-U$, represent the same SO(3) rotation. $\mathrm{SO}(3)\simeq\mathrm{SU}(2)/\mathbb{Z}_2$.
  - SO(3) manifold is real projective space $\mathrm{RP}^3 = S^3/\mathbb{Z}_2$
    (identify antipodal points, $\vec{a}$ and $-\vec{a}$ with $|\vec{a}|=1$, on S^3).
- Haar measure of SU(2): $\mathrm{d}\mu(U) = \delta(\sqrt{\sum_{i=0}^3 a_i^2}-1)\prod_{i=0}^3 \mathrm{d}a_i$.
  This is the proper(up to constant factor) volume element of SU(2) group space.
  - use 4D polar coordinates, $(a_i) = r\cdot(\cos\frac{\theta}{2},\sin\frac{\theta}{2}(\sin\vartheta\cos\phi,\sin\vartheta\sin\phi,\cos\vartheta))$,
    this measure is $\delta(r-1)\cdot|\frac{\partial(a_0,a_1,a_2,a_3)}{\partial(r,\theta,\vartheta,\phi)}|\cdot\mathrm{d}r\mathrm{d}\theta\mathrm{d}\vartheta\mathrm{d}\phi = \frac{1}{2}\sin^2\frac{\theta}{2}\sin\vartheta\,\mathrm{d}\theta\mathrm{d}\vartheta\mathrm{d}\phi$.
    Integral over group space is over $\theta\in[0,2\pi)$, $\vartheta\in[0,\pi]$, $\phi\in[0,2\pi)$. This can be written as $\frac{1}{2}\sin^2\frac{\theta}{2}\mathrm{d}\theta\cdot\mathrm{d}^2\boldsymbol{n}$, where $\mathrm{d}^2\boldsymbol{n}$ means the surface area element on the unit sphere S^2 of rotation axis $\boldsymbol{n}$ with $|\boldsymbol{n}|=1$ in 3D space.

D. SU(2) and SO(3) Groups and Lie Algebras

- The Lie algebras of SU(2) and SO(3) are essentially the same, $\mathfrak{su}(2)=\mathfrak{so}(3)$.
  - Both $\mathfrak{su}(2)$ and $\mathfrak{so}(3)$ are three dimensional, with three basis(generators) $J_{x,y,z}$.
  - $J_{x,y,z}$ satisfy the commutation relation $[J_a,J_b]=\mathrm{i}\epsilon_{abc}J_c$ (Einstein convention), this is sometimes written as $\boldsymbol{J}\times\boldsymbol{J}=\mathrm{i}\boldsymbol{J}$. Here $a,b,c=x,y,z$.
  - For SO(3), $\overleftrightarrow{J}_x = \begin{pmatrix}0&0&0\\0&0&-\mathrm{i}\\0&\mathrm{i}&0\end{pmatrix}$, $\overleftrightarrow{J}_y = \begin{pmatrix}0&0&\mathrm{i}\\0&0&0\\-\mathrm{i}&0&0\end{pmatrix}$, $\overleftrightarrow{J}_z = \begin{pmatrix}0&-\mathrm{i}&0\\\mathrm{i}&0&0\\0&0&0\end{pmatrix}$.
    Or $(\overleftrightarrow{J}_a)_{bc} = -\mathrm{i}\epsilon_{abc}$. And $\overleftrightarrow{R}_{\boldsymbol{n}}(\theta) = \exp(-\mathrm{i}\theta\overleftrightarrow{\boldsymbol{J}}\bullet\boldsymbol{n})$.
  - For SU(2) matrix group, $J_{x,y,z} = \frac{\sigma_{x,y,z}}{2}$, $\boldsymbol{J}$ are usually denoted by $\boldsymbol{S}$ here.
  - If $[J_a,M_b]=\mathrm{i}\epsilon_{abc}M_c$, by the Baker-Hausdorff formula and the above results,
    $e^{-\mathrm{i}\theta\boldsymbol{n}\bullet\boldsymbol{J}}\cdot M_b\cdot e^{\mathrm{i}\theta\boldsymbol{n}\bullet\boldsymbol{J}} = \sum_c M_c\cdot[\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)]_{cb}$.

- Group elements are $\exp(-\mathbb{i}\theta\boldsymbol{J}\bullet\boldsymbol{n})$, with real θ and real unit vector $\boldsymbol{n}$.
  - For SO(3), θ has period 2π ($e^{-\mathbb{i}2\pi\overleftrightarrow{\boldsymbol{J}}\bullet\boldsymbol{n}} = \overleftrightarrow{1}$).
  - For SU(2), θ has period 4π. Roughly means SU(2) is twice as large as SO(3) (note the 2-to-1 mapping between them).
  - SO(3) & SU(2) matrices are *fundamental representations* of the SO(3) & SU(2) group respectively. SO(3) matrices are adjoint representation of both groups.
  - NOTE: $\exp(-\mathbb{i}\theta'\boldsymbol{J}\bullet\boldsymbol{n}')\exp(-\mathbb{i}\theta\boldsymbol{J}\bullet\boldsymbol{n})\exp(\mathbb{i}\theta'\boldsymbol{J}\bullet\boldsymbol{n}') = \exp(-\mathbb{i}\theta\boldsymbol{J}\bullet\overleftrightarrow{R}_{\boldsymbol{n}'}(\theta')\bullet\boldsymbol{n})$, where $\overleftrightarrow{R}_{\boldsymbol{n}'}(\theta')$ is SO(3) rotation matrix (adjoint representation of $e^{-\mathbb{i}\theta'\boldsymbol{J}\cdot\boldsymbol{n}'}$).
  - Therefore, every element of SU(2) [SO(3)] is conjugate to $\exp(-\mathbb{i}\theta J_z)$, (because any rotation axis $\boldsymbol{n}$ can be rotated to z-direction). The conjugacy classes are determined by θ (infinite many classes). Note that θ and $-\theta$ give the same class, therefore the character of any representation must be even functions of θ.

E. Schwinger Boson Representations of SU(2) & SO(3)

- SU(2) matrices act on a 2-dim'l complex linear space as
$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \xrightarrow{U} U\cdot\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} uz_1 + vz_2 \\ -v^*z_1 + u^*z_2 \end{pmatrix} \equiv \begin{pmatrix} z'_1 \\ z'_2 \end{pmatrix}$$

- View this space as the 1-boson states $(z_1\hat{b}^\dagger_\uparrow + z_2\hat{b}^\dagger_\downarrow)|0\rangle = (\hat{b}^\dagger_\uparrow|0\rangle, \hat{b}^\dagger_\downarrow|0\rangle)\cdot\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$, where $\hat{b}_{\uparrow,\downarrow}$ are two orthonormal boson modes. The transformation of (z_1, z_2) can be also viewed as a unitary transformation on the basis, $(\hat{b}^\dagger_\uparrow, \hat{b}^\dagger_\downarrow) \xrightarrow{U} (\hat{b}^\dagger_\uparrow, \hat{b}^\dagger_\downarrow)\cdot U$.

- The single-boson transformation induces transformation in n-boson space according to $\frac{(z_1\hat{b}^\dagger_\uparrow+z_2\hat{b}^\dagger_\downarrow)^n}{\sqrt{n!}}|0\rangle \xrightarrow{U} \frac{(z'_1\hat{b}^\dagger_\uparrow+z'_2\hat{b}^\dagger_\downarrow)^n}{\sqrt{n!}}|0\rangle$, note that the norm $(|z_1|^2+|z_2|^2)^n = (|z'_1|^2+|z'_2|^2)^n$ does not change, because this is unitary transformation in n-boson space.

- Label the occupation basis $|\hat{n}_\uparrow = n_\uparrow, \hat{n}_\downarrow = n - n_\uparrow\rangle$ as $|j = \frac{n}{2}, m = n_\uparrow - \frac{n}{2}\rangle$.
The above state can be expanded in the occupation basis as
$\frac{(z_1\hat{b}^\dagger_\uparrow+z_2\hat{b}^\dagger_\downarrow)^n}{\sqrt{n!}}|0\rangle = \sum_{n_\uparrow=0}^{n} z_1^{n_\uparrow} z_2^{n-n_\uparrow}\frac{\sqrt{n!}}{(n_\uparrow)!(n-n_\uparrow)!}(\hat{b}^\dagger_\uparrow)^{n_\uparrow}(\hat{b}^\dagger_\downarrow)^{n-n_\uparrow}|0\rangle$
$= \sum_{n_\uparrow=0}^{2j} z_1^{n_\uparrow} z_2^{2j-n_\uparrow}\sqrt{\frac{n!}{n_\uparrow!(n-n_\uparrow)!}}|j, n_\uparrow - j\rangle = \sum_m z_1^{j+m} z_2^{j-m}\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}|j,m\rangle$,
where $\sum_m$ means summing over $m = -j, -j+1, \cdots, j-1, j$.

- U induces a unitary transformation on the basis $|j,m\rangle \xrightarrow{U} \sum_{m'} |j,m'\rangle\, D^{(j)}_{m'm}(U)$.

  The D matrix can be solved by considering
  $\sum_m z_1^{j+m} z_2^{j-m} \sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\,|j,m\rangle \xrightarrow{U} \sum_m (z_1')^{j+m}(z_2')^{j-m}\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\,|j,m\rangle$, and
  $\sum_m z_1^{j+m} z_2^{j-m} \sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\,|j,m\rangle \xrightarrow{U} \sum_{m,m'} z_1^{j+m'} z_2^{j-m'}\sqrt{\frac{(2j)!}{(j+m')!(j-m')!}}\, D^{(j)}_{mm'}(U)\,|j,m\rangle$.

  Plug in $z_1' = uz_1 + vz_2$ and $z_2' = -v^* z_1 + u^* z_2$,
  expand $(z_1')^{j+m} = \sum_{k=0}^{j+m} u^k v^{j+m-k} z_1^k z_2^{j+m-k}\binom{j+m}{k}$,
  and $(z_2')^{j-m} = \sum_{k'=0}^{j-m}(-v^*)^{k'}(u^*)^{j+m-k'} z_1^{k'} z_2^{j-m-k'}\binom{j-m}{k'}$, match terms $(k+k'=j+m')$.

  The matrix element of the $(2j+1)\times(2j+1)$ representation is thus
  $D^{(j)}_{mm'}(U) = \sqrt{\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}}\sum_{k=0}^{j+m}\binom{j+m}{k}\binom{j-m}{j+m'-k} u^k v^{j+m-k}(-v^*)^{j+m'-k}(u^*)^{j-m-(j+m'-k)}$.
  Note: invalid binomial coefficients $\binom{n}{m}$ with $m<0$ or $m>n$ shall be zero.

- $D^{(j)}$ is a $(2j+1)$-dimensional *irreducible* unitary representation of SU(2) group.

  Its "irreducibility" will not be proved here.

- $D^{(j)}_{mm'}(U)$ is a homogeneous polynomial of degree $2j$ in terms of u, v, u^*, v^*.

  For integer j, U and $-U$ produce the same D matrix, this is then an irreducible unitary representation of SO(3).

- Relation to spherical harmonics: $D^{(\ell)}_{0m}(e^{\mathrm{i}\phi J_z}e^{\mathrm{i}\theta J_y}) = \sqrt{\frac{4\pi}{2\ell+1}}Y_\ell^m(\theta,\phi)$, for integer ℓ.

- Orthogonality theorem: $\int [D^{(j')}_{\mu'\mu}(U)]^* \cdot D^{(j)}_{m'm}(U)\,\mathrm{d}\mu(U) = \frac{|\mathrm{SU}(2)|}{2j+1}\delta_{j'j}\delta_{\mu'm'}\delta_{\mu m}$,

  $\mathrm{d}\mu(U)$ is the Haar measure, $|\mathrm{SU}(2)| = \int \mathrm{d}\mu(U)$ is the volume of SU(2) group space.

- Character of j-representation: $\chi_j(e^{-\mathrm{i}\theta \boldsymbol{n}\bullet\boldsymbol{J}}) = \chi_j(e^{-\mathrm{i}\theta J_z}) = \sum_{\mu=0}^{2j} e^{-\mathrm{i}(j-\mu)\theta} = \frac{\sin[(j+\frac{1}{2})\theta]}{\sin\frac{1}{2}\theta}$.

  - Proof: $U = e^{-\mathrm{i}\frac{\theta}{2}\sigma_z}$ induces $z_1 \to e^{-\mathrm{i}\frac{\theta}{2}}z_1$ and $z_2 \to e^{\mathrm{i}\frac{\theta}{2}}z_2$. Then
    $\sum_m (z_1')^{j+m}(z_2')^{j-m}\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\,|j,m\rangle$
    $= \sum_m e^{-\mathrm{i}\frac{\theta}{2}[(j+m)-(j-m)]}\, z_1^{j+m} z_2^{j-m}\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\,|j,m\rangle$.
    Therefore $D^{(j)}_{m'm} = \delta_{m'm}e^{-\mathrm{i}m\theta}$ is a diagonal matrix, and its character is $\sum_m e^{-\mathrm{i}m\theta} = \sum_{\mu=0}^{2j} e^{\mathrm{i}(j-\mu)\theta} = \frac{e^{\mathrm{i}j\theta}-e^{\mathrm{i}(-j-1)\theta}}{1-e^{-\mathrm{i}\theta}} = \frac{e^{\mathrm{i}(j+\frac{1}{2})\theta}-e^{\mathrm{i}(-j-\frac{1}{2})\theta}}{e^{\mathrm{i}\theta/2}-e^{-\mathrm{i}\theta/2}} = \frac{\sin[(j+\frac{1}{2})\theta]}{\sin\frac{1}{2}\theta}$.
  - Exercise: check orthogonality relation $\int_0^{2\pi}\chi_{j'}(\theta)^*\chi_j(\theta)\,\sin^2\frac{\theta}{2}\mathrm{d}\theta = \pi\delta_{j'j}$.

II. ANGULAR MOMENTUM AND SPIN

A. Angular Momentum as SO(3) Generators

- The action of spatial rotation $\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)$ on a wavefunction of 3D coordinates $\psi(\boldsymbol{r})$, by our convention of symmetry action, is $(R_{\boldsymbol{n}}(\theta)\psi)(\boldsymbol{r}) = \psi(\overleftrightarrow{R}_{\boldsymbol{n}}(\theta)^{-1} \bullet \boldsymbol{r}) = \psi(e^{\mathrm{i}\theta \overleftrightarrow{\boldsymbol{J}} \cdot \boldsymbol{n}} \bullet \boldsymbol{r})$. Here $\boldsymbol{J}$ are the fundamental representation matrices of $SO(3)$.

- Take $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\theta}$ at $\theta = 0$, this produces the action of symmetry generator $\widehat{\boldsymbol{n} \cdot \boldsymbol{J}}$ on ψ, $\widehat{\boldsymbol{n} \cdot \boldsymbol{J}}$: $\psi \mapsto -((\boldsymbol{n} \cdot \overleftrightarrow{\boldsymbol{J}}) \bullet \boldsymbol{r}) \cdot \frac{\partial}{\partial \boldsymbol{r}}\psi = -n_a(-\mathrm{i}\epsilon_{abc})r_c \frac{\partial}{\partial r_b}\psi = \boldsymbol{n} \cdot (-\mathrm{i}\boldsymbol{r} \times \frac{\partial}{\partial \boldsymbol{r}})\psi$.
  Therefore $\widehat{\boldsymbol{J}} = -\mathrm{i}\boldsymbol{r} \times \frac{\partial}{\partial \boldsymbol{r}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}/\hbar$.
  This is the orbital angular momentum (divided by $\hbar$) and usually denoted as $\widehat{\boldsymbol{L}}$.

- $\hat{L}_{x,y,z}$ are hermitian. $\hat{\boldsymbol{L}}^2 \equiv \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ is hermitian and positive semi-definite.

- Exercise: check $\widehat{\boldsymbol{L}} \times \widehat{\boldsymbol{L}} = \mathrm{i}\widehat{\boldsymbol{L}}$, $[\widehat{L}_a, \hat{r}_b] = \mathrm{i}\epsilon_{abc}\hat{r}_c$, $[\widehat{L}_a, \hat{p}_b] = \mathrm{i}\epsilon_{abc}\hat{p}_c$, $[\widehat{\boldsymbol{L}}^2, \widehat{L}_{x,y,z}] = 0$.

- Ladder operators: $\hat{L}_\pm = \hat{L}_x \pm \mathrm{i}\hat{L}_y$, obviously $(\hat{L}_+)^\dagger = \hat{L}_-$.
  - $[\hat{L}_z, \hat{L}_+] = +\hat{L}_+$, $[\hat{L}_z, \hat{L}_-] = -\hat{L}_-$, namely $\hat{L}_\pm$ changes $\hat{L}_z$ eigenvalues by ± 1.
  - $[\hat{L}_+, \hat{L}_-] = 2\hat{L}_z$, and
    $\widehat{\boldsymbol{L}}^2 = \hat{L}_z^2 + (1/2)(\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+) = \hat{L}_z(\hat{L}_z - 1) + \hat{L}_+\hat{L}_- = \hat{L}_z(\hat{L}_z + 1) + \hat{L}_-\hat{L}_+$.

- Eigenstates of orbital angular momentum:
  suppose $|\hat{\boldsymbol{L}}^2 = \alpha, \hat{L}_z = \beta\rangle$ is the simultaneous eigenstate of $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$, then
  - $\hat{L}_\pm|\hat{\boldsymbol{L}}^2 = \alpha, \hat{L}_z = \beta\rangle \propto |\hat{\boldsymbol{L}}^2 = \alpha, \hat{L}_z = \beta \pm 1\rangle$, from the commutation relations.
  - Use the above formula of $\hat{\boldsymbol{L}}^2$, notice that $\hat{L}_+\hat{L}_-$ and $\hat{L}_-\hat{L}_+$ are both positive semi-definite. Then $\alpha = \langle\alpha, \beta|\hat{\boldsymbol{L}}^2|\alpha, \beta\rangle \geq \langle\alpha, \beta|\hat{L}_z(\hat{L}_z \pm 1)|\alpha, \beta\rangle = \beta \cdot (\beta \pm 1)$.
  - The sequence of $|\alpha, \beta\rangle$ with different β (differ by integers) must be truncated with a minimal $\beta_{\min}$ and maximal $\beta_{\max}$, *s.t.* $\hat{L}_+|\alpha, \beta_{\max}\rangle = 0$ and $\hat{L}_-|\alpha, \beta_{\min}\rangle = 0$. Then $\alpha = \beta_{\max}\cdot(\beta_{\max}+1) = \beta_{\min}\cdot(\beta_{\min}-1)$. So $\beta_{\max} = -\beta_{\min} = -\frac{1}{2}+\sqrt{\alpha + \frac{1}{4}} \equiv \ell$, $\alpha = \ell \cdot (\ell + 1)$, and $2\ell = \beta_{\max} - \beta_{\min}$ is a non-negative integer.
  - $|\hat{\boldsymbol{L}}^2 = \ell(\ell + 1), \hat{L}_z = m\rangle$ are usually denoted by $|L = \ell, L_z = m\rangle$, or just $|\ell, m\rangle$, with $m = -\ell, -\ell + 1, \ldots, \ell - 1, \ell$.

- In polar coodinates (r, θ, ϕ), $\hat{L}_a$ does not depend on radius r.
  $\hat{L}_z = -\mathbb{i}\frac{\partial}{\partial\phi}$, $\hat{L}_\pm = \pm e^{\pm\mathbb{i}\phi}(\frac{\partial}{\partial\theta} \pm \mathbb{i}\frac{\sin\theta}{\cos\theta}\frac{\partial}{\partial\phi})$.
- If a wavefunction $\psi(\boldsymbol{r})$ is the simultaneous eigenstate of $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$, then it must be $R(r)\cdot Y_\ell^m(\theta, \phi)$, where R is the radial wavefunction, Y_ℓ^m is the spherical harmonics. Here ℓ must be integer, due to the periodicity with respect to ϕ with period 2π.

- Matrix elements in orthonormal $|L = \ell, L_z = m\rangle$ basis:
  $\widehat{\boldsymbol{L}}^2|\ell, m\rangle = \ell(\ell+1)\,|\ell, m\rangle, \qquad \widehat{L}_z|\ell, m\rangle = m\,|\ell, m\rangle,$
  Condon-Shortley convention:
  $\widehat{L}_\pm|\ell, m\rangle = \sqrt{\ell(\ell+1) - m(m\pm 1)}|\ell, m\pm 1\rangle = \sqrt{(\ell\mp m)(\ell\pm m+1)}|\ell, m\pm 1\rangle.$
  - The magnitude of matrix element for $\widehat{L}_\pm$ can be computed by,
    $(\widehat{L}_\pm|\ell, m\rangle, \widehat{L}_\pm|\ell, m\rangle) = \langle\ell, m|\widehat{L}_\pm^\dagger\widehat{L}_\pm|\ell, m\rangle = \langle\ell, m|\widehat{L}_\mp\widehat{L}_\pm|\ell, m\rangle$
    $= \langle\ell, m|\widehat{\boldsymbol{L}}^2 - \widehat{L}_z(\widehat{L}_z \pm 1)|\ell, m\rangle = \ell(\ell+1) - m(m\pm 1) = (\ell\mp m)(\ell\pm m+1)$
  - Condon-Shortley convention fixes relative phases between $|\ell, m\rangle$ with different m.

B. Spin-1/2

- "Real" spin - the intrinsic angular momentum - of a particle (*e.g.* spin-1/2 moment of electron) is usually the combined effect of relativity and quantum mechanics. However there are many pseudo-spin-1/2 systems, which are just *two-state* systems.
  - Examples of pseudospin: electron on one of two-sublattices of graphene.

- Spin-1/2 wavefunctions & spin coherent state:
  Generators of rotation in spin-1/2 Hilbert space are "spin operators" $\boldsymbol{S} = \frac{\boldsymbol{\sigma}}{2}$.
  S_z eigenstates form a complete orthonormal basis $|S_z = \pm\frac{1}{2}\rangle$.
  A generic spin-1/2 wavefunction is $z_1|S_z = +\frac{1}{2}\rangle + z_2|S_z = -\frac{1}{2}\rangle$ (with $|z_1|^2 + |z_2|^2 = 1$).
  This two-component "spinor wavefunction" $\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$ corresponds to a "magnetic moment" along $\boldsymbol{n} = (z_1^*, z_2^*)\cdot\boldsymbol{\sigma}\cdot\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$ direction, this is the spin coherent state $|\boldsymbol{n}\rangle$.
  Exercise: check that $\boldsymbol{n}$ defined above is a real unit vector, check that $(\boldsymbol{n}\cdot\hat{\boldsymbol{S}})|\boldsymbol{n}\rangle = \frac{1}{2}|\boldsymbol{n}\rangle$.
  - For $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the spinor wavefunction is usually chosen as $(z_1[\boldsymbol{n}], z_2[\boldsymbol{n}])^T = (e^{-\mathbb{i}\phi/2}\cos\frac{\theta}{2}, e^{\mathbb{i}\phi/2}\sin\frac{\theta}{2})^T$.

- Note that under $\phi \to \phi + 2\pi$ this spinor wavefunction (zs) changes sign (!)
- Resolution of identity: $\int |\boldsymbol{n}\rangle\langle\boldsymbol{n}| \frac{\sin\theta \mathrm{d}\theta \mathrm{d}\phi}{2\pi} = \hat{\mathbb{1}}$. $|\boldsymbol{n}\rangle$ form overcomplete basis.
- ★ Path integral of spin system can be defined in terms of classical vector $\boldsymbol{n}$ using these basis. However Berry phase must be included: *e.g.* Auerbach, Chapter 10.

• Rotation in spin-1/2 space is implemented by SU(2) matrix $e^{-\mathrm{i}\frac{\theta}{2}\boldsymbol{n}'\cdot\boldsymbol{\sigma}}$:
spinor $e^{-\mathrm{i}\frac{\theta}{2}\boldsymbol{n}'\cdot\boldsymbol{\sigma}} \cdot \begin{pmatrix} z_1[\boldsymbol{n}] \\ z_2[\boldsymbol{n}] \end{pmatrix}$ corresponds to moment along $\overleftrightarrow{R}_{\boldsymbol{n}'}(\theta) \bullet \boldsymbol{n}$ direction.

- Rotation by 2π angle operator is $-\mathbb{1}$ (sign change of spinor wavefunction!). This is true for all half-odd-integer spin/angular momentum system.

• ★ Higher spin coherent states: see *e.g.* Auerbach, Chapter 7.
a spin-S moment along $\boldsymbol{n}$ direction can be thought as $2S$ number of spin-1/2 moments along $\boldsymbol{n}$, $|\boldsymbol{n}\rangle_S \sim |\boldsymbol{n}\rangle_{\frac{1}{2}} \otimes \cdots \otimes |\boldsymbol{n}\rangle_{\frac{1}{2}}$ ($2S$ spin-$\frac{1}{2}$). The $2S$ spin-1/2 has to be symmetrized.
It is in fact the state $\frac{(z_1\hat{b}^\dagger_\uparrow + z_2\hat{b}^\dagger_\downarrow)^n}{\sqrt{n!}}|0\rangle$ used before in Schwinger boson representation, if we identify boson occupation basis $|j, m\rangle$ as spin-S basis $|S, S_z\rangle$.

- $|\boldsymbol{n}\rangle_S = \sum_{m=-S}^{S} \sqrt{\frac{(2S)!}{(S+m)!(S-m)!}} z_1^{S+m} z_2^{S-m} |S, S_z = m\rangle$,
where $z_{1,2}$ are components of spin-$\frac{1}{2}$ spinor $(z_1, z_2)^T$ for moment along $\boldsymbol{n}$.
The $(2S+1)$ coefficients are spin-S spinor wavefunction for moment along $\boldsymbol{n}$.
- $(\boldsymbol{n} \cdot \widehat{\boldsymbol{S}})|\boldsymbol{n}\rangle_S = S|\boldsymbol{n}\rangle_S$, where $\widehat{\boldsymbol{S}}$ is spin operator of spin-S.
- Resolution of identity: $\int |\boldsymbol{n}\rangle_S \langle\boldsymbol{n}|_S \frac{(2S+1)\sin\theta \mathrm{d}\theta \mathrm{d}\phi}{4\pi} = \mathbb{1}$.

C. Addition of Angular Momentum

• system of angular momentum j_1 + system of angular momentum j_2:
the tensor product states $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ transform under SU(2) rotation as
$|j_1, m_1\rangle \otimes |j_2, m_2\rangle \xrightarrow{U} \sum_{m_1', m_2'} |j_1, m_1'\rangle \otimes |j_2, m_2'\rangle \, D^{(j_1)}_{m_1' m_1}(U) \, D^{(j_2)}_{m_2' m_2}(U)$.
This $(2j_1+1)(2j_2+1)$-dimensional tensor product representation is usually reducible.

• Label the angular momentum j irrep by $\mathbf{j}$. Then the tensor product representation
$\mathbf{j_1} \otimes \mathbf{j_2} = |\mathbf{j_1} - \mathbf{j_2}| \oplus (|\mathbf{j_1} - \mathbf{j_2}| + \mathbf{1}) \oplus \cdots \oplus (\mathbf{j_1} + \mathbf{j_2})$. - *Clebsch-Gordon.*
This is just the multiplication table of irreps for SU(2)[SO(3)].

- "Proof": assume without loss of generality $j_1 \geq j_2$, use orthogonality of characters, and $\chi_j = \frac{\sin[(j+\frac{1}{2})\theta]}{\sin(\frac{\theta}{2})}$, show that $\chi_{j_1\otimes j_2} = \chi_{(j_1-j_2)\oplus\cdots\oplus(j_1+j_2)}$,
  Method #1: define $x = e^{\mathbb{i}\theta}$, then $\chi_j = \sum_{\mu=0}^{2j} x^{j-\mu}$, represent $\chi_{j_1\otimes j_2} = \chi_{j_1}\cdot\chi_{j_2}$ and $\chi_{(j_1-j_2)\oplus\cdots\oplus(j_1+j_2)} = \sum_J \chi_J$ both as Laurent series of x, then compare coefficients.
  Method #2: $\chi_{j_1\otimes j_2} = \frac{\sin[(j_1+\frac{1}{2})\theta]\cdot\sin[(j_2+\frac{1}{2})\theta]}{\sin(\frac{\theta}{2})\cdot\sin(\frac{\theta}{2})} = \frac{1}{2}\frac{\cos[(j_1-j_2)\theta]-\cos[(j_1+j_2+1)\theta]}{\sin(\frac{\theta}{2})\cdot\sin(\frac{\theta}{2})}$
  $= \sum_{J=j_1-j_2}^{j_1+j_2} \frac{1}{2}\frac{\cos[J\theta]-\cos[(J+1)\theta]}{\sin(\frac{\theta}{2})\cdot\sin(\frac{\theta}{2})} = \sum_{J=j_1-j_2}^{j_1+j_2} \frac{\sin[(J+\frac{1}{2})\theta]}{\sin(\frac{\theta}{2})} = \chi_{(j_1-j_2)\oplus\cdots\oplus(j_1+j_2)}$.

- The total angular momentum operator $\widehat{\boldsymbol{J}} = \widehat{\boldsymbol{J}}_1\otimes\mathbb{1}+\mathbb{1}\otimes\widehat{\boldsymbol{J}}_2$ (just write $\widehat{\boldsymbol{J}}_1+\widehat{\boldsymbol{J}}_2$) satisfies $\widehat{\boldsymbol{J}}\times\widehat{\boldsymbol{J}} = \mathbb{i}\widehat{\boldsymbol{J}}$. By a unitary transformation of basis, $\widehat{\boldsymbol{J}}$ can be block-diagonalized, each block is the angular momentum operator for J between $|J_1-J_2|$ and J_1+J_2. The unitary transformation is given by the ...

- Clebsch-Gordon coefficient: $\langle J_1, m_1; J_2, m_2|J, m\rangle$ (also denoted by $C^{J_1 J_2 J}_{m_1 m_2 m}$), expansion coefficient of total angular momentum J and $\hat{J}_z = m$ basis state $|J, m\rangle$ on tensor product basis $|J_1, m_1; J_2, m_2\rangle \equiv |J_1, m_1\rangle\otimes|J_2, m_2\rangle$, .

  - Definition: $|J, m\rangle = \sum_{m_1,m_2} |J_1, m_1; J_2, m_2\rangle\langle J_1, m_1; J_2, m_2|J, m\rangle$.
  - Orthogonality: as $(2j_1+1)(2j_2+1)$-dimensional unitary matrix,
    $\sum_{J,m}\langle J_1, m_1'; J_2, m_2'|J, m\rangle\langle J, m|J_1, m_1; J_2, m_2\rangle = \delta_{m_1' m_1}\delta_{m_2' m_2}$,
    $\sum_{m_1,m_2}\langle J', m'|J_1, m_1; J_2, m_2\rangle\langle J_1, m_1; J_2, m_2|J, m\rangle = \delta_{J'J}\delta_{m'm}$.
  - Decomposition of the tensor product representation, $D^{(j)}_{m',m}(U)$
    $= \sum_{m_1',m_2',m_1,m_2}\langle J, m'|J_1, m_1'; J_2, m_2'\rangle\cdot D^{(j_1)}_{m_1',m_1}(U)\cdot D^{(j_2)}_{m_2',m_2}(U)\cdot\langle J_1, m_1; J_2, m_2|J, m\rangle$.
  - Then by orthogonality theorem, $\frac{1}{|SU(2)|}\sum_{U\in SU(2)}[D^{(J)}_{m',m}(U)]^* D^{(J_1)}_{m_1',m_1}(U) D^{(J_2)}_{m_2',m_2}(U)$
    $= \frac{1}{2J+1}\langle J_1, m_1'; J_2, m_2'|J, m'\rangle\langle J, m|J_1, m_1; J_2, m_2\rangle$.
  - Selection rule: $\langle J_1, m_1; J_2, m_2|J, m\rangle$ is nonzero only if $m_1+m_2 = m$ ($\hat{J}_z$ conservation), and $|J_1-J_2| \leq J \leq J_1+J_2$ and J_1+J_2-J is integer.
  - Recursion relation: apply $J_\mp = J_{1,\mp}+J_{2,\mp}$ on $|J, m\pm 1\rangle$, use the above definition of C-G coefficient, we have, $\langle J_1, m_1; J_2, m_2|J, m\rangle$
    $= \sqrt{\frac{(J_1-m_1)(J_1+m_1+1)}{(J-m)(J+m+1)}}\langle J_1, m_1+1; J_2, m_2|J, m+1\rangle + \sqrt{\frac{(J_2-m_2)(J_2+m_2+1)}{(J-m)(J+m+1)}}\langle J_1, m_1; J_2, m_2+1|J, m+1\rangle$
    $= \sqrt{\frac{(J_1-m_1+1)(J_1+m_1)}{(J-m+1)(J+m)}}\langle J_1, m_1-1; J_2, m_2|J, m-1\rangle + \sqrt{\frac{(J_2-m_2+1)(J_2+m_2)}{(J-m+1)(J+m)}}\langle J_1, m_1; J_2, m_2-1|J, m-1\rangle$
  - Consider $m = J+1$ (so $|J, m\rangle = 0$) for the above relation after the last "=".
    We have, $\frac{\langle J_1, m_1-1; J_2, J-m_1+1|J, J\rangle}{\langle J_1, m_1; J_2, J-m_1|J, J\rangle} = -\sqrt{\frac{(J_2-(J-m_1)+1)(J_2+(J-m_1))}{(J_1-m_1+1)(J_1+m_1)}}$.

This solves all $\langle J_1, m_1; J_2, m_2 = J - m_1 | J, m = J\rangle$ up to an overall phase factor. $m < J$ case can be obtained by recursion relation after the first "=".

D. Wigner-Eckart Theorem

- If $(2k+1)$ operators $\hat{T}^{(k)}_q$ $(q = -k, -k+1, \cdots, k)$ transform under rotation as the $|J = k, J_z = q\rangle$ angular momentum basis states, namely under SU(2) rotation U, $\hat{T}^{(k)}_q \xrightarrow{U} \hat{U}\hat{T}^{(k)}_q\hat{U}^\dagger = \sum_{q'} \hat{T}^{(k)}_{q'}\, D^{(k)}_{q'q}(U)$,
  then the matrix element of $\hat{T}^{(k)}_q$ between angular momentum j' & j states is
  $\langle j', m'|\hat{T}^{(k)}_q|j, m\rangle = \langle j', m'|j, m; k, q\rangle\langle j'||\hat{T}^{(k)}||j\rangle$,
  $\langle j'||\hat{T}^{(k)}||j\rangle$ is "reduced matrix element" and does not depend on m', q, m, dependence on m', q, m are all in the Clebsch-Gordon coefficient $\langle j', m'|j, m; k, q\rangle$.
  - In some convention a factor $\frac{1}{\sqrt{2j'+1}}$ is on the right-hand-side.
  - Such operators $\hat{T}^{(k)}_q$ are usually called *irreducible tensor operators*.
    Their commutator with rotation generators are $[\hat{\boldsymbol{J}}, \hat{T}^{(k)}_q] = \sum_{q'} \hat{T}^{(k)}_{q'}\langle k, q'|\hat{\boldsymbol{J}}|k, q\rangle$.
    In particular $[\hat{J}_z, \hat{T}^{(k)}_q] = q\hat{T}^{(k)}_q$, $[\hat{J}_\pm, \hat{T}^{(k)}_q] = \sqrt{(k \mp q)(k \pm q + 1)}\hat{T}^{(k)}_{q\pm 1}$.
  - $\sum_{a=x,y,z}[\hat{J}_a, [\hat{J}_a, \hat{T}^{(k)}_q]] = k(k+1)\hat{T}^{(k)}_q$. This can be used to determine the "angular momentum quantum number" k of an operator.
  - Proof: $\langle j', m'|\hat{T}^{(k)}_q|j, m\rangle = \frac{1}{|SU(2)|}\sum_{U\in SU(2)}\langle j', m'|\hat{U}^\dagger\hat{U}\hat{T}^{(k)}_q\hat{U}^\dagger\hat{U}|j, m\rangle$
    $= \frac{1}{|SU(2)|}\sum_{U\in SU(2)}\sum_{n',q',n}[D^{(j')}_{n',m'}(U)]^* D^{(k)}_{q',q}(U) D^{(j)}_{n,m}(U)\langle j', n'|\hat{T}^{(k)}_{q'}|j, n\rangle$
    (use orthogonality theorem for C-G coefficients)
    $= \sum_{n',q',n} \frac{1}{2j'+1}\langle j', m'|j, m; k, q\rangle\langle j, n; k, q'|j', n'\rangle\langle j', n'|\hat{T}^{(k)}_{q'}|j, n\rangle$.
    So $\langle j'||\hat{T}^{(k)}||j\rangle = \frac{1}{2j'+1}\sum_{n',q',n}\langle j, n; k, q'|j', n'\rangle\langle j', n'|\hat{T}^{(k)}_{q'}|j, n\rangle$.

- Special case: $\hat{T}_a$ transform like a vector, $[\hat{J}_a, \hat{T}_b] = \mathbb{i}\epsilon_{abc}\hat{T}_c$, $(a, b, c = x, y, z)$.
  Projection theorem: $\langle j, m'|\hat{T}_a|j, m\rangle = \frac{\langle j,n|\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{T}}|j,n\rangle}{j(j+1)}\langle j, m'|\hat{J}_a|j, m\rangle$. $(a = x, y, z)$
  - Define $\hat{T}^{(1)}_0 \equiv \hat{T}_z$, $\hat{T}^{(1)}_{\pm1} \equiv \frac{1}{\sqrt{2}}(\mp\hat{T}_x - \mathbb{i}\hat{T}_y)$, and similarly $\hat{J}^{(1)}_q$ $(q = -1, 0, 1)$, they are irreducible tensor operators with angular momentum quantum number $k = 1$.
  - $\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{T}} \equiv \hat{J}_x\hat{T}_x + \hat{J}_y\hat{T}_y + \hat{J}_z\hat{T}_z = \sum_{q=-1}^{1}(\hat{J}^{(1)}_q)^\dagger\hat{T}^{(1)}_q$.
  - $\langle j, n|\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{T}}|j, n\rangle$ is independent of n. So $\hat{\boldsymbol{T}}$ is proportional to $\hat{\boldsymbol{J}}$ in $J = j$ space. The proportionality constant can depend on j though.

– Proof: use Wigner-Eckert theorem, and results for C-G coefficient,
$\langle j,m'|j,m;k=1,q\rangle = \frac{\langle j,m'|\hat{J}^{(1)}_q|j,m\rangle}{\sqrt{j(j+1)}}$ (solve $m'=J$ case first), then
$\langle j,m'|\hat{T}^{(1)}_q|j,m\rangle = \sum_{n',q',n} \frac{\langle j,m'|j,m;k=1,q\rangle\langle j,n;k=1,q'|j,n'\rangle}{2j+1}\langle j,n'|\hat{T}^{(1)}_{q'}|j,n\rangle$
$= \frac{\langle j,m'|\hat{J}^{(1)}_q|j,m\rangle}{j(j+1)}\sum_{n',q',n}\frac{1}{2j+1}\langle j,n|(\hat{J}^{(1)}_{q'})^\dagger|j,n'\rangle\langle j,n'|\hat{T}^{(1)}_{q'}|j,n\rangle$
$= \langle j,m'|\hat{J}^{(1)}_q|j,m\rangle\cdot\frac{1}{j(j+1)}\cdot\frac{\sum_n\langle j,n|\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{T}}|j,n\rangle}{2j+1}$.

E. Examples:

- Landé g-factor:
  consider a particle with orbital angular momentum L and spin S,
  the coupling to Zeeman magnetic field $\boldsymbol{B}$ is $\widehat{H} = -\boldsymbol{B}\cdot\mu_B(g_L\widehat{\boldsymbol{L}} + g_S\widehat{\boldsymbol{S}})$,
  where $\mu_B = \frac{e\hbar}{2m}$ is a constant derived from particle charge e and mass m.
  Define total angular momentum $\widehat{\boldsymbol{J}} = \widehat{\boldsymbol{L}} + \widehat{\boldsymbol{S}}$. Then $[\widehat{\boldsymbol{J}}^2, \hat{H}] = 0$. In the subspace of total angular momentum J [namely subspace of $\widehat{\boldsymbol{J}}^2 = J(J+1)$], this Hamiltonian is $\widehat{H}_J = -\boldsymbol{B}\cdot\mu_B g_J\widehat{\boldsymbol{J}}$, where g_J is the Landé g-factor.

  – Define $\widehat{\boldsymbol{M}} = (g_L\widehat{\boldsymbol{L}} + g_S\widehat{\boldsymbol{S}})$. Exercise: check $[\widehat{J}_a, \widehat{M}_b] = \mathbb{i}\epsilon_{abc}\widehat{M}_c$, and $[\widehat{\boldsymbol{J}}^2, \widehat{\boldsymbol{M}}] = 0$.

  – According to the projection theorem, $\widehat{\boldsymbol{M}} = \frac{\langle J,m|\widehat{\boldsymbol{J}}\cdot\widehat{\boldsymbol{M}}|J,m\rangle}{J(J+1)}\widehat{\boldsymbol{J}}$.
  Use $\widehat{\boldsymbol{J}}\cdot\widehat{\boldsymbol{M}} = g_L\widehat{\boldsymbol{L}}^2 + g_S\widehat{\boldsymbol{S}}^2 + (g_L+g_S)\widehat{\boldsymbol{L}}\cdot\widehat{\boldsymbol{S}} = g_L\widehat{\boldsymbol{L}}^2 + g_S\widehat{\boldsymbol{S}}^2 + (g_L+g_S)\frac{\widehat{\boldsymbol{J}}^2-\widehat{\boldsymbol{L}}^2-\widehat{\boldsymbol{S}}^2}{2}$
  $= \frac{g_L-g_S}{2}(\widehat{\boldsymbol{L}}^2 - \widehat{\boldsymbol{S}}^2) + \frac{g_L+g_S}{2}\widehat{\boldsymbol{J}}^2$,
  then we have $g_J = \frac{(g_L-g_S)[L(L+1)-S(S+1)]+(g_L+g_S)J(J+1)}{2J(J+1)}$.

  – For electron, $g_L = 1$, $g_S \approx 2$, $\mu_B = \frac{e\hbar}{2m_e}$ is the Bohr magneton.

III. TIME-REVERSAL SYMMETRY

- Effects of time-reversal in classical physics: changes sign of
  velocity, momentum, angular momentum, electric current, magnetic moment, magnetic field, ...

- Time-reversal for non-relativistic wavefunction in quantum mechanics:
  Take complex conjugate of $\mathbb{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi = \hat{H}\psi$, it becomes $\mathbb{i}\frac{\mathrm{d}}{\mathrm{d}(-t)}\psi^* = \hat{H}^*\psi^*$. *In this case*, time-reversal is just complex conjugation on wavefunction, $\hat{\mathcal{T}}:\ t\to -t,\ \psi\to\psi^*$.

- If the Hamiltonian is "real", the system has **time-reversal symmetry**: $\psi^*(-t)$ is the solution of the same Schrödinger equation as $\psi(t)$.
- With time-reversal symmetry, non-degenerate energy eigenstates $\psi(t)$ are (real function)$\times e^{-\mathrm{i}\phi} e^{-\mathrm{i}Et}$.
  'proof': $\psi(t)$ and $\psi^*(-t)$ are of same energy. So $\psi^*(t=0) = e^{2\mathrm{i}\phi}\psi(t=0)$, then $e^{\mathrm{i}\phi}\psi(t=0)$ is real.

- Complex conjugation operator $\hat{\mathcal{K}}$: anti-linear operator ($\hat{\mathcal{K}}\lambda|\psi\rangle = \lambda^*\hat{\mathcal{K}}|\psi\rangle$) defined in coordinate basis as $\hat{\mathcal{K}}|x\rangle = |x\rangle$. Note that $\hat{\mathcal{K}}^\dagger = \hat{\mathcal{K}}^{-1} = \hat{\mathcal{K}}$. For anti-linear operator $\hat{\mathcal{K}}$, the Hermitian conjugate is defined by $(\hat{\mathcal{K}}^\dagger\psi, \phi) = (\psi, \hat{\mathcal{K}}\phi)^*$.
  - "**Real states**" are states invariant under time-reversal: $\hat{\mathcal{K}}|\phi\rangle = |\phi\rangle$.
  - $\langle x|\hat{\mathcal{K}}|\psi\rangle = \langle x|\hat{\mathcal{K}}\left(\int \psi(x')|x'\rangle\,\mathrm{d}x'\right) = \langle x|\left(\int \psi^*(x')|x'\rangle\,\mathrm{d}x'\right) = \psi(x)^*$.
  - $\hat{\mathcal{K}}|p\rangle = \hat{\mathcal{K}}\left(\int \frac{e^{\mathrm{i}px}}{\sqrt{2\pi}}|x\rangle\,\mathrm{d}x\right) = \int \frac{e^{-\mathrm{i}px}}{\sqrt{2\pi}}|x\rangle\,\mathrm{d}x = |-p\rangle$.
  - For linear operator $\hat{O}$, $\hat{\mathcal{K}}\hat{O} = \hat{O}^*\hat{\mathcal{K}}$, or $\hat{\mathcal{K}}\hat{O}\hat{\mathcal{K}}^{-1} = \hat{O}^*$.
    Note: $\langle\phi|\hat{O}^*|\psi\rangle = (\langle\phi|\hat{O}|\psi\rangle)^*$ only for real states.
  - Any anti-linear operator $\hat{O} = \hat{O}\hat{\mathcal{K}}\cdot\hat{\mathcal{K}}$, where $\hat{O}\hat{\mathcal{K}}$ is a linear operator.
    Any anti-unitary operator is of the form $\hat{U}\hat{\mathcal{K}}$ where $\hat{U}$ is a unitary operator.

A. Time-reversal Symmetry and Angular Momentum

- Time-reversal operation on states should change sign of measured angular momentum, $\langle J, m'|\widehat{\mathcal{T}}^\dagger\,\widehat{\boldsymbol{J}}\,\widehat{\mathcal{T}}|J, m\rangle = -\langle J, m'|\widehat{\boldsymbol{J}}|J, m\rangle$.
  - Consider $\widehat{J}_z$, $\langle J, m'|\widehat{J}_z|J, m\rangle = \delta_{m'm}m$, the above relation shows that $\widehat{\mathcal{T}}|J, m\rangle = c_m|J, -m\rangle$, where c_m is a phase factor.
  - Consider $\widehat{J}_x$, $\langle J, m'|\widehat{J}_x|J, m\rangle$
    $= \frac{1}{2}(\delta_{m',m+1}\sqrt{(J-m)(J+m+1)} + \delta_{m'+1,m}\sqrt{(J-m')(J+m'+1)})$.
    $\langle J, m'|\widehat{\mathcal{T}}^\dagger\,\widehat{J}_x\,\widehat{\mathcal{T}}|J, m\rangle = c^*_{m'}c_m\langle J, -m'|\widehat{J}_x|J, -m\rangle$
    $= c^*_{m'}c_m\frac{1}{2}(\delta_{-m',-m+1}\sqrt{(J+m)(J-m+1)} + \delta_{-m'+1,-m}\sqrt{(J+m')(J-m'+1)})$.
    Comparing terms, *e.g.* for $m' = m+1$, we must have $c_{m+1} = -c_m$.
  - Finally $\widehat{\mathcal{T}}|J, m\rangle = c\,(-1)^{J-m}|J, -m\rangle$, where c is a constant phase.

- For integer J, Condon-Shortley convention is $[c = (-1)^J]$
  $\widehat{\mathcal{T}}|J, m\rangle = (-1)^m |J, -m\rangle$.
- For spin-1/2, the usual convention is $c = 1$, $\widehat{\mathcal{T}}|\uparrow\rangle = |\downarrow\rangle$, $\widehat{\mathcal{T}}|\downarrow\rangle = -|\uparrow\rangle$.
- $\widehat{\mathcal{T}}\widehat{\mathcal{T}}|J, m\rangle = \widehat{\mathcal{T}} c\,(-1)^{J-m}|J, -m\rangle = c^* c\,(-1)^{J-m}(-1)^{J+m}|J, m\rangle = (-1)^{2J}|J, m\rangle$.
  For half-odd-integer J states, $\widehat{\mathcal{T}}^2 = -\mathbb{1}$.

- Time-reversal operations on operators: time-reversal operator $\widehat{\mathcal{T}} = \widehat{U}_T \widehat{\mathcal{K}}$,
  where $\widehat{U}_T$ is some unitary operator, $\widehat{\mathcal{K}}$ is complex conjugation.
  We need $(\widehat{U}_T)_{ij}(\widehat{\boldsymbol{J}})^*_{jk}(\widehat{U}_T^\dagger)_{k\ell} = -(\widehat{\boldsymbol{J}})_{i\ell}$. However $\widehat{U}_T$ would depend on basis choice (!).
  - Using $|J, J_z\rangle$ basis, $\widehat{U}_T = e^{\mathrm{i}\pi \widehat{J}_y}$ (Condon-Shortley convention). In this basis, $\widehat{J}_y$ are purely imaginary in this basis, so changes sign under complex conjugation; $\widehat{J}_{x,z}$ matrix elements are real, but $e^{\mathrm{i}\pi\widehat{J}_y}\widehat{J}_{x,z}e^{-\mathrm{i}\pi\widehat{J}_y} = -\widehat{J}_{x,z}$.
  - For spin-1/2, the common convention is $\widehat{U}_T = \mathrm{i}\sigma^y$.
  - However if "real" basis are used, *e.g.*, for $L = 1$, use p-orbital basis, $|p_x\rangle = \frac{|L=1,m=-1\rangle - |L=1,m=1\rangle}{\sqrt{2}}$, $|p_y\rangle = \frac{|L=1,m=-1\rangle + |L=1,m=1\rangle}{-\sqrt{2}\mathrm{i}}$, $|p_z\rangle = |L = 1, m = 0\rangle$, the matrix elements of $\widehat{\boldsymbol{L}}$ are all purely imaginary. Time-reversal is just complex conjugation on matrix elements, without further unitary transformation.

B. Time-reversal Symmetry: Kramers Degeneracy

- Kramers theorem (Kramers degeneracy):
  for system with time-reversal symmetry and of half-odd-integer angular momentum, all energy levels are (at least) doubly degenerate.
  - Suppose energy eigenstate $|E\rangle$ is non-degenerate, time-reversal symmetry dictates that $\widehat{\mathcal{T}}|E\rangle$ is also energy E eigenstate, so $\widehat{\mathcal{T}}|E\rangle = e^{\mathrm{i}\phi}|E\rangle$, then $\widehat{\mathcal{T}}\widehat{\mathcal{T}}|E\rangle = e^{\mathrm{i}\phi}e^{-\mathrm{i}\phi}|E\rangle = |E\rangle$, this contradicts $\widehat{\mathcal{T}}^2 = -\mathbb{1}$ for half-odd-integer spin.
  - In fact, the inner product $(|E\rangle, \mathcal{T}|E\rangle)$ vanishes. By the definition of anti-unitary operator, $(|E\rangle, \mathcal{T}|E\rangle) = (\mathcal{T}|E\rangle, \mathcal{T}\mathcal{T}|E\rangle)^* = (\mathcal{T}|E\rangle, -|E\rangle)^* = -(|E\rangle, \mathcal{T}|E\rangle)$.
  - For system with odd number of electrons and time-reversal symmetry, the energy levels must be doubly degenerate. Because odd number of spin-1/2 can only produce half-odd-integer total spin.

Summary of Lecture #6: perturbation theory

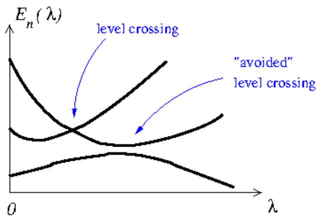
The Goals and The Requirements

- Understand the generic and formal approach to perturbative expansion for time-independent perturbations.
  - Viewpoint #1: perturbative expansion as a (asymptotic) series expansion of energy eigenvalues and eigenstates.
  - Viewpoint #2: perturbative expansion as a sequence of unitary transformations, trying to separate coupled modes/degrees of freedom.
- Understand the basic tools for dealing with time-dependent perturbations:
  the interaction picture for Hamiltonian(Schrödinger picture) $\hat{H}_S(t) = \hat{H}_0 + \hat{V}_S(t)$.
  - Definitions: $|\psi(t)\rangle_I = e^{\mathbb{i}\hat{H}_0 t/\hbar}|\psi(t)\rangle_S$, $\hat{O}_I(t) = e^{\mathbb{i}\hat{H}_0 t/\hbar}\hat{O}_S e^{-\mathbb{i}\hat{H}_0 t/\hbar}$.
    Relation to Schrödinger picture: $\langle\psi(t)|_S\hat{O}_S|\phi(t)\rangle_S = \langle\psi(t)|_I\hat{O}_I(t)|\phi(t)\rangle_I$.
  - Time evolution: $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_I = \hat{V}_I(t)|\psi(t)\rangle_I$.
    $|\psi(t)\rangle_I = \hat{U}_I(t)|\psi(t=0)\rangle_I = \hat{U}_I(t)|\psi(t=0)\rangle_S$, formally $\hat{U}_I(t) = \mathcal{T}e^{-\frac{\mathbb{i}}{\hbar}\int_0^t \hat{V}_I(t')\,\mathrm{d}t'}$,
    Dyson series: $\hat{U}_I(t) = \mathbb{1} + \frac{-\mathbb{i}}{\hbar}\int_{t_1=0}^{t}\hat{V}_I(t_1)\,\mathrm{d}t_1 + (\frac{-\mathbb{i}}{\hbar})^2\int_{t_1=0}^{t}\int_{t_2=0}^{t_1}\hat{V}_I(t_1)\hat{V}_I(t_2)\,\mathrm{d}t_1\mathrm{d}t_2 + \ldots$
  - Note the similarity and difference to the Heisenberg picture (lecture notes #3).
- Optional references:
  J.J. Sakurai, *Modern Quantum Mechanics*, Chapter 5.
  Landau & Lifschitz, *Quantum Mechanics: Non-relativistic Theory*, Chapter VI.

I. TIME-INDEPENDENT PERTURBATION THEORY FOR DISCRETE LEVELS

A. Nondegenerate Perturbation Theory: The Goal

- Given a Hamiltonian $\hat{H}_0$ with nondegenerate energy eigenvalues $E_n^{(0)}$ and corresponding normalized eigenstates $|\psi_n^{(0)}\rangle$ $(n = 0, 1, \cdots)$, compute the energy eigenvalues and eigenstates of $\hat{H} = \hat{H}_0 + \lambda\hat{V}$, in terms of series of the "small parameter" λ.
  - In the $|n\rangle$ basis, $\hat{H}_0$ is a diagonal matrix $(H_0)_{mn} = E_n\delta_{mn}$ with nondegenerate diagonal entries. $\hat{V}$ is a generic matrix with matrix element $V_{mn} = \langle\psi_m^{(0)}|\hat{V}|\psi_n^{(0)}\rangle$.
  - Diagonal and off-diagonal matrix elements of $\hat{V}$ play different roles: diagonal V_{nn} shifts energy of n-th level without changing eigenstate; off-diagonal V_{mn} mixes n-th and m-th eigenstates and shifts their energies.
  - "Level repulsion": eigenvalues of $\begin{pmatrix} E_0 & V_{12} \\ V_{12}^* & E_1 \end{pmatrix}$ is $\frac{E_0+E_1}{2} \pm \sqrt{(\frac{E_0-E_1}{2})^2 + |V_{12}|^2}$, the difference is $\sqrt{(E_0 - E_1)^2 + 4|V_{12}|^2} \geq |E_1 - E_0|$, adding off-diagonal perturbation tends to increase level distance.
  - It is usually assumed that for sufficiently small λ, the n-th eigenstates $|n, \lambda\rangle$ of $\hat{H}$ is *adiabatically* connected to $|\psi_n^{(0)}\rangle$ (no level-crossing with increasing λ).

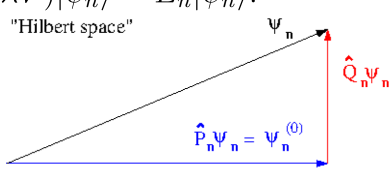


  - *Assume* the n-th eigenvalue and n-th eigenstate are, $E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$, $|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \cdots$. Note that $|\psi_n\rangle$ here is *not* normalized, and it is usually assumed that all perturbations $|\psi_n^{(k>0)}\rangle$ are orthogonal to $|\psi_n^{(0)}\rangle$.

B. Formal Perturbative Expansion

- Define projection operators $\hat{P}_n = |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|$ and $\hat{Q}_n = \mathbb{1} - \hat{P}_n = \sum_{m\neq n} |\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|$. Note that $\hat{H}_0\hat{P}_n = \hat{P}_n\hat{H}_0 = E_n^{(0)}\hat{P}_n$, $[\hat{H}_0, \hat{Q}_n] = 0$ and $\hat{P}_n\hat{Q}_n = \hat{Q}_n\hat{P}_n = 0$.

- Consider the stationary state Schrödinger equation: $(\hat{H}_0 + \lambda\hat{V})|\psi_n\rangle = E_n|\psi_n\rangle$. Use $|\psi_n\rangle = \hat{P}_n|\psi_n\rangle + \hat{Q}_n|\psi_n\rangle$, *assume* $\hat{Q}_n|\psi_n\rangle$ is a small perturbation to be solved. Rearrange terms,



  $(E_n - \hat{H}_0)\hat{Q}_n|\psi_n\rangle = (E_n^{(0)} - E_n)\hat{P}|\psi_n\rangle + \lambda\hat{V}|\psi_n\rangle \quad (*)$.
  Apply $\hat{Q}_n$ on both sides of $(*)$, $\hat{Q}_n(E_n - \hat{H}_0)\hat{Q}_n \cdot \hat{Q}_n|\psi_n\rangle = 0 + \lambda\hat{Q}_n\hat{V}|\psi_n\rangle$.

- The non-trivial eigenvalues of $\hat{Q}_n(E_n - \hat{H}_0)\hat{Q}_n$ are $E_n - E_m^{(0)}$ with $m \neq n$, *assume* all these eigenvalues are nonzero, then this operator has an "inverse" $\hat{G}_n = \hat{Q}_n \frac{1}{E_n - \hat{H}_0} \hat{Q}_n$. defined on the space orthogonal to $|\psi_n^{(0)}\rangle$, $\hat{G}_n \cdot \hat{Q}_n(E_n - \hat{H}_0)\hat{Q}_n = \hat{Q}_n$. Note that $\hat{G}_n\hat{Q}_n = \hat{Q}_n\hat{G}_n = \hat{G}_n$, and $\hat{G}_n\hat{P}_n = \hat{P}_n\hat{G}_n = 0$.

- We can now "solve" the perturbation as $\hat{Q}_n|\psi_n\rangle = \hat{G}_n\hat{Q}_n\lambda\hat{V}|\psi_n\rangle = \hat{G}_n\lambda\hat{V}|\psi_n\rangle$. Then $|\psi_n\rangle = \hat{P}_n|\psi_n\rangle + \hat{G}_n\lambda\hat{V}|\psi_n\rangle$, or $(\mathbb{1} - \hat{G}_n\lambda\hat{V})|\psi_n\rangle = \hat{P}_n|\psi_n\rangle$, or formally
$|\psi_n\rangle = (\mathbb{1} - \hat{G}_n\lambda\hat{V})^{-1}\,\hat{P}_n|\psi_n\rangle = \sum_{k=0}^{\infty}(\hat{G}_n\lambda\hat{V})^k\,\hat{P}_n|\psi_n\rangle$ [1].

- Take inner product with $\hat{P}_n|\psi_n\rangle$ on both sides of $(*)$, we can "solve" the energy shift, $(E_n - E_n^{(0)})\langle\psi_n|\hat{P}_n|\psi_n\rangle = \langle\psi_n|\hat{P}_n\lambda\hat{V}|\psi_n\rangle = \sum_{k=0}^{\infty}\langle\psi_n|\hat{P}_n\lambda\hat{V}(\hat{G}_n\lambda\hat{V})^k\hat{P}_n|\psi_n\rangle$ [2].

- $\hat{P}_n|\psi_n\rangle \propto |\psi_n^{(0)}\rangle$, usually just choose $\hat{P}_n|\psi_n\rangle = |\psi_n^{(0)}\rangle$. Then $\langle\psi_n|\psi_n\rangle \geq \langle\psi_n|\hat{P}_n|\psi_n\rangle = 1$.

- Example: 3-level problem, under the basis of $(|\psi_1^{(0)}\rangle, |\psi_2^{(0)}\rangle, \psi_3^{(0)}\rangle)$, $\hat{H}_0$ is diagonal. For $n = 1$, $\hat{P}_{n=1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, $\hat{Q}_{n=1} = \mathbb{1}_{3\times 3} - \hat{P}_{n=1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, $\hat{G}_{n=1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{E_1 - E_2^{(0)}} & 0 \\ 0 & 0 & \frac{1}{E_1 - E_3^{(0)}} \end{pmatrix}$.

C. Formal Perturbative Expansion: Summary

- Summary:
$|\psi_n\rangle = (\mathbb{1} - \lambda\hat{G}_n\hat{V})^{-1}\,\hat{P}_n|\psi_n\rangle = \sum_{k=0}^{\infty}\lambda^k(\hat{G}_n\hat{V})^k\,\hat{P}_n|\psi_n\rangle$ [1],
$(E_n - E_n^{(0)})\langle\psi_n|\hat{P}_n|\psi_n\rangle = \sum_{k=0}^{\infty}\langle\psi_n|\hat{P}_n\lambda\hat{V}(\hat{G}_n\lambda\hat{V})^k\hat{P}_n|\psi_n\rangle$ [2], where $\hat{G}_n = \hat{Q}_n\frac{1}{E_n - \hat{H}_0}\hat{Q}_n$.

- Note that [1] and [2] do not really solve $|\psi_n\rangle$ and E_n in terms of known quantities. Because $\hat{G}_n$ contains the unknown E_n.

- 1st-order perturbation: approximate $|\psi_n\rangle = \hat{P}_n|\psi_n\rangle + O(\lambda) = |\psi_n^{(0)}\rangle + O(\lambda)$. Then $E_n - E_n^{(0)} = \lambda\langle\psi_n^{(0)}|\hat{V}|\psi_n^{(0)}\rangle + O(\lambda^2) = \lambda V_{nn} + O(\lambda^2)$.

- 2nd-order perturbation: $|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda\hat{G}_n\hat{V}|\psi_n^{(0)}\rangle + O(\lambda^2)$
$= |\psi_n^{(0)}\rangle + \lambda\hat{Q}_n\frac{1}{E_n^{(0)} - \hat{H}_0}\hat{Q}_n\hat{V}|\psi_n^{(0)}\rangle + O(\lambda^2) = |\psi_n^{(0)}\rangle + \lambda\sum_{m\neq n}\frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}|\psi_m^{(0)}\rangle + O(\lambda^2)$.
$E_n - E_n^{(0)} = \lambda V_{nn} + \lambda^2\sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n^{(0)} - E_m^{(0)}} + O(\lambda^3)$.
Note that off-diagonal V_{nm} always lowers ground state energy (level repulsion).

- For higher order perturbation, more accurate E_n should be used in $\hat{G}_n$. For example, the 3rd-order energy shift is $E_n - E_n^{(0)} = \lambda V_{nn} + \langle\psi_n^{(0)}|\lambda\hat{V}\hat{G}_n\lambda\hat{V}|\psi_n^{(0)}\rangle +$

$\langle\psi_n^{(0)}|\lambda\hat{V}\hat{G}_n\lambda\hat{V}\hat{G}_n\lambda\hat{V}|\psi_n^{(0)}\rangle + O(\lambda^4)$. In the $\langle\psi_n^{(0)}|\lambda\hat{V}\hat{G}_n\lambda\hat{V}|\psi_n^{(0)}\rangle$ term, you need to use λ^1-order approximation of $\hat{G}_n$, then you need to use $E_n \approx E_n^{(0)} + \lambda V_{nn}$, and $\frac{1}{E_n - E_m^{(0)}} \approx \frac{1}{E_n^{(0)}+\lambda V_{nn}-E_m^{(0)}} \approx \frac{1}{E_n^{(0)}-E_m^{(0)}} - \frac{\lambda V_{nn}}{(E_n^{(0)}-E_m^{(0)})^2}$ in $\hat{G}_n$. In the $\langle\psi_n^{(0)}|\lambda\hat{V}\hat{G}_n\lambda\hat{V}\hat{G}_n\lambda\hat{V}|\psi_n^{(0)}\rangle$ term, you can use the 0^{th}-order approximation of $\hat{G}_n$.

- Wavefunction re-normalization: $\langle\psi_n|\psi_n\rangle = \frac{1}{Z_n}$, $Z_n \le 1$ is the weight of unperturbed state $|\psi_n^{(0)}\rangle$ in $|\psi_n\rangle$. Perturbative expansion is good when Z_n is close to unity.
  Z_n is related to $Z_n = \frac{\partial}{\partial E_n^{(0)}} E_n$.
  - 'Proof': $\frac{1}{Z_n} = \langle\psi_n|\psi_n\rangle = \sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\lambda^{k+k'}\langle\psi_n^{(0)}|(\hat{V}\hat{G}_n)^k(\hat{G}_n\hat{V})^{k'}|\psi_n^{(0)}\rangle = 1 + \sum_{k=1}^{\infty}\sum_{k'=1}^{\infty}\lambda^{k+k'}\langle\psi_n^{(0)}|(\hat{V}\hat{G}_n)^k(\hat{G}_n\hat{V})^{k'}|\psi_n^{(0)}\rangle$. Note that $\hat{G}_n|\psi_n^{(0)}\rangle = 0$, so the $k=0, k'\neq 0$ or $k'=0, k\neq 0$ terms do not contribute.
    Take $\frac{\partial}{\partial E_n^{(0)}}$ on both sides of [2] (fix $E_m^{(0)}$ for $m \neq n$, $|\psi_m^{(0)}\rangle$, $\hat{V}$), note that $\frac{\partial}{\partial E_n^{(0)}}\hat{G}_n = \frac{\partial}{\partial E_n^{(0)}}(\hat{Q}_n\frac{1}{E_n-\hat{H}_0}\hat{Q}_n) = \sum_{m\neq n}|\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|\frac{-1}{(E_n-E_m^{(0)})^2}\frac{\partial}{\partial E_n^{(0)}}E_n = -(\hat{G}_n)^2\frac{\partial}{\partial E_n^{(0)}}E_n$, then $\frac{\partial}{\partial E_n^{(0)}}E_n - 1 = \lambda\langle\psi_n^{(0)}|\hat{V}\left(\frac{\partial}{\partial E_n^{(0)}}|\psi_n\rangle\right) = \lambda\langle\psi_n^{(0)}|\hat{V}\sum_{k=1}^{\infty}\lambda^k\left(\frac{\partial}{\partial E_n^{(0)}}(\hat{G}_n\hat{V})^k\right)|\psi_n^{(0)}\rangle = -\frac{\partial}{\partial E_n^{(0)}}E_n \cdot \langle\psi_n^{(0)}|\hat{V}\sum_{k=1}^{\infty}\lambda^{k+1}\sum_{k'=0}^{k-1}(\hat{G}_n\hat{V})^{k'}\hat{G}_n(\hat{G}_n\hat{V})^{k-k'}|\psi_n^{(0)}\rangle$. Therefore $(\frac{\partial}{\partial E_n^{(0)}}E_n)^{-1} = 1 + \sum_{k=2}^{\infty}\lambda^k\sum_{k'=1}^{k-1}\langle\psi_n^{(0)}|(\hat{V}\hat{G}_n)^{k'}(\hat{G}_n\hat{V})^{k-k'}|\psi_n^{(0)}\rangle = \langle\psi_n|\psi_n\rangle$.
- Non-degenerate perturbation is a good approximation when the off-diagonal terms are much smaller than original energy differences, $|\lambda V_{n,m}| \ll |E_n^{(0)} - E_m^{(0)}|$ $(n \neq m)$.

D. Example: Harmonic Oscillator Plus Linear Potential

- $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = \hbar\omega(\hat{b}^\dagger\hat{b} + \frac{1}{2})$, with non-degenerate energy levels $E_n^{(0)} = (n+\frac{1}{2})\hbar\omega$, and unperturbed eigenstates $|\psi_n^{(0)}\rangle = \frac{1}{\sqrt{n!}}(\hat{b}^\dagger)^n|\psi_0^{(0)}\rangle$, and $\hat{b}|\psi_0^{(0)}\rangle = 0$,
- Perturbation $\lambda\hat{V} = \lambda\hat{x} = \lambda\sqrt{\frac{\hbar}{2m\omega}}(\hat{b}+\hat{b}^\dagger)$, $V_{nm} = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{m}\delta_{n+1,m} + \sqrt{n}\delta_{n,m+1})$.
- 1st-order perturbation vanishes. 2nd-order perturbation correction to energy is $E_n \approx E_n^{(0)} + \sum_{m\neq n}\frac{\lambda^2|V_{nm}|^2}{E_n - E_m} = E_n^{(0)} + \frac{\lambda^2}{2m\omega}(\frac{n+1}{-\omega} - \frac{n}{\omega}) = E_n^{(0)} - \frac{\lambda^2}{2m\omega^2}$.
- This happens to be the exact result. $\hat{H}_0 + \lambda\hat{V} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + \lambda\hat{x}$ $= \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}(\hat{x} + \frac{\lambda}{m\omega^2})^2 - \frac{\lambda^2}{2m\omega^2} = \hbar\omega(\hat{b}'^\dagger\hat{b}' + \frac{1}{2}) - \frac{\lambda^2}{2m\omega^2}$, with $\hat{b}' = \hat{b} + \frac{\lambda}{\sqrt{2\hbar m\omega^3}}$.
- Due to inversion symmetry $\hat{I}:\ |x\rangle \mapsto |-x\rangle$, $\hat{I}(\hat{H}_0 + \lambda\hat{V})\hat{I}^\dagger = \hat{H}_0 - \lambda\hat{V}$. Eigenvalues of $\hat{H}_0 + \lambda\hat{V}$ must be even function of λ. Therefore all odd-order perturbations vanish.

- Exercise: compute the 4th order correction and check that it vanishes.

E. Degenerate Perturbation Theory

- If energy level $E_n^{(0)}$ has g-fold degenerate orthonormal eigenstates $|\psi_{n\alpha}^{(0)}\rangle$, $\alpha = 1, \cdots, g$, define $\hat{P}_n = \sum_\alpha |\psi_{n\alpha}^{(0)}\rangle\langle\psi_{n\alpha}^{(0)}|$ and $\hat{Q}_n = \mathbb{1} - \hat{P}_n$. The expansion is the same, except...

- $\hat{P}_n|\psi_n\rangle = \sum_\alpha c_\alpha |\psi_{n\alpha}^{(0)}\rangle$ is a linear combination with unknown coefficients c_α to be solved.

- $|\psi_n\rangle = (\mathbb{1} - \lambda\hat{G}_n\hat{V})^{-1}\,\hat{P}_n|\psi_n\rangle = \sum_\beta \sum_{k=0}^{\infty} \lambda^k (\hat{G}_n\hat{V})^k\,|\psi_{n\beta}^{(0)}\rangle\, c_\beta \qquad [1'].$

- Take inner product with $|\psi_{n\alpha}^{(0)}\rangle$ on both sides of $(*)$, we have the "secular equation", $(E_n - E_n^{(0)}) \cdot (c_\alpha) = \sum_\beta \langle\psi_{n\alpha}^{(0)}|\hat{V}\sum_{k=0}^{\infty}\lambda^{k+1}(\hat{G}_n\hat{V})^k|\psi_{n\beta}^{(0)}\rangle \cdot (c_\beta) \qquad [2'].$

- 1st-order perturbation: $|\psi_n\rangle = \sum_\alpha c_\alpha|\psi_{n\alpha}^{(0)}\rangle + O(\lambda)$, the secular equation is $(E_n - E_n^{(0)}) \cdot c_\alpha = \sum_\beta \lambda V_{n\alpha,n\beta} \cdot c_\beta + O(\lambda^2)$, diagonalize the $g \times g$ matrix $V_{n\alpha,n\beta} = \langle\psi_{n\alpha}^{(0)}|\hat{V}|\psi_{n\beta}^{(0)}\rangle$ to get the energy shift and c_α.

- 2nd-order perturbation: $|\psi_n\rangle = \sum_\alpha c_\alpha(|\psi_{n\alpha}^{(0)}\rangle + \sum_{m\neq n}\frac{\lambda V_{m,n\alpha}}{E_n^{(0)}-E_m^{(0)}}|\psi_m^{(0)}\rangle) + O(\lambda^2)$, the secular equation is $(E_n - E_n^{(0)})c_\alpha = \sum_\beta(\lambda V_{n\alpha,n\beta} + \sum_{m\neq n}\frac{\lambda^2 V_{n\alpha,m}V_{m,n\beta}}{E_n^{(0)}-E_m^{(0)}}) \cdot c_\beta + O(\lambda^3)$.

- If 1st order perturbation *completely* removes degeneracy, we can use *normalized* c_α ($\sum_\alpha |c_\alpha|^2 = 1$) from 1st order perturbation here to compute 2nd-order energy shift, $E_n - E_n^{(0)} = \lambda\sum_{\alpha,\beta} c_\alpha^* V_{n\alpha,n\beta}c_\beta + \lambda^2\sum_{m\neq n}\frac{c_\alpha^* V_{n\alpha,m}V_{m,n\beta}c_\beta}{E_n^{(0)}-E_m^{(0)}} + O(\lambda^3)$.

- Almost-degenerate perturbation: for $E_n^{(0)} \neq E_m^{(0)}$, if $|\lambda V_{n,m}| \gg |E_n^{(0)} - E_m^{(0)}|$, we need to use degenerate perturbation theory, and treat the original energy difference as perturbation. For example, for $\hat{H} = \begin{pmatrix} E_0 & \lambda V \\ \lambda V & E_1 \end{pmatrix}$, when $|\lambda V| \gg |E_1 - E_0|$, we should define $\hat{H}_0 = E_0\mathbb{1}_{2\times 2}$, and $\begin{pmatrix} 0 & \lambda V \\ \lambda V & E_1 - E_0 \end{pmatrix}$ as perturbation.

F. Example: Heisenberg Exchange from Hubbard Model

- For two sites $i = 1, 2$, on each site we have spin-1/2 electron modes $\hat{c}_{is}$, $s =\uparrow,\downarrow$. The unperturbed Hamiltonian is onsite Coulomb repulsion (Hubbard interaction), $\hat{H}_0 = U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow})$. Consider electron number $\sum_{i,s}\hat{n}_{is} = \sum_{i,s}\hat{c}_{is}^\dagger\hat{c}_{is} = 2$ subspace.

- The spectrum of $\hat{H}_0$ is illustrated on the right.
  The ground states are 4-fold degenerate, $E_0^{(0)} = 0$,
  $|\psi_{0\alpha}^{(0)}\rangle = (\hat{c}_{1\uparrow}^\dagger \hat{c}_{2\uparrow}^\dagger|0\rangle,\, \hat{c}_{1\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger|0\rangle,\, \hat{c}_{1\downarrow}^\dagger \hat{c}_{2\uparrow}^\dagger|0\rangle,\, \hat{c}_{1\downarrow}^\dagger \hat{c}_{2\downarrow}^\dagger|0\rangle)$,
  The excited states are two-fold degenerate, $E_1^{(0)} = U$,
  $|\psi_{1\alpha}^{(0)}\rangle = (\hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger|0\rangle,\, \hat{c}_{2\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger|0\rangle)$.

- Consider electron hoppings, $\hat{V} = -t\sum_{s=\uparrow,\downarrow}(\hat{c}_{1s}^\dagger \hat{c}_{2s} + \hat{c}_{2s}^\dagger \hat{c}_{1s})$. 1st-order perturbation vanishes. We have to solve the 2nd-order secular equation. For the ground states subspace, $(E_0 - E_0^{(0)})c_\alpha = \sum_\beta \sum_\gamma \frac{\langle\psi_{0\alpha}^{(0)}|\hat{V}|\psi_{1\gamma}^{(0)}\rangle\langle\psi_{1\gamma}^{(0)}|\hat{V}|\psi_{0\beta}^{(0)}\rangle}{E_0^{(0)} - E_1^{(0)}} \cdot c_\beta$. The 4×4 matrix is $-\frac{2t^2}{U}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$. The lowest energy state is spin singlet $\frac{1}{\sqrt{2}}(\hat{c}_{1\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger - \hat{c}_{1\downarrow}^\dagger \hat{c}_{2\uparrow}^\dagger)|0\rangle$, with energy $-\frac{4t^2}{U}$, the remaining three spin triplet states have zero energy.

- This energy difference between spin singlet and triplets is effectively captured by Heisenberg exchange, $\frac{4t^2}{U}(\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 - \frac{1}{4})$, where $\hat{\boldsymbol{S}}_i = \frac{1}{2}\sum_{s,s'} \hat{c}_{is}^\dagger (\boldsymbol{\sigma})_{ss'} \hat{c}_{is'}$.

- Degenerate perturbation may be avoided by symmetry analysis. Define unitary operator $\hat{I}$: $\hat{c}_{1s} \leftrightarrow \hat{c}_{2s}$, which swaps the two sites. Then $\hat{I}\hat{H}\hat{I}^\dagger = \hat{H}$, and $\hat{I}^2 = \mathbb{1}$. $\hat{I}$ generates a Z_2 group $\{\mathbb{1}, \hat{I}\}$ with two irreps $(\Gamma_{1,2})$, $R_{\Gamma_1}(I) = 1$ and $R_{\Gamma_2}(I) = -1$. Define $\hat{S}_z \equiv \frac{1}{2}\sum_i(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$, then $\hat{S}_z$ commutes with $\hat{H}$ and $\hat{I}$. Then we can divide the Hilbert space by $\hat{S}_z$ eigenvalues and irreps of the Z_2 group, and solve the perturbation theory in each subspace.

$\hat{S}_z$	$\hat{I}$	states	$\hat{H}_0$	$\hat{V}$
1	-1	$\hat{c}_{1\uparrow}^\dagger \hat{c}_{2\uparrow}^\dagger\|0\rangle$	(0)	(0)
-1	-1	$\hat{c}_{1\downarrow}^\dagger \hat{c}_{2\downarrow}^\dagger\|0\rangle$	(0)	(0)
0	1	$\frac{1}{\sqrt{2}}(\hat{c}_{1\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger - \hat{c}_{1\downarrow}^\dagger \hat{c}_{2\uparrow}^\dagger)\|0\rangle$ $\frac{1}{\sqrt{2}}(\hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger + \hat{c}_{2\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger)\|0\rangle$	$\begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix}$	$\begin{pmatrix} 0 & -2t \\ -2t & 0 \end{pmatrix}$
0	-1	$\frac{1}{\sqrt{2}}(\hat{c}_{1\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger + \hat{c}_{1\downarrow}^\dagger \hat{c}_{2\uparrow}^\dagger)\|0\rangle$ $\frac{1}{\sqrt{2}}(\hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger - \hat{c}_{2\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger)\|0\rangle$	$\begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix}$	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

II. PERTURBATIVE EXPANSION AS UNITARY TRANSFORMATIONS

A. Prelude: A Harder Way to Solve a 2×2 Problem

- Given $\hat{H} = \hat{H}_0 + \lambda\hat{V} = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix} + \lambda \begin{pmatrix} 0 & V \\ V & 0 \end{pmatrix} = \frac{E_0+E_1}{2}\sigma_0 + \frac{E_0-E_1}{2}\sigma_z + \lambda V \sigma_x$, in orthonormal basis $(|\psi_0^{(0)}\rangle, |\psi_1^{(0)}\rangle)$. Try to "decouple" the two levels by unitary transformations.

- Consider $(|\psi_0^{(1)}\rangle, |\psi_1^{(1)}\rangle) = e^{\mathbb{i}\lambda\hat{S}_0}(|\psi_0^{(0)}\rangle, |\psi_1^{(0)}\rangle)$, Hamiltonian in this basis is $\hat{H}^{(1)} = e^{\mathbb{i}\lambda\hat{S}_0}\hat{H}e^{-\mathbb{i}\lambda\hat{S}_0} = \hat{H}_0 + \lambda([\mathbb{i}\hat{S}_0, \hat{H}_0] + \hat{V}) + \lambda^2(\frac{1}{2}[\mathbb{i}\hat{S}_0, [\mathbb{i}\hat{S}_0, \hat{H}_0]] + [\mathbb{i}\hat{S}_0, \hat{V}]) + \cdots$, demand that $\hat{H}^{(1)}$ has no off-diagonal term of order $O(\lambda)$. Then we need $[\mathbb{i}\hat{S}_0, \hat{H}_0] + \hat{V} = 0$, which is $\hat{S}_0 = \frac{V}{E_0-E_1}\sigma_y$.

- $\hat{H}^{(1)} = \hat{H}_0 + \frac{\lambda^2 V^2}{E_0-E_1}\sigma_z - \frac{4}{3}\frac{\lambda^3 V^3}{(E_0-E_1)^2}\sigma_x - \frac{\lambda^4 V^4}{(E_0-E_1)^3}\sigma_z + O(\lambda^5)$, eigenvalues up to $O(\lambda^2)$ are $E_0 + \frac{\lambda^2 V^2}{E_0-E_1}$ and $E_1 - \frac{\lambda^2 V^2}{E_0-E_1}$.

- This procedure can be continued: define $\hat{H}^{(2)} = e^{\mathbb{i}\lambda^3\hat{S}_1}\hat{H}^{(1)}e^{-\mathbb{i}\lambda^3\hat{S}_1}$, and choose $\hat{S}_1$ to cancel the off-diagonal terms in $\hat{H}^{(1)}$ of order λ^3, $\hat{H}^{(2)}$ is then diagonal up to $O(\lambda^4)$, the diagonal entries give approximate eigenvalues up to $O(\lambda^4)$, and the new basis $(|\psi_0^{(2)}\rangle, |\psi_1^{(2)}\rangle) = e^{\mathbb{i}\lambda^3\hat{S}_1}e^{\mathbb{i}\lambda\hat{S}_0}(|\psi_0^{(0)}\rangle, |\psi_1^{(0)}\rangle)$ are the approximate eigenstates up to $O(\lambda^3)$.

- Note: Because $\hat{H}^{(1)}$ contains off-diagonal terms of only order λ^3 and higher, the difference between $\hat{H}^{(2)}$ diagonal terms and $\hat{H}^{(1)}$ diagonal terms will be at least of order λ^6, coming from $[\mathbb{i}\lambda^3\hat{S}_1, (\text{order } \lambda^3 \text{ off-diagonal terms of } \hat{H}^{(1)})]$ and $\frac{1}{2}[\mathbb{i}\lambda^3\hat{S}_1, [\mathbb{i}\lambda^3\hat{S}_1, \hat{H}_0]]$. Therefore the diagonal term of $\hat{H}^{(1)}$ is already accurate up to order λ^4.

B. The General Idea

- Given $\hat{H} = \hat{H}_0 + \lambda\hat{V}$, $\hat{H}_0$ has known energy levels E_n (may be degenerate). Try to use a sequence of unitary transformations to remove "off-diagonal terms".

- Here "off-diagonal terms" means terms connecting eigenstates of $\hat{H}_0$ with *different* energy. Therefore the procedure only block-diagonalizes the Hamiltonian. Terms (diagonal and off-diagonal) connecting eigenstates of $\hat{H}_0$ with the same energy, namely the matrix in the secular equation of degenerate perturbation theory, will be produced.

- Define the projection operators $\hat{P}_n$ projecting onto E_n eigenstate space. Then $\mathbb{1} = \sum_n \hat{P}_n$. Define $\hat{V}_{nm} = \hat{P}_n \hat{V} \hat{P}_m$ (related to matrix element V_{nm} by $\hat{V}_{nm} = V_{nm}|\psi_n^{(0)}\rangle\langle\psi_m^{(0)}|$), then $\hat{V} = \sum_{n,m} \hat{V}_{nm}$. Note that $[\hat{H}_0, \hat{V}_{nm}] = (E_n - E_m)\hat{V}_{nm}$.

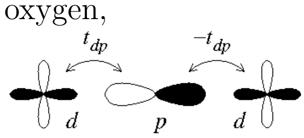
- Consider $\hat{H}^{(1)} = e^{\mathbb{i}\lambda\hat{S}_0}\hat{H}e^{-\mathbb{i}\lambda\hat{S}_0}$, we want to cancel $\hat{V}_{nm}$ terms with $n \neq m$ in $\hat{H}^{(1)}$, then we need $[\mathbb{i}\hat{S}_0, \hat{H}_0] + \sum_{n\neq m} \hat{V}_{nm} = 0$. The solution is $\mathbb{i}\hat{S}_0 = \sum_{n\neq m} \frac{\hat{V}_{nm}}{E_n - E_m}$.

- $\hat{H}^{(1)} = \hat{H}_0 + \lambda\sum_n \hat{V}_{nn} + \frac{\lambda^2}{2}[\mathbb{i}\hat{S}_0, \sum_{m\neq n} \hat{V}_{mn}] + \lambda^2[\mathbb{i}\hat{S}_0, \sum_n \hat{V}_{nn}] + O(\lambda^3) = \hat{H}_0 + \lambda\sum_n \hat{V}_{nn} + \frac{\lambda^2}{2}\sum_{n'\neq m, m\neq n}(\frac{\hat{V}_{n'm}\hat{V}_{mn}}{E_{n'} - E_m} - \frac{\hat{V}_{n'm}\hat{V}_{mn}}{E_m - E_n}) + \lambda^2\sum_{m\neq n}\frac{\hat{V}_{mn}\hat{V}_{nn} - \hat{V}_{mm}\hat{V}_{mn}}{E_m - E_n} + O(\lambda^3)$. The diagonal terms are $\hat{H}_0 + \lambda\sum_n \hat{V}_{nn} + \lambda^2\sum_{m\neq n}\frac{\hat{V}_{nm}\hat{V}_{mn}}{E_n - E_m} + O(\lambda^3)$, same as series expansion result.

- This abstract procedure can be carried out to arbitrary order of λ (by computers). For next order, $\hat{H}^{(2)} = e^{\mathbb{i}\lambda^2\hat{S}_2}\hat{H}^{(1)}e^{-\mathbb{i}\lambda^2\hat{S}_2}$, we demand that $[\mathbb{i}\lambda^2\hat{S}_2, \hat{H}_0]$ cancels the order λ^2 off-diagonal terms of $\hat{H}^{(1)}$. Note that $[\hat{H}_0, \hat{V}_{n'm}\hat{V}_{mn}] = (E_{n'} - E_n)\hat{V}_{n'm}\hat{V}_{mn}$. Then $\mathbb{i}\hat{S}_2 = \sum_{n'\neq m, m\neq n, n'\neq n}\frac{1}{2(E_{n'} - E_n)}(\frac{\hat{V}_{n'm}\hat{V}_{mn}}{E_{n'} - E_m} - \frac{\hat{V}_{n'm}\hat{V}_{mn}}{E_m - E_n}) + \sum_{m\neq n}\frac{1}{E_m - E_n}\frac{\hat{V}_{mn}\hat{V}_{nn} - \hat{V}_{mm}\hat{V}_{mn}}{E_m - E_n}$. But the generated corrections to diagonal terms will be $O(\lambda^4)$. So diagonal terms in $\hat{H}^{(1)}$ is already accurate up to $O(\lambda^3)$.

C. Example: d-d Hoppings Mediated by d-p Hybridization

- Consider two transition metal(TM) ions connected by an oxygen, the d-electrons can hop between the two TM ions through oxygen p-orbitals. Ignore spin here.



$\hat{H}_0 = \epsilon_d(\hat{d}_1^\dagger\hat{d}_1 + \hat{d}_2^\dagger\hat{d}_2) + \epsilon_p\,\hat{c}^\dagger\hat{c}$. Here $\hat{d}_{1,2}$ are d-electrons, $\hat{c}$ is p-electron.

- The perturbation is d-p hybridization, $\hat{V} = t_{dp}(\hat{d}_1^\dagger\hat{c} - \hat{d}_2^\dagger\hat{c} + h.c.)$. NOTE the signs. Define $\hat{V}_+ = t_{dp}(\hat{d}_1^\dagger\hat{c} - \hat{d}_2^\dagger\hat{c})$ and $\hat{V}_- = (\hat{V}_+)^\dagger$. Then $[\hat{H}_0, \hat{V}_\pm] = \pm(\epsilon_d - \epsilon_p)\hat{V}_\pm$, $\hat{V} = \hat{V}_+ + \hat{V}_-$. Note $\hat{V}$ has no diagonal component (always change eigenvalues of $\hat{H}_0$).

- $\hat{H}^{(1)} = e^{\mathbb{i}\hat{S}_0}\hat{H}e^{-\mathbb{i}\hat{S}_0}$, and demand $[\mathbb{i}\hat{S}_0, \hat{H}_0] + \hat{V} = 0$. Then $\mathbb{i}\hat{S}_0 = \frac{1}{\epsilon_d - \epsilon_p}(\hat{V}_+ - \hat{V}_-)$. $\hat{H}^{(1)} \approx \hat{H}_0 + \frac{1}{2}[\mathbb{i}\hat{S}_0, \hat{V}] = \hat{H}_0 + \frac{1}{2(\epsilon_d - \epsilon_p)}[\hat{V}_+ - \hat{V}_-, \hat{V}_+ + \hat{V}_-] = \hat{H}_0 + \frac{1}{\epsilon_d - \epsilon_p}[\hat{V}_+, \hat{V}_-]$.

- $[\hat{V}_+, \hat{V}_-] = t_{dp}^2\sum_{i,j=1}^2(-1)^{i+j}[\hat{d}_i^\dagger\hat{c}, \hat{c}^\dagger\hat{d}_j] = t_{dp}^2\sum_{i,j=1}^2(-1)^{i+j}(\hat{d}_i^\dagger\hat{d}_j - \delta_{ij}c^\dagger c)$ $= t_{dp}^2(\sum_i \hat{d}_i^\dagger\hat{d}_i - 2\hat{c}^\dagger\hat{c}) - t_{dp}^2(\hat{d}_1^\dagger\hat{d}_2 + h.c.)$.

- The 2nd-order perturbation generates effective d-d hopping $-\frac{t_{dp}^2}{\epsilon_d - \epsilon_p}(\hat{d}_1^\dagger\hat{d}_2 + h.c.)$.

D. Example: Spin Interactions from Hubbard Model (Not Required)

- Reference: A.H. MacDonald, *et al.*, *Phys. Rev. B* **37**, 9753 (1988).

- Consider the Hubbard model, $\hat{H}_0 = U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow})$, $\hat{V} = -t\sum_{s=\uparrow,\downarrow}(\hat{c}^\dagger_{1s}\hat{c}_{2s} + h.c.)$. Define $\hat{V}_{+1} = -t\sum_{s=\uparrow,\downarrow}(\hat{n}_{1,-s}\hat{c}^\dagger_{1s}\hat{c}_{2s}(1-\hat{n}_{2,-s}) + h.c.)$,
  $\hat{V}_{-1} = -t\sum_{s=\uparrow,\downarrow}((1-\hat{n}_{1,-s})\hat{c}^\dagger_{1s}\hat{c}_{2s}\hat{n}_{2,-s} + h.c.)$,
  $\hat{V}_0 = -t\sum_{s=\uparrow,\downarrow}((1-\hat{n}_{1,-s})\hat{c}^\dagger_{1s}\hat{c}_{2s}(1-\hat{n}_{2,-s}) + \hat{n}_{1,-s}\hat{c}^\dagger_{1s}\hat{c}_{2s}\hat{n}_{2,-s} + h.c.)$,
  then $[\hat{H}_0, \hat{V}_m] = mU\,\hat{V}_m$, and $\hat{V} = \sum_m \hat{V}_m$.
  Note that by definition $\hat{V}_m$ changes the number of "double-occupancy" by m.

- We want $[\mathbb{i}\hat{S}_0, \hat{H}_0] + \hat{V}_{+1} + \hat{V}_{-1} = 0$, then $\mathbb{i}\hat{S}_0 = \frac{1}{U}(\hat{V}_{+1} - \hat{V}_{-1})$. $\hat{H}^{(1)} = e^{\mathbb{i}\hat{S}_0}\hat{H}e^{-\mathbb{i}\hat{S}_0} \approx \hat{H}_0 + \hat{V}_0 + \frac{1}{2}[\mathbb{i}\hat{S}_0, \hat{V}_{+1} + \hat{V}_{-1}] + [\mathbb{i}\hat{S}_0, \hat{V}_0]$

- The diagonal terms (those commute with $\hat{H}_0$) are $\hat{H}_0 + \hat{V}_0 + \frac{1}{U}[\hat{V}_{+1}, \hat{V}_{-1}]$.

- Consider the action of these terms on the H_0 ground states (single-occupancy states, with $\hat{n}_1 = \hat{n}_{1\uparrow} + \hat{n}_{1\downarrow} = 1$ and $\hat{n}_2 = \hat{n}_{2\uparrow} + \hat{n}_{2\downarrow} = 1$), then only $-\frac{1}{U}\hat{V}_{-1}\hat{V}_{+1}$ is effective, because $\hat{V}_{-1}$ acting on single-occupancy states will vanish ($\hat{V}_{-1}$ will decrease the number of double-occupancy by 1). $\hat{V}_{+1}$ can move an electron from site i to site j, create a double-occupancy on site j, then $\hat{V}_{-1}$ must move an electron from site j back to site i, to remove this double-occupancy. The effect of this term is then $-\frac{t^2}{U}\sum_{s,s',i\neq j}(\hat{c}^\dagger_{is}\hat{c}_{js})(\hat{c}^\dagger_{js'}\hat{c}_{is'}) = \frac{t^2}{U}[\sum_{s,s',i\neq j}\hat{c}^\dagger_{is}\hat{c}^\dagger_{js'}\hat{c}_{js}\hat{c}_{is'} - \sum_{s,i\neq j}\hat{n}_{is}]$ $= \frac{t^2}{U}[\sum_{i\neq j}(2\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j + \frac{1}{2}) - 2] = \frac{4t^2}{U}(\hat{\boldsymbol{S}}_1\cdot\hat{\boldsymbol{S}}_2 - \frac{1}{4})$.

- Exercise: check the spin exchange $\sum_{s,s'}\hat{c}^\dagger_{is}\hat{c}^\dagger_{js'}\hat{c}_{js}\hat{c}_{is'} = 2\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j + \frac{1}{2}$, in the single-occupancy subspace. Here $\hat{\boldsymbol{S}}_i = \frac{1}{2}\sum_{s,s'}\hat{c}^\dagger_{is}(\boldsymbol{\sigma})_{ss'}\hat{c}_{is'}$.

III. TIME-DEPENDENT PERTURBATION THEORY

A. The interaction picture

- Given the Schrödinger picture time-dependent Hamiltonian $\hat{H}_S(t) = \hat{H}_0 + \hat{V}_S(t)$, where $\hat{H}_0$ is independent of time t, The time evolution is $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_S = [\hat{H}_0 + \hat{V}_S(t)]|\psi(t)\rangle_S$. The goal is to "eliminate" $\hat{H}_0$ from this equation.

- Define the "interaction picture" states $|\psi(t)\rangle_I = e^{\mathbb{i}\hat{H}_0 t/\hbar}|\psi(t)\rangle_S$.
  Define the "interaction picture" operators $\hat{O}_I(t) = e^{\mathbb{i}\hat{H}_0 t/\hbar}\hat{O}_S e^{-\mathbb{i}\hat{H}_0 t/\hbar}$.
  Note the similarity to the Heisenberg picture, and
  $\langle\psi(t)|_S\hat{O}_S|\phi(t)\rangle_S = \langle\psi(t)|_I\hat{O}_I(t)|\phi(t)\rangle_I$.

- Time evolution of states: $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_I = \hat{V}_I(t)|\psi(t)\rangle_I$.
  - "Proof": $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_I = (\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}e^{\mathbb{i}\hat{H}_0 t/\hbar})|\psi(t)\rangle_S + e^{\mathbb{i}\hat{H}_0 t/\hbar}\cdot\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_S$
    $= e^{\mathbb{i}\hat{H}_0 t/\hbar}(-\hat{H}_0)|\psi(t)\rangle_S + e^{\mathbb{i}\hat{H}_0 t/\hbar}[\hat{H}_0 + \hat{V}_S(t)]|\psi(t)\rangle_S = e^{\mathbb{i}\hat{H}_0 t/\hbar}\hat{V}_S(t)|\psi(t)\rangle_S$
    $= e^{\mathbb{i}\hat{H}_0 t/\hbar}\hat{V}_S(t)e^{-\mathbb{i}\hat{H}_0 t/\hbar}\cdot e^{\mathbb{i}\hat{H}_0 t/\hbar}|\psi(t)\rangle_S = \hat{V}_I(t)|\psi(t)\rangle_I$.

- Define the unitary time evolution operator in the interaction picture $\hat{U}_I(t)$, $|\psi(t)\rangle_I = \hat{U}_I(t)|\psi(t=0)\rangle_I = \hat{U}_I(t)|\psi(t=0)\rangle_S$. Then $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t} = \hat{V}_I(t)\hat{U}_I(t)$. The formal solution is the time-ordered exponential $\hat{U}_I(t) = \mathcal{T}\exp[-\frac{\mathbb{i}}{\hbar}\int_0^t \hat{V}_I(t')\,\mathrm{d}t']$, or ...

- Dyson series: $\hat{U}_I(t) = \mathbb{1} + \frac{-\mathbb{i}}{\hbar}\int_{t_1=0}^t \hat{V}_I(t_1)\,\mathrm{d}t_1 + (\frac{-\mathbb{i}}{\hbar})^2\int_{t_1=0}^t\int_{t_2=0}^{t_1}\hat{V}_I(t_1)\hat{V}_I(t_2)\,\mathrm{d}t_1\mathrm{d}t_2 + \ldots$

- Relation to Schrödinger picture time evolution operator: $\hat{U}_I(t) = e^{\mathbb{i}\hat{H}_0 t/\hbar}\hat{U}_S(t)$.

- Transition probability:
  Let $|i\rangle$ and $|f\rangle$ be normalized eigenstates of $\hat{H}_0$, $\hat{H}_0|i\rangle = E_i|i\rangle$, $\hat{H}_0|f\rangle = E_f|f\rangle$.
  Start at state $|i\rangle$ at $t=0$, evolve over time t, the probability of final state $|f\rangle$ is
  $P(i\to f,t) = |\langle f|U_S(t)|i\rangle|^2 = |\langle f|e^{-\frac{\mathbb{i}}{\hbar}\hat{H}_0 t}\hat{U}_I(t)|i\rangle|^2 = |\langle f|e^{-\frac{\mathbb{i}}{\hbar}E_f t}\hat{U}_I(t)|i\rangle|^2$
  $= |\langle f|\hat{U}_I(t)|i\rangle|^2$

B. Transition probability: constant perturbation

- $\hat{H}_S(t) = \begin{cases}\hat{H}_0, & t<0,\\ \hat{H}_0 + \hat{V}, & t>0.\end{cases}$
  $\hat{V}$ is hermitian and t-independent. This is a constant perturbation turned on at $t=0$.

- Keep up to 1st order term in the Dyson series of $\hat{U}_I(t)$.
  $\langle f|\hat{U}_I(t)|i\rangle = \langle f|i\rangle + \frac{-\mathbb{i}}{\hbar}\int_{t_1=0}^t e^{\mathbb{i}(E_f-E_i)t_1/\hbar}\langle f|\hat{V}|i\rangle\,\mathrm{d}t_1 + O(V^2)$
  $= \langle f|i\rangle + \frac{-\mathbb{i}}{\hbar}\frac{\hbar}{\mathbb{i}(E_f-E_i)}(e^{\mathbb{i}(E_f-E_i)t/\hbar} - 1)V_{fi} + O(V^2)$. Here $V_{fi} \equiv \langle f|\hat{V}|i\rangle$.
  The probability is (for $f\neq i$ case), $P(i\to f,t) = \frac{4\sin^2(\frac{E_f-E_i}{2\hbar}t)}{(E_f-E_i)^2}|V_{fi}|^2$

- Transition rate: $P(i \to f, t)/t = \frac{4\sin^2(\frac{\Delta E}{2\hbar}t)}{t\cdot(\Delta E)^2}|V_{fi}|^2$, where $\Delta E = E_f - E_i$.
  Take $t \to +\infty$ limit, use $\lim_{a\to+\infty} \frac{\sin^2(ax)}{ax^2} = \pi\delta(x)$, then we have

- Fermi's golden rule: transition rate is
  $\Gamma(i \to f) \equiv \lim_{t\to+\infty} \frac{P(i\to f,t)}{t} = \frac{2\pi}{\hbar}\delta(E_f - E_i)|V_{fi}|^2$.

- Exercise: keep up to 2nd order terms in Dyson series, redo the calculation.

- The meaning of the $\delta(E_f - E_i)$:
  The total transition rate to *leave* the initial state is, $\Gamma_i \equiv \sum_{f,\ f\neq i}\Gamma(i \to f)$. Then $P(i \to i, t) \sim (1 - \Gamma_i t) \sim e^{-\Gamma_i t}$. The *lifetime* of state i is $\frac{1}{\Gamma_i}$. Formally the energy of state i has imaginary part $-\mathbb{i}\frac{\hbar}{2\Gamma_i}$. Γ_i equals to $\int \mathrm{d}E_f\, \rho'(E_f)\Gamma(i \to f)$, where $\rho'(E_f)$ is the *density of state*, $\rho'(E) = \sum_{f',\ f'\neq i}\delta(E - E_{f'})$. Here f' may be a continuous label, then $\sum_{f'}$ is an integral. The Fermi golden rule means that the *decay rate* of the initial state is (to lowest order of perturbation), $\frac{2\pi}{\hbar}\rho'(E_i)\cdot$ (average of $|V_{fi}|^2$ for $E_f = E_i$).

C. Transition probability: harmonic perturbation

- $\hat{H}_S(t) = \begin{cases} \hat{H}_0, & t < 0, \\ \hat{H}_0 + \hat{V}e^{\mathbb{i}\omega t} + \hat{V}^\dagger e^{-\mathbb{i}\omega t}, & t > 0. \end{cases}$
  ω is a nonzero real constant. $\hat{V}$ may not be hermitian, but is t-independent.

- Keep up to 1st order term in the Dyson series of $\hat{U}_I(t)$.
  $\langle f|\hat{U}_I(t)|i\rangle = \langle f|i\rangle + \frac{-\mathbb{i}}{\hbar}\int_{t_1=0}^{t} e^{\mathbb{i}(E_f-E_i)t_1/\hbar}(e^{\mathbb{i}\omega t}V_{fi} + e^{-\mathbb{i}\omega t}V_{fi}^\dagger)\,\mathrm{d}t_1 + O(V^2)$
  $= \langle f|i\rangle - \left[\frac{V_{fi}}{(E_f-E_i+\hbar\omega)}(e^{\frac{\mathbb{i}}{\hbar}(E_f-E_i+\hbar\omega)t} - 1) + \frac{V_{fi}^\dagger}{(E_f-E_i-\hbar\omega)}(e^{\frac{\mathbb{i}}{\hbar}(E_f-E_i-\hbar\omega)t} - 1)\right] + O(V^2)$.
  The probability is (for $f \neq i$ case),
  $$P(i \to f, t) = \frac{4\sin^2(\frac{\Delta E+\hbar\omega}{2\hbar}t)}{(\Delta E+\hbar\omega)^2}|V_{fi}|^2 + \frac{4\sin^2(\frac{\Delta E-\hbar\omega}{2\hbar}t)}{(\Delta E-\hbar\omega)^2}|V_{fi}^\dagger|^2 + \frac{4\sin(\frac{\Delta E+\hbar\omega}{2\hbar}t)\sin(\frac{\Delta E-\hbar\omega}{2\hbar}t)}{(\Delta E)^2-\hbar^2\omega^2}(V_{fi}^* V_{fi}^\dagger e^{-\mathbb{i}\omega t} + (V_{fi}^\dagger)^* V_{fi}e^{\mathbb{i}\omega t}).$$
  Take $t \to +\infty$ limit, the transition rate is given by

- Fermi's golden rule: transition rate is
  $\Gamma(i \to f) \equiv \lim_{t\to+\infty}\frac{P(i\to f,t)}{t} = \frac{2\pi}{\hbar}[\delta(E_f - E_i + \hbar\omega)|V_{fi}|^2 + \delta(E_f - E_i - \hbar\omega)|V_{fi}^\dagger|^2]$.

- Exercise: keep up to 2nd order terms in Dyson series, redo the calculation.

- Detailed balance (see Sakurai, section 5.7): note that $\Gamma(i \to f)$ equals to $\Gamma(f \to i)$. Roughly speaking, absorption(of energy $\hbar\omega$) rate = emission rate.

D. Relation to time-independent theory

- $\hat{H} = \hat{H}_0 + \hat{V}$.
  Denote normalized eigenstates of $\hat{H}_0$ as $|\psi_n^{(0)}\rangle$, $\hat{H}_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle$, and normalized eigenstates of $\hat{H}$ as $|\psi_n\rangle$, $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$.
  For simplicity denote $\langle\psi_n^{(0)}|\hat{V}|\psi_m^{(0)}\rangle$ as V_{nm}.

- Consider $\langle\psi_n^{(0)}|\hat{U}_I(t)|\psi_n^{(0)}\rangle = \langle\psi_n^{(0)}|e^{\mathbb{i}\hat{H}_0 t/\hbar}\hat{U}_S(t)|\psi_n^{(0)}\rangle$
  $= e^{\mathbb{i}E_n^{(0)}t/\hbar}\langle\psi_n^{(0)}|(\sum_m |\psi_m\rangle\langle\psi_m|e^{-\mathbb{i}E_m t/\hbar})|\psi_n^{(0)}\rangle = \sum_m |\langle\psi_n^{(0)}|\psi_m\rangle|^2 e^{-\mathbb{i}E_m t/\hbar}e^{\mathbb{i}E_n^{(0)}t/\hbar}$.
  Consider non-degenerate case, $|\psi_n\rangle$ has large overlap with only $|\psi_n^{(0)}\rangle$,
  $\langle\psi_n^{(0)}|\hat{U}_I(t)|\psi_n^{(0)}\rangle = Z_n e^{-\mathbb{i}(E_n - E_n^{(0)})t/\hbar} + \sum_{m,\ m\neq n} |\langle\psi_n^{(0)}|\psi_m\rangle|^2 e^{-\mathbb{i}E_m t/\hbar}e^{\mathbb{i}E_n^{(0)}t/\hbar}$
  $\approx Z_n + Z_n\frac{-\mathbb{i}}{\hbar}(E_n - E_n^{(0)})t + Z_n\frac{1}{2}(\frac{-\mathbb{i}(E_n - E_n^{(0)})t}{\hbar})^2 + \sum_{m,\ m\neq n} |\langle\psi_n^{(0)}|\psi_m\rangle|^2 e^{-\mathbb{i}E_m t/\hbar}e^{\mathbb{i}E_n^{(0)}t/\hbar}$.
  Here $Z_n = |\langle\psi_n^{(0)}|\psi_n\rangle|^2$ is close to unity.

- Compute $\langle\psi_n^{(0)}|\hat{U}_I(t)|\psi_n^{(0)}\rangle$ by Dyson series. Up to 2nd order this is $\langle\psi_n^{(0)}|\hat{U}_I(t)|\psi_n^{(0)}\rangle$
  $= 1 + \frac{-\mathbb{i}}{\hbar}\int_{t_1=0}^{t} \mathrm{d}t_1 \langle\psi_n^{(0)}|\hat{V}_I(t_1)|\psi_n^{(0)}\rangle + (\frac{-\mathbb{i}}{\hbar})^2 \int_{t_1=0}^{t} \mathrm{d}t_1 \int_{t_2=0}^{t_1} \mathrm{d}t_2 \langle\psi_n^{(0)}|\hat{V}_I(t_1)\hat{V}_I(t_2)|\psi_n^{(0)}\rangle$
  $= 1 + \frac{-\mathbb{i}}{\hbar}V_{nn}t + (\frac{-\mathbb{i}}{\hbar})^2 \int_{t_1=0}^{t} \mathrm{d}t_1 \int_{t_2=0}^{t_1} \mathrm{d}t_2 \sum_m e^{\mathbb{i}E_n^{(0)}t_1/\hbar}V_{nm}e^{-\mathbb{i}E_m^{(0)}t_1/\hbar} \cdot e^{\mathbb{i}E_m^{(0)}t_2/\hbar}V_{mn}e^{-\mathbb{i}E_m^{(0)}t_2/\hbar}$
  $= 1 + \frac{-\mathbb{i}}{\hbar}V_{nn}t + \frac{1}{2}(\frac{-\mathbb{i}V_{nn}t}{\hbar})^2 + (\frac{-\mathbb{i}}{\hbar})^2 \sum_{m\neq n} V_{nm}V_{mn} \int_{t_1=0}^{t} \mathrm{d}t_1\, e^{\mathbb{i}(E_n^{(0)} - E_m^{(0)})t_1/\hbar}\frac{e^{\mathbb{i}(E_m^{(0)} - E_n^{(0)})t_1/\hbar} - 1}{\mathbb{i}(E_m^{(0)} - E_n^{(0)})/\hbar}$
  $= 1 + \frac{-\mathbb{i}}{\hbar}(V_{nn} + \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n^{(0)} - E_m^{(0)}}) \cdot t + \frac{1}{2}(\frac{-\mathbb{i}V_{nn}t}{\hbar})^2$
  $\quad - (\frac{-\mathbb{i}}{\hbar})^2 \sum_{m\neq n} V_{nm}V_{mn}\frac{e^{\mathbb{i}(E_n^{(0)} - E_m^{(0)})t/\hbar} - 1}{\mathbb{i}(E_m^{(0)} - E_n^{(0)})/\hbar \cdot \mathbb{i}(E_n^{(0)} - E_m^{(0)})/\hbar}$
  $= [1 - \sum_{m\neq n}\frac{V_{nm}V_{mn}}{(E_n^{(0)} - E_m^{(0)})^2}] + \frac{-\mathbb{i}}{\hbar}(V_{nn} + \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n^{(0)} - E_m^{(0)}}) \cdot t + \frac{1}{2}(\frac{-\mathbb{i}V_{nn}t}{\hbar})^2$
  $\quad - (\frac{-\mathbb{i}}{\hbar})^2 \sum_{m\neq n} V_{nm}V_{mn}\frac{e^{\mathbb{i}(E_n^{(0)} - E_m^{(0)})t/\hbar}}{\mathbb{i}(E_m^{(0)} - E_n^{(0)})/\hbar \cdot \mathbb{i}(E_n^{(0)} - E_m^{(0)})/\hbar}$.
  Compare with previous results, we see that up to 2nd order,

- $E_n - E_n^{(0)} = V_{nn} + \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n^{(0)} - E_m^{(0)}}$,
  $Z_n = 1 - \sum_{m\neq n}\frac{V_{nm}V_{mn}}{(E_n^{(0)} - E_m^{(0)})^2}$.
  Consistent with time-independent perturbation theory.

Summary of Lecture #7: scattering theory

The Goals and The Requirements

- Understand the basic tools in scattering theory:
  perturbation theory applied to continuous spectrum of
  the Hamiltonian of (free particle $\hat{H}_0$ + scattering potential $\hat{V}$)
  - For sufficiently short-ranged potential, scattering state energy is the same as plane wave state energy for $\hat{H}_0$.
  - Lippmann-Schwinger equation: $|\psi\rangle = |\boldsymbol{k}\rangle + \frac{1}{E_0 - \hat{H}_0 + \mathbb{i}\epsilon}\hat{V}|\psi\rangle$.
    Note the $+\mathbb{i}\epsilon$ produces correct $t \to \pm\infty$ limit.
  - Born approximation: $|\psi\rangle \approx |\boldsymbol{k}\rangle + \frac{1}{E_0 - \hat{H}_0 + \mathbb{i}\epsilon}\hat{V}|\boldsymbol{k}\rangle$.
  - Scattering matrix (S-matrix): unitary time evolution operator in interaction picture.
- Note: we will assume that the space is three dimensional.
- Understand some basic concepts in scattering theory
  - Scattering cross section, σ: total scattered particle current under unit incoming particle current density.
  - Differential scattering cross section, $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$: scattered particle current $\mathrm{d}\sigma$ into the solid angle element $\mathrm{d}\Omega$, divided by $\mathrm{d}\Omega$, under unit incoming current density.
  - Optical theorem: $\sigma = \frac{4\pi}{k}\mathrm{Im}[f(\boldsymbol{k}, \boldsymbol{k})]$.
    Total cross section is related to the forward scattering amplitude.
- We will not be dealing with inelastic scattering in class.
- Optional references:
  J.J. Sakurai, *Modern Quantum Mechanics*, Chapter 7.
  Landau & Lifschitz, *Quantum Mechanics: Non-relativistic Theory*, Chapter XVII.

I. SETUP OF SCATTERING PROBLEM

- Rough picture (time-dependent):
  particle beam (plane wave packet) $|\psi(t=0)\rangle$ coming in, interacting with $\hat{V}$;
  scattered particles (scattered wave) $|\psi(t \to +\infty)\rangle$ going out.

- Rough picture (time-independent):
  a (short-ranged) scattering potential $\hat{V}$ as a perturbation to free particle Hamiltonian $\hat{H}_0$. The unperturbed state is momentum eigenstate $|\boldsymbol{k}\rangle$ ($\boldsymbol{k}$ is wavevector, $\hbar\boldsymbol{k}$ is momentum). The perturbed state contains scattered waves.

  - difficulties in treating scattering theory as perturbation theory: infinite degeneracy, because there are infinitely many $|\boldsymbol{k}'\rangle$ with the same energy ($|\boldsymbol{k}'| = |\boldsymbol{k}|$) under $\hat{H}_0$ as $|\boldsymbol{k}\rangle$.

- We will consider non-relativistic particles only. $\hat{H}_0 = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2$.

- Particle number (probability) current is $\mathrm{Re}[\psi^*(\boldsymbol{r})(-\mathrm{i}\frac{\hbar}{m}\boldsymbol{\nabla})\psi(\boldsymbol{r})]$.

A. Scattering cross section

- Differential cross section: $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$.
  $\mathrm{d}\sigma$ is the particle current being scattered into the solid angle element $\mathrm{d}\Omega$, under unit incoming particle current density.

- Cross section: $\sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\,\mathrm{d}\Omega$.
  Total scattered particle current, under unit incoming particle current density.

- Incoming plane wave $|\boldsymbol{k}\rangle$ is not normalizable. Probability is not easily defined. To overcome this, one can use free wave packet instead of plane wave. See *e.g.* Sakurai, Chapter 7.

II. LIPPMANN-SCHWINGER EQUATION

- Take the time-independent approach, $(\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle$.

- Assume that $\hat{V}$ is sufficiently short-ranged, namely for position $\boldsymbol{r}$ at a large distance from the scatterer, $\hat{V}(\boldsymbol{r}) \approx 0$. And $|\psi\rangle$ has the plane wave component $|\boldsymbol{k}\rangle$. Consider the Schrödinger equation around $\boldsymbol{r}$ (where we can ignore $\hat{V}$), we conclude that $E = E_0 = \frac{\hbar^2 \boldsymbol{k}^2}{2m}$.

- Formally (see also series expansion approach to time-independent perturbation), $|\psi\rangle = |\psi_0\rangle + \frac{1}{E-\hat{H}_0}\hat{V}|\psi\rangle$, where $|\psi_0\rangle$ is $\hat{H}_0$ eigenstate, usually taken as $|\boldsymbol{k}\rangle$. We however need to avoid the singularity of $\frac{1}{E-\hat{H}_0}$.

- Lippmann-Schwinger equation: $|\psi\rangle = |\boldsymbol{k}\rangle + \frac{1}{E-\hat{H}_0+\mathrm{i}\epsilon}\hat{V}|\psi\rangle$, where $\epsilon \to 0+$.

- Understanding $+\mathrm{i}\epsilon$ (not rigorous):
  Lippmann-Schwinger equation can be rewritten as $(\hat{H}_0 + \hat{V})|\psi\rangle = (E + \mathrm{i}\epsilon)|\psi\rangle - \mathrm{i}\epsilon|\boldsymbol{k}\rangle$.
  Consider Schrödinger equation $\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = (\hat{H}_0 + \hat{V})|\psi\rangle$, we have $\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}(e^{\mathrm{i}Et/\hbar-\epsilon t/\hbar}|\psi\rangle) = -e^{\mathrm{i}Et/\hbar-\epsilon t/\hbar}\cdot \mathrm{i}\epsilon|\boldsymbol{k}\rangle$, solution is $e^{\mathrm{i}Et/\hbar-\epsilon t/\hbar}|\psi\rangle = |\psi(t=0)\rangle - \frac{e^{\mathrm{i}Et/\hbar-\epsilon t/\hbar}-1}{\mathrm{i}E-\epsilon}\cdot \mathrm{i}\epsilon|\boldsymbol{k}\rangle$, or $|\psi\rangle = e^{-\mathrm{i}Et/\hbar+\epsilon t/\hbar}(|\psi(t=0)\rangle + \frac{\epsilon}{E+\mathrm{i}\epsilon}|\boldsymbol{k}\rangle) - \frac{\epsilon}{E+\mathrm{i}\epsilon}|\boldsymbol{k}\rangle$.
  Then $|\psi\rangle$ becomes the plane wave when $t \to -\infty$, mimic the scattering process.

- Insert resolution of identity into Lippmann-Schwinger equation
  $\langle\boldsymbol{r}|\psi\rangle = \langle\boldsymbol{r}|\boldsymbol{k}\rangle + \int \mathrm{d}^3\boldsymbol{r}' \int \mathrm{d}^3\boldsymbol{p}\, \langle\boldsymbol{r}|\frac{1}{\frac{\hbar^2\boldsymbol{k}^2}{2m} - \frac{\hbar^2\boldsymbol{p}^2}{2m} + \mathrm{i}\epsilon}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\hat{V}|\psi\rangle$.
  Note that $\langle\boldsymbol{r}|\psi\rangle = \psi(\boldsymbol{r})$, $\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \frac{1}{(2\pi)^{3/2}}e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}$, $\langle\boldsymbol{r}'|\hat{V} = V(\boldsymbol{r}')\langle\boldsymbol{r}'|$ (assume $\hat{V}$ depends on position only), then $\psi(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + \int \mathrm{d}^3\boldsymbol{r}' \int \mathrm{d}^3\boldsymbol{p}\, \frac{e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{\boldsymbol{k}^2-\boldsymbol{p}^2+\mathrm{i}\epsilon}\cdot\frac{2m}{(2\pi)^3\hbar^2}\cdot V(\boldsymbol{r}')\psi(\boldsymbol{r}')$. The integration over $\boldsymbol{p}$ can be done. Use polar coordinates and define the $+z$ direction along $\boldsymbol{r}-\boldsymbol{r}'$. We have $\int \mathrm{d}^3\boldsymbol{p}\,\frac{e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{\boldsymbol{k}^2-\boldsymbol{p}^2+\mathrm{i}\epsilon} = \int_0^\infty p^2\mathrm{d}p \int_0^\pi \sin\theta\,\mathrm{d}\theta \int_0^{2\pi}\mathrm{d}\phi\,\frac{e^{\mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|\cos\theta}}{k^2-p^2+\mathrm{i}\epsilon} = \int_0^\infty p^2\mathrm{d}p \int_{-1}^1 \mathrm{d}(\cos\theta)\,2\pi\frac{e^{\mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|\cos\theta}}{k^2-p^2+\mathrm{i}\epsilon} = \int_0^\infty p^2\mathrm{d}p\,\frac{2\pi}{\mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|}\frac{(e^{\mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|}-e^{-\mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|})}{k^2-p^2+\mathrm{i}\epsilon} = \int_{-\infty}^\infty p\mathrm{d}p\,\frac{2\pi}{\mathrm{i}|\boldsymbol{r}-\boldsymbol{r}'|}\frac{e^{\mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|}}{k^2-p^2+\mathrm{i}\epsilon} = 2\pi\mathrm{i}\,\mathrm{Res}_{z=+\sqrt{k^2+\mathrm{i}\epsilon}}(z\cdot\frac{2\pi}{\mathrm{i}|\boldsymbol{r}-\boldsymbol{r}'|}\cdot\frac{e^{\mathrm{i}z|\boldsymbol{r}-\boldsymbol{r}'|}}{k^2+\mathrm{i}\epsilon-z^2}) = -\frac{2\pi^2}{|\boldsymbol{r}-\boldsymbol{r}'|}e^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}$.
  Finally

- $\psi(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} - \frac{2m}{\hbar^2}\int \mathrm{d}^3\boldsymbol{r}'\,\frac{e^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\cdot V(\boldsymbol{r}')\psi(\boldsymbol{r}')$.

- Further approximation: $|\boldsymbol{r}| \gg |\boldsymbol{r}'|$, the position where we measure the scattered wave is very far(compared to the range of $\hat{V}$) from the scattering potential, $|\boldsymbol{r}-\boldsymbol{r}'| \approx |\boldsymbol{r}| - \frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{|\boldsymbol{r}|}$, $\psi(\boldsymbol{r}) \approx \frac{1}{(2\pi)^{3/2}}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} - \frac{2m}{\hbar^2}\frac{e^{\mathrm{i}kr}}{4\pi r}\int \mathrm{d}^3\boldsymbol{r}'\,e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi(\boldsymbol{r}')$, where $\boldsymbol{k}' = |\boldsymbol{k}|\frac{\boldsymbol{r}}{|\boldsymbol{r}|}$. This is usually written as

- $\psi(\boldsymbol{r}) \approx \frac{1}{(2\pi)^{3/2}}\left(e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f(\boldsymbol{k}', \boldsymbol{k})\frac{e^{\mathrm{i}kr}}{r}\right)$, where $\boldsymbol{k}' = |\boldsymbol{k}|\frac{\boldsymbol{r}}{|\boldsymbol{r}|}$. This looks like superposition of incoming plane wave and outgoing spherical wave (with angle dependent amplitude). $f(\boldsymbol{k}', \boldsymbol{k}) = -\frac{(2\pi)^{3/2}}{4\pi}\frac{2m}{\hbar^2}\int \mathrm{d}^3\boldsymbol{r}'\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi(\boldsymbol{r}')$, has the unit of length.

- The outgoing particle current in solid angle element $\mathrm{d}\Omega$ along $\boldsymbol{k}'$ direction at distance r is $\mathrm{Re}\{[\frac{1}{(2\pi)^{3/2}}f(\boldsymbol{k}', \boldsymbol{k})\frac{e^{\mathrm{i}kr}}{r}]^*(-\mathrm{i}\frac{\hbar}{m}\frac{\partial}{\partial r})[\frac{1}{(2\pi)^{3/2}}f(\boldsymbol{k}', \boldsymbol{k})\frac{e^{\mathrm{i}kr}}{r}]\} \cdot r^2\mathrm{d}\Omega = \frac{\hbar k}{m}\frac{1}{(2\pi)^3}|f(\boldsymbol{k}', \boldsymbol{k})|^2\,\mathrm{d}\Omega$. The incoming particle current density is $\mathrm{Re}[(\frac{1}{(2\pi)^{3/2}}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}})^*(-\mathrm{i}\frac{\hbar}{m}\boldsymbol{\nabla})(\frac{1}{(2\pi)^{3/2}}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}})] = \frac{\hbar\boldsymbol{k}}{m}\frac{1}{(2\pi)^3}$. The differential cross section is the ratio of the two,

- $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\boldsymbol{k}', \boldsymbol{k})|^2$

III. OPTICAL THEOREM

- Not very rigorous derivation (see *e.g.* Prof. Murayama's notes for rigorous one): Consider a sphere of radius r, the total outgoing particle current should be zero, $\int r^2\mathrm{d}\Omega\,\mathrm{Re}[\psi^*(\boldsymbol{r})(-\mathrm{i}\frac{\hbar}{m}\frac{\partial}{\partial r})\psi(\boldsymbol{r})] = 0$, where $\psi = \frac{1}{(2\pi)^{3/2}}\left(e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f(\boldsymbol{k}', \boldsymbol{k})\frac{e^{\mathrm{i}kr}}{r}\right)$.
  Use polar coordinates and define $+z$ direction along $\boldsymbol{k}$, $0 = r^2\int_0^\pi \sin\theta\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi$ $\frac{\hbar}{m}\frac{1}{(2\pi)^3}\{k\cos\theta + k\frac{|f(\theta,\phi)|^2}{r^2} + \mathrm{Re}[\frac{k\cos\theta}{r}f^*(\theta,\phi)e^{\mathrm{i}k(\cos\theta-1)r} + (\frac{k}{r}+\frac{-\mathrm{i}}{r^2})f(\theta,\phi)e^{-\mathrm{i}k(\cos\theta-1)r}]\}$, so $\sigma = \int_0^\pi \sin\theta\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi\,|f(\theta,\phi)|^2 = -r\cdot\int_0^\pi\sin\theta\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi\,\mathrm{Re}[\cos\theta\cdot f^*(\theta,\phi)e^{\mathrm{i}k(\cos\theta-1)r} + (1+\frac{-\mathrm{i}}{kr})f(\theta,\phi)e^{-\mathrm{i}k(\cos\theta-1)r}]$.
  Consider the case $kr \gg 1$ and average over r, the contribution to the integral comes mainly from $\theta \approx 0$ region, and ϕ dependence of f is small there. Define $x = 1 - \cos\theta$, $\sigma \approx -r\cdot\int_0^2\mathrm{d}x\,2\pi\,\mathrm{Re}[f^*(0,0)e^{-\mathrm{i}krx} + f(0,0)e^{\mathrm{i}krx}] = -r\cdot 2\pi\,\mathrm{Re}[f^*(0,0)\frac{e^{-2\mathrm{i}kr}-1}{-\mathrm{i}kr} + f(0,0)\frac{e^{2\mathrm{i}kr}-1}{\mathrm{i}kr}]$, ignore the fast oscillating factor $e^{\pm 2\mathrm{i}kr}$ (for averaging over r), we have

- Optical theorem: $\sigma = \frac{4\pi}{k}\mathrm{Im}[f(\boldsymbol{k}, \boldsymbol{k})]$.
  Total cross section is related to the forward scattering amplitude.

IV. BORN APPROXIMATION

- Like in 1st order approximation in the series expansion approach to time-independent perturbation theory, approximate the unknown $|\psi\rangle$ on the right-hand-side of Lippmann-Schwinger equation by the incoming plane wave, we have the

- Born approximation: $|\psi\rangle = |\boldsymbol{k}\rangle + \frac{1}{E-\hat{H}_0+\mathbb{i}\epsilon}\hat{V}|\boldsymbol{k}\rangle$

- $f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{(2\pi)^{3/2}}{4\pi}\frac{2m}{\hbar^2}\int \mathrm{d}^3\boldsymbol{r}'\, e^{-\mathbb{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\frac{e^{\mathbb{i}\boldsymbol{k}\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}} = -\frac{2m}{4\pi\hbar^2}\int \mathrm{d}^3\boldsymbol{r}'\, V(\boldsymbol{r}')\, e^{-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{r}'}$,
  where $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$ is the *momentum transfer*. So $f(\boldsymbol{k}',\boldsymbol{k})$ is proportional to the Fourier transform of $V(\boldsymbol{r})$ at momentum transfer wavevector.

- If the scattering potential $V(\boldsymbol{r})$ is central (depends on $r = |\boldsymbol{r}|$ only),
  $f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{2m}{4\pi\hbar^2}\int r^2\mathrm{d}r \int \sin\theta\mathrm{d}\theta \int \mathrm{d}\phi\, V(r)\, e^{-\mathbb{i}qr\cos\theta}$
  $= -\frac{2m}{4\pi\hbar^2}\int r^2\mathrm{d}r\, 2\pi\frac{e^{-\mathbb{i}qr}-e^{\mathbb{i}qr}}{-\mathbb{i}qr}V(r) = -\frac{2m}{\hbar^2}\int \mathrm{d}r\, \frac{r\sin(qr)}{q}V(r)$

- One can apply higher order approximation to the Lippmann-Schwinger equation, and obtain the *Born expansion*, $|\psi\rangle = |\boldsymbol{k}\rangle + \frac{1}{E-\hat{H}_0+\mathbb{i}\epsilon}\hat{V}|\boldsymbol{k}\rangle + \frac{1}{E-\hat{H}_0+\mathbb{i}\epsilon}\hat{V}\frac{1}{E-\hat{H}_0+\mathbb{i}\epsilon}\hat{V}|\boldsymbol{k}\rangle + \ldots$.

V. PARTIAL WAVE EXPANSION

- Consider the case of central potential $V(\boldsymbol{r}) = V(r)$, then $f(\boldsymbol{k}',\boldsymbol{k})$ is only function of the angle θ between $\boldsymbol{k}'$ and $\boldsymbol{k}$, define the $\boldsymbol{k}$ direction as $+z$ direction,
  $\psi(\boldsymbol{r}) \sim e^{\mathbb{i}kz} + f(\theta)\frac{e^{\mathbb{i}kr}}{r}$.

- Expand the plane wave into spherical waves,
  $e^{\mathbb{i}kz} = \sum_{l=0}^{\infty}(2l+1)\mathbb{i}^l j_l(kr)P_l(\cos\theta)$,
  where P_l is Legendre polynomial, j_l is spherical Bessel function.

- For large r, $e^{\mathbb{i}kz} \sim \frac{1}{2\mathbb{i}kr}\sum_{l=0}^{\infty}(2l+1)(e^{\mathbb{i}kr} - (-1)^l e^{-\mathbb{i}kr})P_l(\cos\theta)$,

- Expand $f(\theta)$ into Legendre polynomials, $f(\theta) = \sum_{l=0}^{\infty}(2l+1)f_l P_l(\cos\theta)$.

- $\sigma = \int \mathrm{d}\Omega\, |f|^2 = 4\pi\sum_l (2l+1)|f_l|^2$,
  where we have used $\int_0^\pi \sin\theta\mathrm{d}\theta\, P_{l'}(\cos\theta)P_l(\cos\theta) = \frac{2}{2l+1}\delta_{l'l}$.

- By optical theorem, $\sigma = \frac{4\pi}{k}\mathrm{Im}[f(0)] = \frac{4\pi}{k}\sum_l (2l+1)\mathrm{Im}(f_l)$,
  where we have used $P_l(1) = 1$.

- Comparing the two results, $|f_l|^2 = \frac{1}{k}\mathrm{Im}(f_l)$, or $|1 + 2\mathbb{i}kf_l|^2 = 1$.
  Define phase shift δ_l such that $1 + 2\mathbb{i}kf_l = e^{2\mathbb{i}\delta_l}$, then $f_l = \frac{1}{k}e^{\mathbb{i}\delta_l}\sin\delta_l$.

- $\psi(\boldsymbol{r}) \sim \frac{1}{2\mathbb{i}kr}\sum_l (2l+1)P_l(\cos\theta)[e^{2\mathbb{i}\delta_l}e^{\mathbb{i}kr} - (-1)^l e^{-\mathbb{i}kr}]$.
  $\sigma = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l$.

- Expand $\psi(\boldsymbol{r}) = \sum_l Y_l^0(\theta,\phi) R_l(r)$, where $Y_l^0(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$, then the radial wavefunction satisfies $\left[-\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2} r + \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} V(r)\right] R_l(r) = k^2 R_l(r)$, and $R_l(r) \sim \frac{1}{2\mathbb{i}kr}\frac{1}{\sqrt{4\pi(2l+1)}}[e^{2\mathbb{i}\delta_l} e^{\mathbb{i}kr} - (-1)^l e^{-\mathbb{i}kr}]$ as $r \to \infty$.

- To solve δ_l, solve the radial wavefunction $R_l(r)$ first, expand its asymptotic ($r \to \infty$) form by spherical Bessel functions $j_l(kr)$ and $n_l(kr)$, $R_l(r) \sim j_l(kr)\cos\delta_l + n_l(kr)\sin\delta_l$.

  - Reminder about spherical Bessel function: $j_l(\rho)$ and $n_l(\rho)$, solutions to $\left[-\frac{1}{\rho}\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}\rho + \frac{l(l+1)}{\rho^2}\right] R(\rho) = R(\rho)$. $j_l(\rho) = (-\rho)^l (\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho})^l (\frac{\sin\rho}{\rho})$, $n_l(\rho) = -(-\rho)^l(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho})^l(\frac{\cos\rho}{\rho})$.
  - Asymptotic behavior:
    $\rho \to 0$, $j_l(\rho) \sim \frac{\rho^l}{(2l+1)!!}$, $n_l(\rho) \sim -\frac{(2l-1)!!}{\rho^l}$.
    $\rho \to \infty$, $j_l(\rho) \sim \frac{\sin(\rho - l\pi/2)}{\rho}$, $n_l(\rho) \sim -\frac{\cos(\rho - l\pi/2)}{\rho}$.

VI. SCATTERING MATRIX (S-MATRIX)

- $\hat{S}$ is the unitary time evolution operator in interaction picture, under the limit that the initial time $t_i \to -\infty$ and the final time $t_f \to +\infty$, $\hat{S} \sim \lim_{t_i\to-\infty, t_f\to+\infty} \hat{U}_I(t_f, t_i)$.

- From Dyson series, $\hat{S} = \mathbb{1} + \frac{-\mathbb{i}}{\hbar}\int_{t_i}^{t_f} \mathrm{d}t_1\, \hat{V}_I(t_1) + (\frac{-\mathbb{i}}{\hbar})^2 \int_{t_i}^{t_f}\mathrm{d}t_1 \int_{t_i}^{t_1} \mathrm{d}t_2\, \hat{V}_I(t_1)\hat{V}_I(t_2) + \ldots$, with $\hat{V}_I(t) = e^{\mathbb{i}\hat{H}_0 t/\hbar}\hat{V} e^{-\mathbb{i}\hat{H}_0 t/\hbar}$.

- The limit $t_i \to -\infty$ and $t_f \to +\infty$ will formally cause non-convergent integrals. To avoid this, assume that the potential (in Schrödinger picture) $\hat{V}$ depends on time and decays to zero as $t \to \pm\infty$, $\hat{V}(t) = \hat{V} e^{-\epsilon|t|}$ with $\epsilon > 0$.

- The 1st order term in Dyson series is $\frac{-\mathbb{i}}{\hbar}\int_{-\infty}^{+\infty}\mathrm{d}t_1\, e^{\mathbb{i}\hat{H}_0 t_1/\hbar}\hat{V} e^{-\epsilon|t|} e^{-\mathbb{i}\hat{H}_0 t_1/\hbar}$
$= \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{-\mathbb{i}}{\hbar}\int_{-\infty}^{+\infty}\mathrm{d}t_1\, |\boldsymbol{k}\rangle e^{\mathbb{i}E_{\boldsymbol{k}} t_1/\hbar}\langle\boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle e^{-\epsilon|t_1|} e^{-\mathbb{i}E_{\boldsymbol{k}'} t_1/\hbar}\langle\boldsymbol{k}'|$
$= \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{-\mathbb{i}}{\hbar}|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|(\int_{-\infty}^0 \mathrm{d}t_1\, e^{\mathbb{i}(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})/\hbar\cdot t_1 + \epsilon t_1} + \int_0^{+\infty}\mathrm{d}t_1\, e^{\mathbb{i}(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})/\hbar\cdot t_1 - \epsilon t_1})$
$= \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{-\mathbb{i}}{\hbar}|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|(\frac{1}{\mathbb{i}(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})/\hbar+\epsilon} - \frac{1}{\mathbb{i}(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})/\hbar-\epsilon})$
$= \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{-\mathbb{i}}{\hbar}|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|\frac{2\epsilon}{(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})^2/\hbar^2+\epsilon^2}$
$\sim \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{-\mathbb{i}}{\hbar}|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|\cdot 2\pi\delta(\frac{E_{\boldsymbol{k}}-E_{\boldsymbol{k}'}}{\hbar}) = -\sum_{\boldsymbol{k},\boldsymbol{k}'}|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|\cdot 2\pi\mathbb{i}\delta(E_{\boldsymbol{k}} - E_{\boldsymbol{k}'})$,
note that formally $\lim_{\epsilon\to+0}\frac{2\epsilon}{x^2+\epsilon^2} = 2\pi\delta(x)$.

- The 2nd order term in Dyson series is $(\frac{-\mathbb{i}}{\hbar})^2\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\,\hat{V}_I(t_1)\hat{V}_I(t_2)$
$= (\frac{-\mathbb{i}}{\hbar})^2\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\,\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3}|\boldsymbol{k}_1\rangle e^{\mathbb{i}E_{\boldsymbol{k}_1}t_1/\hbar}\langle\boldsymbol{k}_1|\hat{V}|\boldsymbol{k}_2\rangle e^{-\epsilon|t_1|}e^{-\mathbb{i}E_{\boldsymbol{k}_2}t_1/\hbar}$
$\times\, e^{\mathbb{i}E_{\boldsymbol{k}_2}t_2/\hbar}\langle\boldsymbol{k}_2|\hat{V}|\boldsymbol{k}_3\rangle e^{-\epsilon|t_2|}e^{-\mathbb{i}E_{\boldsymbol{k}_3}t_2/\hbar}\langle\boldsymbol{k}_3|$
$= (\frac{-\mathbb{i}}{\hbar})^2\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3}|\boldsymbol{k}_1\rangle\langle\boldsymbol{k}_1|\hat{V}|\boldsymbol{k}_2\rangle\langle\boldsymbol{k}_2|\hat{V}|\boldsymbol{k}_3\rangle\langle\boldsymbol{k}_3|$
$\times\Big[\int_{-\infty}^{0}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2+\int_0^{\infty}\mathrm{d}t_1(\int_{-\infty}^{0}\mathrm{d}t_2+\int_0^{t_1}\mathrm{d}t_2)\Big]\,e^{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_2})t_1/\hbar-\epsilon|t_1|}e^{\mathbb{i}(E_{\boldsymbol{k}_2}-E_{\boldsymbol{k}_3})t_2/\hbar-\epsilon|t_2|}$
$= (\frac{-\mathbb{i}}{\hbar})^2\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3}|\boldsymbol{k}_1\rangle\langle\boldsymbol{k}_1|\hat{V}|\boldsymbol{k}_2\rangle\langle\boldsymbol{k}_2|\hat{V}|\boldsymbol{k}_3\rangle\langle\boldsymbol{k}_3|\times[\int_{-\infty}^{0}\mathrm{d}t_1\frac{e^{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_3})t_1/\hbar+\epsilon t_1}}{\mathbb{i}(E_{\boldsymbol{k}_2}-E_{\boldsymbol{k}_3})/\hbar+\epsilon}$
$+\int_0^{\infty}\mathrm{d}t_1(\frac{e^{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_2})t_1/\hbar-\epsilon t_1}}{\mathbb{i}(E_{\boldsymbol{k}_2}-E_{\boldsymbol{k}_3})/\hbar+\epsilon}+\frac{e^{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_3})t_1/\hbar-\epsilon t_1}-e^{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_2})t_1/\hbar-\epsilon t_1}}{\mathbb{i}(E_{\boldsymbol{k}_2}-E_{\boldsymbol{k}_3})/\hbar-\epsilon})]$
$= (\frac{-\mathbb{i}}{\hbar})^2\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3}|\boldsymbol{k}_1\rangle\langle\boldsymbol{k}_1|\hat{V}|\boldsymbol{k}_2\rangle\langle\boldsymbol{k}_2|\hat{V}|\boldsymbol{k}_3\rangle\langle\boldsymbol{k}_3|$
$\times\,[\frac{1}{\mathbb{i}(E_{\boldsymbol{k}_2}-E_{\boldsymbol{k}_3})/\hbar+\epsilon}(\frac{1}{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_3})/\hbar+\epsilon}-\frac{1}{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_2})/\hbar-\epsilon})$
$-\frac{1}{\mathbb{i}(E_{\boldsymbol{k}_2}-E_{\boldsymbol{k}_3})/\hbar-\epsilon}(\frac{1}{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_3})/\hbar-\epsilon}-\frac{1}{\mathbb{i}(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_2})/\hbar-\epsilon})].$
Consider $\lim_{\epsilon\to+0}\frac{1}{x+\mathbb{i}\epsilon}=-\mathbb{i}\pi\delta(x)+\mathcal{P}(\frac{1}{x})$ where $\mathcal{P}$ means Cauchy principal value, above result is $-\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3}|\boldsymbol{k}_1\rangle\langle\boldsymbol{k}_1|\hat{V}|\boldsymbol{k}_2\rangle\frac{1}{E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_2}+\mathbb{i}\epsilon}\langle\boldsymbol{k}_2|\hat{V}|\boldsymbol{k}_3\rangle\langle\boldsymbol{k}_3|\times 2\pi\mathbb{i}\delta(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_3})$
$=-\sum_{\boldsymbol{k}_1,\boldsymbol{k}_3}|\boldsymbol{k}_1\rangle\langle\boldsymbol{k}_1|\hat{V}\frac{1}{E_{\boldsymbol{k}_1}-\hat{H}_0+\mathbb{i}\epsilon}\hat{V}|\boldsymbol{k}_3\rangle\langle\boldsymbol{k}_3|\times 2\pi\mathbb{i}\delta(E_{\boldsymbol{k}_1}-E_{\boldsymbol{k}_3})$

- Finally $\langle\boldsymbol{k}|(\hat{S}-\mathbb{1})|\boldsymbol{k}'\rangle=-2\pi\mathbb{i}\delta(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})\langle\boldsymbol{k}|(\hat{V}+\hat{V}\frac{1}{E_{\boldsymbol{k}}-\hat{H}_0+\mathbb{i}\epsilon}\hat{V}+\dots)|\boldsymbol{k}'\rangle$.
Note the similarity to Born expansion.

- From $\sum_{\boldsymbol{k}'}\langle\boldsymbol{k}|\hat{S}^\dagger|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|\hat{S}|\boldsymbol{k}\rangle=\langle\boldsymbol{k}|\boldsymbol{k}\rangle$ (because $\hat{S}$ is unitary), we have $\sum_{\boldsymbol{k}'}[\langle\boldsymbol{k}|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|(\hat{S}-\mathbb{1})|\boldsymbol{k}\rangle+\langle\boldsymbol{k}|(\hat{S}^\dagger-\mathbb{1})|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|\boldsymbol{k}\rangle+|\langle\boldsymbol{k}'|(\hat{S}-\mathbb{1})|\boldsymbol{k}\rangle|^2]=0$, or $-\sum_{\boldsymbol{k}'}4\pi\delta(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})\mathrm{Im}[\langle\boldsymbol{k}|\boldsymbol{k}'\rangle T(\boldsymbol{k}',\boldsymbol{k})]=\sum_{\boldsymbol{k}'}[2\pi\delta(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})]^2|T(\boldsymbol{k}',\boldsymbol{k})|^2$, where $T(\boldsymbol{k}',\boldsymbol{k})=\langle\boldsymbol{k}'|(\hat{V}+\hat{V}\frac{1}{E_{\boldsymbol{k}'}-\hat{H}_0+\mathbb{i}\epsilon}\hat{V}+\dots)|\boldsymbol{k}\rangle$. This is formally the *optical theorem* $-\mathrm{Im}[T(\boldsymbol{k},\boldsymbol{k})]=\sum_{\boldsymbol{k}'}\pi\delta(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})|T(\boldsymbol{k}',\boldsymbol{k})|^2$.
In 3D space, $f(\boldsymbol{k}',\boldsymbol{k})=-\frac{2m}{\hbar^2}\cdot 2\pi^2\cdot T(\boldsymbol{k}',\boldsymbol{k})$, and $\sum_{\boldsymbol{k}'}\delta(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})\cdots=\int\mathrm{d}\Omega\,\frac{2m}{\hbar^2}\frac{k}{2}\dots$, this recovers the previous optical theorem.

- For central potential problem, the S-matrix is block-diagonal in the basis of angular momentum ℓ free spherical waves, the matrix element of $\hat{S}$ between inward spherical wave and outward spherical wave is $\exp(2\mathbb{i}\delta_\ell)$ where δ_ℓ is the phase shift.
See *e.g.* Prof. Murayama's lecture notes for more details.

VII. EXAMPLES

A. Coulomb potential scattering: Born approximation

- $V(\boldsymbol{r}) = V(r) = \frac{ZZ'e^2}{r}$, Z and Z' are charges (in unit of elementary charge e) of the point-like scatterer and the incoming particle respectively, Gauss unit is used (to change to SI unit, replace e^2 by $e^2/4\pi\epsilon_0$).

- Under Born approximation:
  $f(\boldsymbol{k}', \boldsymbol{k}) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty \mathrm{d}r\, rV(r)\sin(qr) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty \mathrm{d}r\,(ZZ'e^2)\sin(qr)$.
  This however does not seem to converge.

- Consider a short-ranged Yukawa potential $V(r) = (ZZ'e^2)\frac{\exp(-\mu r)}{r}$.
  Under Born approximation:
  $f(\boldsymbol{k}', \boldsymbol{k}) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty \mathrm{d}r\,(ZZ'e^2)\exp(-\mu r)\sin(qr) = -\frac{2m}{\hbar^2}(ZZ'e^2)\frac{1}{q^2+\mu^2}$.
  Note that $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$, so $q = 2k\sin(\theta/2)$ where θ is the scattering angle (between $\boldsymbol{k}'$ and $\boldsymbol{k}$),
  $f(\theta) = -\frac{2m}{\hbar^2}(ZZ'e^2)\frac{1}{4k^2\sin^2(\theta/2)+\mu^2}$.

- Differential cross section: $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\theta)|^2 = [\frac{2m}{\hbar^2}(ZZ'e^2)]^2(\frac{1}{4k^2\sin^2(\theta/2)+\mu^2})^2$.

- Total cross section: $\sigma = \int \sin\theta \mathrm{d}\theta \int \mathrm{d}\phi\, \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = 2\pi \int \mathrm{d}(\cos\theta)[\frac{2m}{\hbar^2}(ZZ'e^2)]^2(\frac{1}{2k^2(1-\cos\theta)+\mu^2})^2$
  $= [\frac{2m}{\hbar^2}(ZZ'e^2)]^2\frac{4\pi}{4k^2\mu^2+\mu^4}$

- Finally take the limit that $\mu \to 0$,
  $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = [\frac{2m}{\hbar^2}(ZZ'e^2)]^2\frac{1}{q^4} = [\frac{2m}{\hbar^2}(ZZ'e^2)]^2\frac{1}{16k^4\sin^4(\theta/2)}$;
  $\sigma \to \infty$.

- σ diverges because Coulomb potential is a long-ranged, no matter how off-target the incoming particle is from the scatterer, it will be affected.

- Form factor:
  if the scatterer's charge has a distribution $\rho(\boldsymbol{r}')$ $[Z = \int \mathrm{d}^3\boldsymbol{r}'\,\rho(\boldsymbol{r}')]$, $V(\boldsymbol{r}) = \int \mathrm{d}^3\boldsymbol{r}\,\frac{Z'e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\rho(\boldsymbol{r}')$. This is a convolution of Coulomb potential with $\rho(\boldsymbol{r}')$, under Born approximation, the scattering amplitude is the Fourier transform of V, so is the product of Fourier transforms of Coulomb potential and ρ,

$f(\theta) = -\frac{2m}{\hbar^2}\frac{Z'e^2}{q^2}\int \mathrm{d}^3\boldsymbol{r}'\,\rho(\boldsymbol{r}')\exp(-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{r}') = f_{\text{point scatterer}}(\theta)\cdot F(\boldsymbol{q})$,
where the form factor $F(\boldsymbol{q}) = \frac{1}{Z}\int \mathrm{d}^3\boldsymbol{r}'\,\rho(\boldsymbol{r}')\exp(-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{r}')$.
By measuring differential cross section and comparing with that of point scatterer, one can measure $|F(\boldsymbol{q})|^2$ and obtain information about the charge distribution ρ.

- Bragg scattering: *e.g.* X-ray or neutron diffraction on crystal,
  if the scatterer has a periodic density distribution, *e.g.* electrons in crystals, $\rho(\boldsymbol{r}') = \rho(\boldsymbol{r}'+\boldsymbol{a}_1) = \rho(\boldsymbol{r}'+\boldsymbol{a}_2) = \rho(\boldsymbol{r}'+\boldsymbol{a}_3)$ when the arguments are within the parallelepiped spanned by $L\boldsymbol{a}_1$, $L\boldsymbol{a}_2$, $L\boldsymbol{a}_3$. Under Born approximation, the scattering amplitude is $f(\boldsymbol{q}) = f_{\text{point scatterer}}(\boldsymbol{q})\int \mathrm{d}^3\boldsymbol{r}'\,\rho(\boldsymbol{r}')\exp(-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{r}')$. The total form factor is $F(\boldsymbol{q}) = \int_{\text{unit cell}} \mathrm{d}^3\boldsymbol{r}'\,\rho(\boldsymbol{r}')\exp(-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{r}')\sum_{x=0}^{L-1}\sum_{y=0}^{L-1}\sum_{z=0}^{L-1}\exp[-\mathbb{i}\boldsymbol{q}\cdot(x\boldsymbol{a}_1+y\boldsymbol{a}_2+z\boldsymbol{a}_3)]$ $= F_{\text{unit cell}}(\boldsymbol{q})\cdot\frac{1-e^{-L\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{a}_1}}{1-e^{-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{a}_1}}\frac{1-e^{-L\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{a}_2}}{1-e^{-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{a}_2}}\frac{1-e^{-L\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{a}_3}}{1-e^{-\mathbb{i}\boldsymbol{q}\cdot\boldsymbol{a}_3}}$, differential cross section is proportional to $|F(\boldsymbol{q})|^2 = |F_{\text{unit cell}}(\boldsymbol{q})|^2\frac{\sin^2(L\boldsymbol{q}\cdot\boldsymbol{a}_1/2)}{\sin^2(\boldsymbol{q}\cdot\boldsymbol{a}_1/2)}\frac{\sin^2(L\boldsymbol{q}\cdot\boldsymbol{a}_2/2)}{\sin^2(\boldsymbol{q}\cdot\boldsymbol{a}_2/2)}\frac{\sin^2(L\boldsymbol{q}\cdot\boldsymbol{a}_3/2)}{\sin^2(\boldsymbol{q}\cdot\boldsymbol{a}_3/2)}$. The differential cross section is peaked when $\boldsymbol{q}\cdot\boldsymbol{a}_{1,2,3} = 0 \mod 2\pi$, namely $\boldsymbol{q}$ is a reciprocal lattice vector (Bragg's law). The peak width (in $\boldsymbol{k}$-space) is proportional to $1/L$ namely inverse of sample's linear size.

B. Hard sphere: s-wave scattering

- $V(r) = \begin{cases} 0, & r > a; \\ V_0, & r < a. \end{cases}$
- For small momentum $k \ll 1/a$, scattering happens mainly in the s-wave channel ($l = 0$). The radial Schrödinger equation is $[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2m}{\hbar^2}V(r)](r\,R_0(r)) = k^2(r\,R_0(r))$.
- Repulsive case: $V_0 > 0$, define $K = \sqrt{\frac{2mV_0}{\hbar^2}}$.
  - For $k > K$, $r\,R(r) = \begin{cases} \sin(\sqrt{k^2-K^2}r), & r < a; \\ A\sin(ka+\delta_0), & r > a. \end{cases}$
    The phase shift $\delta_0 = \arctan[\frac{k}{\sqrt{k^2-K^2}}\tan(\sqrt{k^2-K^2}a)] - ka$.
    For $k \gg K$, δ_0 vanishes (as K^2/k^2) and so does the cross section.
  - For $k < K$, $r\,R(r) = \begin{cases} \sinh(\sqrt{K^2-k^2}r), & r < a; \\ A\sin(ka+\delta_0), & r > a. \end{cases}$
    The phase shift $\delta_0 = \arctan[\frac{k}{\sqrt{K^2-k^2}}\tanh(\sqrt{K^2-k^2}a)] - ka$.

For $k \ll K$, $\delta_0 \sim ka[\frac{\tanh(Ka)}{Ka} - 1]$.

Define the s-wave *scattering length*, $a_0 = -\lim_{k\to 0}\frac{\mathrm{d}\delta_0}{\mathrm{d}k}$, in this case $a_0 = a\,[1 - \frac{\tanh(Ka)}{Ka}] > 0$. For infinitely repulsive potential ($V_0 \to +\infty$, $K \to +\infty$), $a_0 = a$.

- Attractive case: $V_0 < 0$, define $K = \sqrt{-\frac{2mV_0}{\hbar^2}}$.
  - $r\,R(r) = \begin{cases} \sin(\sqrt{K^2+k^2}r), & r < a; \\ A\,\sin(ka+\delta_0), & r > a. \end{cases}$

    The phase shift $\delta_0 = \arctan[\frac{k}{\sqrt{K^2+k^2}}\tan(\sqrt{K^2+k^2}a)] - ka$.

    The scattering length $a_0 = -\lim_{k\to 0}\frac{\mathrm{d}\delta_0}{\mathrm{d}k} = a\,[1 - \frac{\tan(Ka)}{Ka}]$.

    For small $Ka \ll 1$, this is negative.
  - For $Ka = \pi/2 + n\pi$, $n = 0, 1, \ldots$, the scattering length a_0 diverges. This is the condition to have a zero energy bound state $r\,R(r) = \begin{cases} \sin(Kr), & r < a; \\ \text{constant}, & r > a. \end{cases}$
  - The S-matrix element $e^{2\mathbb{i}\delta_0} = e^{-2\mathbb{i}ka}\frac{1+\mathbb{i}\frac{k}{\sqrt{k^2+K^2}}\tan(\sqrt{k^2+K^2}a)}{1-\mathbb{i}\frac{k}{\sqrt{k^2+K^2}}\tan(\sqrt{k^2+K^2}a)}$ can have a pole at $k = \mathbb{i}\kappa$, if $\kappa = -\frac{\sqrt{K^2-\kappa^2}}{\tan(\sqrt{K^2-\kappa^2}a)}$. This is the condition to have a energy $-\frac{\hbar^2\kappa^2}{2m}$ bound state $r\,R(r) = \begin{cases} \sin(\sqrt{K^2-\kappa^2}r), & r < a; \\ A\,\exp(-\kappa r), & r > a. \end{cases}$

- In summary,

  the scattering length is positive(usually negative) for repulsive(attractive) potential;

  scattering length can diverge if a bound state energy approaches zero;

  poles of S-matrix (with complex k) indicate bound states.

Summary of Lecture #8: introduction to relativistic quantum mechanics

The Goals and The Requirements

- Have some basic understanding about the Dirac equation:
  - One way to reconcile special relativity $E = \sqrt{m^2c^4 + c^2p^2}$ and quantum mechanics $\psi \sim \exp[\mathbb{i}(\boldsymbol{p} \cdot \boldsymbol{x} - E \cdot t)/\hbar]$.
  - $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = (c\boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} + mc^2\beta)\psi$.
    α_i and β anti-commute, are hermitian, and square to identity.
    Use Dirac's convention $\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix}$.
- Get to know some basic consequences of the Dirac equation:
  - Orbital angular momentum $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$ is not conserved.
    Angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ is conserved. Spin $S_a = \frac{\hbar}{4\mathbb{i}}\epsilon_{abc}\alpha_b\alpha_c$.
    $S_a = \frac{\hbar}{2}\begin{pmatrix} \sigma_a & 0 \\ 0 & \sigma_a \end{pmatrix}$ under Dirac's convention.
  - Zeeman coupling term $-\frac{q}{m}\boldsymbol{S} \cdot \boldsymbol{B}$ with $g = 2$.
  - Spin-orbit coupling: under potential $V(\boldsymbol{x})$, the low energy effective Hamiltonian include $-\frac{q}{2m^2c^2}\hat{\boldsymbol{S}} \cdot (\boldsymbol{E} \times \hat{\boldsymbol{p}})$, where $\boldsymbol{E} = -\frac{\partial}{\partial \boldsymbol{r}}V$.
  - Zitterbewegung: Dirac particle cannot be "at rest" in the classical sense. Even with $\boldsymbol{p} = 0$ and without external potential, it seems to be oscillating, $\boldsymbol{x}(t) = \boldsymbol{x}(0) + \frac{\hbar}{2mc}(\boldsymbol{\alpha}\sin\frac{2mc^2t}{\hbar} + \mathbb{i}\boldsymbol{\alpha}\beta\cos\frac{2mc^2t}{\hbar})$.
- Optional references:

  M.E. Peskin, D.V. Schroeder, *An Introduction to Quantum Field Theory*, Chapter 3.

  J.J. Sakurai, *Advanced Quantum Mechanics*, Chapter 3.

  P.A.M. Dirac, *The Principle of Quantum Mechanics*, Chapter XI.

I. REMINDER ABOUT BASICS OF SPECIAL RELATIVITY

- Lorentz group: $O(1,3)$ group,
  $(ct,x,y,z) \to (ct,x,y,z)\cdot\Lambda_{4\times4}$, preserving $(ct)^2 - x^2 - y^2 - z^2$.

- Use metric $\eta_{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$ where diag means diagonal matrix. $\Lambda\cdot\eta\cdot\Lambda^T = \eta$.

- Contra-variant 4-vectors: index $\mu = 0,1,2,3$,
  4-position $x^\mu = (ct,x,y,z)$;
  4-momentum $p^\mu = (\frac{E}{c}, p_x, p_y, p_z)$, E is energy;
  4-potential $A^\mu = (\frac{\phi}{c}, A_x, A_y, A_z)$, ϕ and $\boldsymbol{A}$ are electrostatic and vector potentials;
  4-current density $j^\mu = (c\rho, \boldsymbol{j})$, ρ and $\boldsymbol{j}$ are density and current density.

- Covariant 4-vectors are obtained by contravariant ones as $v_\nu = v^\mu\eta_{\mu\nu}$. Einstein's convention of implicit summation over repeated indices is used. $\partial_\mu \equiv \frac{\partial}{\partial x^\mu}$. Greek indices take values of $0,1,2,3$, Roman indices take values of $1,2,3$ (or x,y,z).

- Proper time element $\mathrm{d}\tau$ is given by $(\mathrm{d}\tau)^2 = \mathrm{d}x^\mu\,\eta_{\mu\nu}\,\mathrm{d}x^\nu$.

- Lorentz invariant quantities:
  for example $p^\mu p_\mu = E^2/c^2 - \boldsymbol{p}^2 = m^2c^2$

- Classical mechanics and electromagnetism can be cast into Lorentz covariant form. Maxwell's equations: $\epsilon^{\mu\nu\rho}\partial_\mu F_{\nu\rho} = 0$, $\partial^\mu F_{\mu\nu} = \mu_0 j_\nu$ where μ_0 is vacuum permeability. $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu = -F_{\nu\mu}$ is electromagnetic field tensor. $F_{0a} = E_a/c$ for $a = 1,2,3$ and $\boldsymbol{E}$ is electric field; $F_{ab} = -\epsilon_{abc}B_c$ for $a,b,c = 1,2,3$ and $\boldsymbol{B}$ is magnetic field.

- A moving particle in electric field will experience an effective magnetic field, the magnetic moment of the particle will precess (Thomas precession).

II. KLEIN-GORDON EQUATION

- The plane wave states are $\psi \sim e^{\mathbb{i}(\boldsymbol{p}\cdot\boldsymbol{x} - E\cdot t)/\hbar}$, suggesting $\boldsymbol{p} \to -\mathbb{i}\hbar\boldsymbol{\nabla}$ and $E \to \mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}$.

- For non-relativistic particle, dispersion relation is $E = \frac{\boldsymbol{p}^2}{2m}$, suggesting non-relativistic Schrödinger equation $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi$.

- The first attempt to reconcile with relativistic dispersion relation $E^2 - \boldsymbol{p}^2c^2 = m^2c^4$ is the *Klein-Gordon equation* $\hbar^2\left(-\frac{1}{c^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \boldsymbol{\nabla}^2\right)\psi = m^2c^2\psi$, or $(\hbar^2\partial^\mu\partial_\mu + m^2c^2)\psi = 0$.
- The ψ in Klein-Gordon equation cannot be treated as probability amplitude.
  - In non-relativistic case, $\int \psi^*\psi\,\mathrm{d}^3\boldsymbol{x}$ is conserved, and $\psi^*\psi$ is non-negative, so can be interpreted as probability density.
  - Under Klein-Gordon equation, $\int(\mathbb{i}\psi^*\frac{\mathrm{d}}{\mathrm{d}t}\psi - \mathbb{i}\psi\frac{\mathrm{d}}{\mathrm{d}t}\psi^*)\,\mathrm{d}^3\boldsymbol{x}$ is conserved, however the integrand is not positive semidefinite and cannot be interpreted as probability density.

III. DIRAC EQUATION

- The trouble with probability interpretation of Klein-Gordon equation is the appearance of 2nd time derivative. Then it is tempting to consider the dispersion relation, $E = \sqrt{\boldsymbol{p}^2c^2 + m^2c^4}$ and replace E and $\boldsymbol{p}$ as before. However quantum mechanics should allow linear superposition of wave functions, the square root does not allow that. Dirac formally solved the square root as linear function of $\boldsymbol{p}$ and obtain
- Dirac equation: $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = (c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + mc^2\beta)\psi$.
- To be consistent with $E^2 = \boldsymbol{p}^2c^2 + m^2c^4$, we need
  $\{\alpha_i, \alpha_j\} = 2\delta_{ij}$, $\{\alpha_i, \beta\} = 0$, and $\beta^2 = 1$.
  Then α_i and β must be matrices, and ψ is a vector.
- Dirac's convention: $\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix}$. $\sigma_{0,1,2,3}$ are Pauli matrices.
  Dirac equation becomes $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = \begin{pmatrix} mc^2 & c\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} \\ c\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} & -mc^2 \end{pmatrix} \cdot \psi$.
- $\psi^\dagger \cdot \psi$ can be interpreted as probability density.
- Lorentz covariant form of Dirac equation: $(\mathbb{i}\hbar\gamma^\mu\partial_\mu - mc^2)\tilde{\psi} = 0$,
  where $\gamma^\mu = (\beta, \beta\boldsymbol{\alpha})$ and $\tilde{\psi} = \beta\psi$. Note that $\{\gamma^\mu, \gamma^\nu\} = \eta^{\mu\nu}$.
  Under Lorentz transformations (including spatial rotations) the vector wave function $\tilde{\psi}$ shall transform non-trivially (not only changing argument t and $\boldsymbol{x}$).

- Conserved quantities for $\hat{H} = c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + mc^2\beta$,
  - momentum $\hat{\boldsymbol{p}} = -\mathbb{i}\hbar\boldsymbol{\nabla}$.
  - angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, $\boldsymbol{L} = \boldsymbol{x}\times\hat{\boldsymbol{p}}$ is orbital angular momentum, $S_a = \frac{\hbar}{4\mathbb{i}}\epsilon_{abc}\alpha_b\alpha_c$ is "spin" angular momentum. $\boldsymbol{L}$ (or $\boldsymbol{S}$) alone is not conserved. Spin has eigenvalues $\pm\frac{\hbar}{2}$ (Dirac particles are spin-1/2).
    $[J_a, J_b] = \mathbb{i}\hbar\epsilon_{abc}J_c$, $[L_a, L_b] = \mathbb{i}\hbar\epsilon_{abc}L_c$, $[S_a, S_b] = \mathbb{i}\hbar\epsilon_{abc}S_c$, $[L_a, S_b] = 0$.
    Spatial rotation corresponds to $\exp(-\mathbb{i}\theta\boldsymbol{n}\cdot\boldsymbol{J}/\hbar)$.
  - helicity $\boldsymbol{J}\cdot\frac{\boldsymbol{p}}{|\boldsymbol{p}|} = \boldsymbol{S}\cdot\frac{\boldsymbol{p}}{|\boldsymbol{p}|}$, projection of (spin) angular momentum onto direction of momentum. Helicity can be $\pm\frac{\hbar}{2}$.
- Weyl equation: when mass $m = 0$, the Dirac equation can be block-diagonalized into two 2×2 equations $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = \pm(c\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})\psi$. $\pm$ signs correspond to right(left)-handed Weyl fermions.
- Majorana fermions: it is possible to choose $\boldsymbol{\alpha}$ to be real and β to be purely imaginary (*e.g.* $\beta = \sigma_1\otimes\sigma_2$, $\alpha_1 = \sigma_1\otimes\sigma_3$, $\alpha_2 = -\sigma_3\otimes\sigma_0$, $\alpha_3 = -\sigma_1\otimes\sigma_1$), in this case the Dirac equation divided $\mathbb{i}$ on both sides becomes real, so has real wave function solutions.
- Zitterbewegung:
  consider the Heisenberg picture equation of motion, $\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x} = \frac{\mathbb{i}}{\hbar}[\hat{H}, \boldsymbol{x}] = c\boldsymbol{\alpha}$, so the velocity operator has eigenvalue $\pm c$ and different components of velocity do not commute! Consider the case that $\boldsymbol{p} = 0$, further use of Heisenberg equations of motion produces $(\frac{\mathrm{d}}{\mathrm{d}t})^2\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x} = -\frac{4m^2c^4}{\hbar^2}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}$. solution is $\boldsymbol{x}(t) = \boldsymbol{x}(0) + \frac{\hbar}{2mc}(\boldsymbol{\alpha}\sin\frac{2mc^2t}{\hbar} + \mathbb{i}\boldsymbol{\alpha}\beta\cos\frac{2mc^2t}{\hbar})$.
  Dirac particle "at rest" seems to be oscillating very rapidly.

A. Solutions to Dirac equation

- let $\psi(t, \boldsymbol{x}) = e^{\mathbb{i}(\boldsymbol{p}\cdot\boldsymbol{x} - E\cdot t)/\hbar}u(\boldsymbol{p})$. Then $\begin{pmatrix} mc^2 & c\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\boldsymbol{\sigma}\cdot\boldsymbol{p} & -mc^2 \end{pmatrix}\cdot u(\boldsymbol{p}) = E\,u(\boldsymbol{p})$
  Note that $\boldsymbol{\sigma}\cdot\boldsymbol{p}$ has eigenvalues $\pm|\boldsymbol{p}|$, denote the corresponding eigenvectors as $\chi_\pm(\boldsymbol{p})$, $(\boldsymbol{\sigma}\cdot\boldsymbol{p})\chi_\pm(\boldsymbol{p}) = \pm|\boldsymbol{p}|\chi_\pm(\boldsymbol{p})$, if $\boldsymbol{p} = |\boldsymbol{p}|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, one can choose $\chi_+(\boldsymbol{p}) = \begin{pmatrix} \cos(\theta/2) \\ e^{\mathbb{i}\phi}\sin(\theta/2) \end{pmatrix}$, $\chi_-(\boldsymbol{p}) = \begin{pmatrix} -e^{-\mathbb{i}\phi}\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}$, the two solutions to $u(\boldsymbol{p})$ with

$E = \sqrt{\boldsymbol{p}^2c^2 + m^2c^4}$ are $u_+(\boldsymbol{p}) = \begin{pmatrix} \sqrt{\frac{E+mc^2}{2mc^2}}\chi_+(\boldsymbol{p}) \\ \sqrt{\frac{E-mc^2}{2mc^2}}\chi_+(\boldsymbol{p}) \end{pmatrix}$ and $u_-(\boldsymbol{p}) = \begin{pmatrix} \sqrt{\frac{E+mc^2}{2mc^2}}\chi_-(\boldsymbol{p}) \\ -\sqrt{\frac{E-mc^2}{2mc^2}}\chi_-(\boldsymbol{p}) \end{pmatrix}$, the subscript $\pm$ of u indicate helicity states.

- Negative energy solutions:
  let $\psi(t, \boldsymbol{x}) = e^{-\mathbb{i}(\boldsymbol{p}\cdot\boldsymbol{x} - E\cdot t)/\hbar}v(\boldsymbol{p})$. Then $\begin{pmatrix} -mc^2 & c\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\boldsymbol{\sigma}\cdot\boldsymbol{p} & mc^2 \end{pmatrix} \cdot v(\boldsymbol{p}) = E\, v(\boldsymbol{p})$. For $E = \sqrt{\boldsymbol{p}^2c^2 + m^2c^4}$, $v_+(\boldsymbol{p}) = \begin{pmatrix} \sqrt{\frac{E-mc^2}{2mc^2}}\chi_+(\boldsymbol{p}) \\ \sqrt{\frac{E+mc^2}{2mc^2}}\chi_+(\boldsymbol{p}) \end{pmatrix}$ and $v_-(\boldsymbol{p}) = \begin{pmatrix} -\sqrt{\frac{E-mc^2}{2mc^2}}\chi_-(\boldsymbol{p}) \\ \sqrt{\frac{E+mc^2}{2mc^2}}\chi_-(\boldsymbol{p}) \end{pmatrix}$.
  Because of the way we define ψ here, this seems nagative energy $-E$ solution of the Dirac equation, with momentum $-\boldsymbol{p}$. This ψ should be interpreted as the conjugate of the "positron" wave function.

B. Non-relativistic limit of Dirac equation

- The Dirac equation of charge q particle in electromagnetic field is
  $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = [c\boldsymbol{\alpha}\cdot(-\mathbb{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A}) + mc^2\beta + qV]\psi$.
  V is electrostatic potential, $\boldsymbol{A}$ is vector potential, both depend on space and time.

- Consider the case that $|\boldsymbol{p}| \ll mc$. Separate the "diagonal" and "off-diagonal" parts of Hamiltonian, $\hat{H} = \hat{H}_0 + \hat{H}_1$ where $\hat{H}_0 = mc^2\beta + qV$ and $\hat{H}_1 = c\boldsymbol{\alpha}\cdot(-\mathbb{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A})$.

- Eliminate the off-diagonal parts $\hat{H}_1$ by sequences of unitary transformations,
  $\psi' = e^{\mathbb{i}\hat{S}}\psi$, then $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi' = \hat{H}'\psi'$ where $\hat{H}' = e^{\mathbb{i}\hat{S}}\hat{H}e^{-\mathbb{i}\hat{S}} - \mathbb{i}\hbar e^{\mathbb{i}\hat{S}}\frac{\partial}{\partial t}e^{-\mathbb{i}\hat{S}}$
  $= \hat{H} + [\mathbb{i}\hat{S}, \hat{H}] + \frac{1}{2}[\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, \hat{H}]] + \frac{1}{6}[\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, \hat{H}]]] + \frac{1}{24}[\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, \hat{H}]]]] + \ldots$
  $-\hbar\frac{\partial}{\partial t}\hat{S} - \hbar\frac{1}{2}[\mathbb{i}\hat{S}, \frac{\partial}{\partial t}\hat{S}] - \hbar\frac{1}{6}[\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, \frac{\partial}{\partial t}\hat{S}]] + \ldots$

- $\hat{H}_1$ anti-commutes with β. Choose $\mathbb{i}\hat{S} = \beta\boldsymbol{\alpha}\cdot(\hat{\boldsymbol{p}} - q\boldsymbol{A})/2mc = \beta\hat{H}_1/2mc^2$, so that $[\mathbb{i}\hat{S}, mc^2\beta] = -\hat{H}_1$, note that $[\mathbb{i}\hat{S}, \hat{H}_1] = \frac{\beta}{mc^2}(\hat{H}_1)^2$, $[\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, \hat{H}_1]] = -\frac{1}{m^2c^4}(\hat{H}_1)^3$, $\ldots$;
  $\hat{H}' = mc^2\beta + (qV + \frac{\beta}{2mc^2}[\hat{H}_1, qV] - \frac{1}{(2mc^2)^2}[\hat{H}_1, [\hat{H}_1, qV]] + \ldots)$
  $+(\frac{\beta}{2mc^2}(\hat{H}_1)^2 - \frac{1}{3m^2c^4}(\hat{H}_1)^3 + \frac{\beta}{8m^2c^4}(\hat{H}_1)^3 + \ldots)$
  $+(\mathbb{i}\hbar\frac{\beta}{2mc^2}\frac{\partial}{\partial t}\hat{H}_1 - \frac{\mathbb{i}\hbar}{8m^2c^4}[\hat{H}_1, \frac{\partial}{\partial t}\hat{H}_1] + \ldots)$

- The diagonal terms up to $\frac{1}{m^2}$ are (no need for further unitary transformation)
  $\beta\,(mc^2 + \frac{(\hat{H}_1)^2}{2mc^2}) + q\,V - \frac{1}{8m^2c^4}[\hat{H}_1, [\hat{H}_1, q\,V]] - \frac{\mathbb{i}\hbar}{8m^2c^4}[\hat{H}_1, \frac{\partial}{\partial t}\hat{H}_1]$.

- $\frac{(\hat{H}_1)^2}{2mc^2} = \frac{1}{2m}\,\alpha_i\,(\hat{p}_i - qA_i)\cdot\alpha_j\,(\hat{p}_j - qA_j) = \frac{1}{2m}\,(\delta_{ij} + \mathbb{i}\frac{2\hat{S}_k}{\hbar}\epsilon_{ijk})(\hat{p}_i - qA_i)(\hat{p}_j - qA_j)$ $= \frac{1}{2m}[(\hat{\boldsymbol{p}} - q\boldsymbol{A})^2 - 2\hat{S}_k\epsilon_{ijk}\cdot q\,\partial_i A_j] = \frac{1}{2m}[(\hat{\boldsymbol{p}} - q\boldsymbol{A})^2 - 2q\hat{\boldsymbol{S}}\cdot\boldsymbol{B}]$, this gives the non-relativistic kinetic energy and the Zeeman term with Landé g-factor $g = 2$.

- For the last two terms, $[\hat{H}_1, q\,V] = -\mathbb{i}\hbar qc\boldsymbol{\alpha}\cdot(\nabla V)$, $[\hat{H}_1, \frac{\partial}{\partial t}\hat{H}_1] = [\hat{H}_1, -qc\boldsymbol{\alpha}\cdot\frac{\partial}{\partial t}\boldsymbol{A}]$, $[\hat{H}_1, [\hat{H}_1, q\,V]] = [\hat{H}_1, -\mathbb{i}\hbar qc\boldsymbol{\alpha}\cdot(\nabla V)]$, so $-\frac{1}{8m^2c^4}[\hat{H}_1, [\hat{H}_1, q\,V]] - \frac{\mathbb{i}\hbar}{8m^2c^4}[\hat{H}_1, \frac{\partial}{\partial t}\hat{H}_1]$
$= -\frac{\mathbb{i}}{8m^2c^4}[\hat{H}_1, \mathbb{i}\hbar qc\boldsymbol{\alpha}\cdot(-\nabla V - \frac{\partial}{\partial t}\boldsymbol{A})] = -\frac{\mathbb{i}}{8m^2c^4}[\hat{H}_1, \mathbb{i}\hbar qc\boldsymbol{\alpha}\cdot\boldsymbol{E}]$
$= -\frac{\mathbb{i}\hbar c^2 q}{8m^2c^4}[\alpha_i(\hat{p}_i - qA_i), \alpha_j E_j]$
$= -\frac{\mathbb{i}\hbar q}{8m^2c^2}((\delta_{ij} + \mathbb{i}\frac{2\hat{S}_k}{\hbar}\epsilon_{ijk})(\hat{p}_i - qA_i)E_j - (\delta_{ij} - \mathbb{i}\frac{2\hat{S}_k}{\hbar}\epsilon_{ijk})E_j(\hat{p}_i - qA_i))$
$= -\frac{\hbar^2 q}{8m^2c^2}(\boldsymbol{\nabla}\cdot\boldsymbol{E}) + \frac{q}{2m^2c^2}\epsilon_{ijk}\hat{S}_k E_j(\hat{p}_i - qA_i) - \frac{\mathbb{i}\hbar q}{4m^2c^2}(\hat{S}_k\epsilon_{ijk}\partial_i E_j)$
$= -\frac{\hbar^2 q}{8m^2c^2}(\boldsymbol{\nabla}\cdot\boldsymbol{E}) - \frac{q}{2m^2c^2}\hat{\boldsymbol{S}}\cdot(\boldsymbol{E}\times\hat{\boldsymbol{P}}) - \frac{\mathbb{i}\hbar q}{4m^2c^2}\hat{\boldsymbol{S}}\cdot(\boldsymbol{\nabla}\times\boldsymbol{E})$.
The 1st term is the Darwin term. The 2nd term is the spin-orbit coupling. The last term vanishes for static electromagnetic field.

- For static central potential $V(\boldsymbol{r}) = V(r)$, $\boldsymbol{E} = -\nabla V = -\frac{\boldsymbol{r}}{r}\frac{\partial}{\partial r}V(r)$, the spin-orbit coupling becomes $-\frac{q}{2m^2c^2}\hat{\boldsymbol{S}}\cdot(\boldsymbol{E}\times\hat{\boldsymbol{P}}) = \frac{q}{2m^2c^2}\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\hat{\boldsymbol{S}}\cdot(\boldsymbol{r}\times\hat{\boldsymbol{P}}) = \frac{q}{2m^2c^2}\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{L}}$.