Matteo Veneziano – Quantum Physics II Formula Sheet

General single qubit state

- ⋆ $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, or $|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$, $|\alpha|^2 + |\beta|^2 = 1$
- ⋆ $|\psi\rangle$ is an eigenstate of $\boldsymbol{\sigma}\cdot\boldsymbol{n}$ with eigenvalue 1

Evolution

- ⋆ $i\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle$ (Schrödinger)
- ⋆ if H time-independent then $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, $U(t) = e^{-iHt}$

Pauli matrices

- ⋆ $\sigma_0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$
- ⋆ $\mathrm{Tr}[\sigma_0] = 2$, $\mathrm{Tr}[\sigma_i] = 0$ for $i = 1, 2, 3$ $\qquad S_i = \frac{\hbar}{2}\sigma_i$
- ⋆ $\sigma_i\sigma_j = \delta_{ij}\mathbb{I} + i\epsilon_{ijk}\sigma_k \quad [\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$ $\qquad$ ⋆ $V = \boldsymbol{v}\cdot\boldsymbol{\sigma} \Rightarrow V^2 = \mathbb{I}$
- ⋆ $\{\sigma_i, \sigma_j\} = \sigma_i\sigma_J + \sigma_j\sigma_i = 2\delta_{ij}\mathbb{I}$
- ⋆ Paulis form an orthonormal basis with $\mathrm{Tr}[\sigma_i, \sigma_j] = 2\delta_{ij}$
- ⋆ The Pauli α operator, $\alpha \in \{x, y, z\}$, rotates the state by π around the α-axis.
- ⋆ Paulis as generators: any single qubit hamiltonian can be written as $H = \omega\boldsymbol{n}\cdot\boldsymbol{\sigma}$
  $U = \exp(-i\omega\boldsymbol{\sigma}\cdot\boldsymbol{n}t) = \cos(\omega t)\mathbb{I} - i\sin(\omega t)\boldsymbol{n}\cdot\boldsymbol{\sigma}$
  Causes a qubit state to rotate around $\boldsymbol{n}$ at a rate $2\omega t$.

Observables

- ⋆ $M = \sum_k \lambda_k |\lambda_k\rangle\langle\lambda_k|$ Hermitian
- ⋆ $\langle M\rangle = \langle\psi|M|\psi\rangle = \sum_k \lambda_k P_k$, $P_k = |\langle\lambda_k|\psi\rangle|^2$
- ⋆ $\Pi_k = |\lambda_k\rangle\langle\lambda_k|$ Projector $\Rightarrow P_k = \langle\psi|\Pi_k|\psi\rangle$, $\sum_k \Pi_k = 1$
- ⋆ Measurement $\Rightarrow$ State collapses to $\frac{\Pi_k|\psi_k\rangle}{\sqrt{P_k}}$

Composite systems $\quad \mathcal{H}_{ABC\ldots} = \mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_c \ldots$

- ⋆ The resulting space has dimension $n_A n_B n_C \ldots$
- ⋆ Operators $T_{AB}|\lambda_i j\rangle = (T_a \otimes T_b)(|\mu_i \otimes \nu_j\rangle) = T_A|\mu_i\rangle \otimes |\nu_k\rangle$
- ⋆ $[T_A \otimes \mathbb{I}_B, \mathbb{I}_A \otimes T_B] = 0, \quad \{T_A \otimes \mathbb{I}_B, \mathbb{I}_A \otimes T_B\} = 2(T_A \otimes T_B)$
  $e^{A\otimes\mathbb{I}+\mathbb{I}\otimes B} = e^A \otimes e^B$
- ⋆ Global measurem. $T = T_A \otimes T_B \to T|T_i\rangle = t_i|T_i\rangle$, $\quad |\psi\rangle = \sum_i |T_i\rangle\langle T_i|\psi\rangle$
- ⋆ Partial measurement T_A: if $|\psi\rangle = \sum_{ij}|T_{A,i}\rangle \otimes |T_{B,j}\rangle = \sum_i |T_{A,i}\rangle \otimes |\phi_{B,i}\rangle$
  then $P_i = \sum_j |c_{ij}|^2$ and system collapses to $|\psi\rangle' \propto |T_{A,i}\rangle \otimes |\phi_{B,i}\rangle$
- ⋆ $P_{\hat{O}}(\lambda|\psi) = \langle\psi|\Pi^A_\lambda|\psi\rangle$ is the probability of a measurement of operator $\hat{O}$ yielding its eigenvalue λ, with A the subspace of the meas., $\Pi^A_\lambda = |\lambda\rangle\langle\lambda|_A \otimes \mathbb{I}_B$ and $|\lambda\rangle$ the eigenket corresponding to eigenvalue λ
  For measurements on both subspaces use $\Pi_\lambda = |\lambda\rangle\langle\lambda|_A \otimes |\kappa\rangle\langle\kappa|_B$
- ⋆ *Entangled* state: its coefficients cannot be written as the product of two independent coefficients. *Separable* state: the global wave function can be written as the product of two wavefunctions corresponding to subsystems A and B (measures performed on one part do not affect the other).
- ⋆ Condition of separability for 2 qubits: if $c_{ij} = c_i^{(A)}c_j^{(B)}$, with $i, j \in \{0, 1\}$, then $\det\begin{pmatrix}c_{00} & c_{01}\\ c_{10} & c_{11}\end{pmatrix} = 0 \Leftrightarrow$ separable. E.g. in $(\alpha|0\rangle_A \otimes \beta|0\rangle_B)$, $c_{00} = \alpha\beta$.
- ⋆ $H_{AB} = H_A \otimes \mathbb{I}_B + \mathbb{I}_A \otimes H_B \Longrightarrow e^{-itH_{AB}} = e^{-itH_A} \otimes e^{-ith_B}$
  A separable unitary generates no entanglement when applied to a separable state.

Quantum eraser

- ⋆ $|\nearrow\rangle = \frac{1}{\sqrt{2}}(|H\rangle + |V\rangle)$, $|\swarrow\rangle = \frac{1}{\sqrt{2}}(|H\rangle - |V\rangle)$
- ⋆ $|H\rangle = \frac{1}{\sqrt{2}}(|\nearrow\rangle + |\swarrow\rangle)$, $|V\rangle = \frac{1}{\sqrt{2}}(|\nearrow\rangle - |\swarrow\rangle)$
- ⋆ $P(x) = \langle\psi(x,t)|(|x\rangle\langle x| \otimes \mathbb{I})|\psi(x,t)\rangle$ Probability density on screen

Bell states

- ⋆ $|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B\right)$ $\qquad$ maximally entangled
  $|\Phi^-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |0\rangle_B - |1\rangle_A \otimes |1\rangle_B\right)$
  $|\Psi^+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B\right)$
  $|\Psi^-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B\right)$
- ⋆ They form an orthonormal basis of the Hilbert space of the two spins $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$
- ⋆ Non separable
- ⋆ Eigenstates of $\hat{H} = \mu_x\hat{S}_x^{(A)} \otimes \hat{S}_x^{(B)} + \mu_y\hat{S}_y^{(A)} \otimes \hat{S}_y^{(B)}$
- ⋆ $P_{\hat{S}_x^{(A)}}(\pm\frac{\hbar}{2}|\psi) = \frac{1}{2} \quad \forall|\psi\rangle$ a Bell state.

CHSH Inequality

- ⋆ Bipartite system with LHS measuring device, which can measure either A or A', and RHS device which can measure B or B'. The probability of a result combination is written as $P(l, r|L, R)$ with L, R the settings on LHS and RHS device and l and r the results of the measures (±1).
- ⋆ Bell inequalities define a correlation coefficient C and then place an upper bound on possible values this coefficient can take if you assume factorisability
- ⋆ Factorisability: $p(l, r|L, R) = \int P(l|L, \lambda)P(r|R, \lambda)P(\lambda)d\lambda$ where λ incorporates all effects from the system's shared history. Two necessary conditions for factorisability to hold: Setting Independence $P(l|L, B, \lambda) = P(l|L, B', \lambda)$ and Outcome Indipendence $P(l, A, R, r, \lambda) = P(l|A, R, r', \lambda)$.
- ⋆ $C := |\langle LR\rangle - \langle LR'\rangle| + |\langle LR\rangle + \langle L'R\rangle|$ with $\langle LR\rangle = \sum_{l,r=\pm1} lrP(l, r|L, R)$
- ⋆ $C \leq 2$ in the classical case, violated in quantum case (Tsirelson's bound: $C \leq 2\sqrt{2}$)
  Quantum Mechanics violates outcome indipendence.

Reduced and mixed quantum states

- ⋆ Density operator: $\rho = |\psi\rangle\langle\psi| \Longrightarrow \langle O\rangle = \mathrm{Tr}(\rho O)$ for any observable O
- ⋆ General single qubit: $\rho = \begin{pmatrix}cos(\theta/2)^2 & \cos(\theta/2)\sin(\theta/2)e^{-i\phi}\\ \cos(\theta/2)\sin(\theta/2)e^{i\phi} & \sin(\theta/2)^2\end{pmatrix} =$
  $= \frac{1}{2}\sigma_0 + \frac{1}{2}\sum_{i=1}^3 v_i\sigma_i$ with $\boldsymbol{v} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$; $v_i = \mathrm{Tr}[\rho\sigma_i]$
- ⋆ $\rho = \sum_k p_k|\psi_k\rangle\langle\psi_k|$ System prepared in state $|\psi_k\rangle$ with prob. p_k (**mixed** state)
- ⋆ Maximally mixed: $\frac{\mathbb{I}}{2} = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$
- ⋆ If $\rho = p|\psi\rangle\langle\psi| + (1-p)|\phi\rangle\langle\phi|$ where ψ, ϕ have Bloch vectors $\boldsymbol{v}, \boldsymbol{u}$ of pure states, the mixed state has Bloch vector $\boldsymbol{w} = p\boldsymbol{v} + (1-p)\boldsymbol{u}$; $|\boldsymbol{w}|^2 \leq 1$
- ⋆ $\rho_A = \sum_{k=1}^{d_B}(\mathbb{I}_A \otimes \langle k|)\rho_{AB}(\mathbb{I}_A \otimes |k\rangle) = \mathrm{Tr}_B[\rho_{AB}]$ $\qquad$ **Reduced** state
- ⋆ $\mathrm{Tr}_B[|ij\rangle\langle kl|] = |i\rangle\langle k|\,\mathrm{Tr}[|j\rangle\langle l|]$
- ⋆ **Props**: (i) $\rho_A^\dagger = \rho_A$ (self-adj.) $\qquad$ (ii)$\mathrm{Tr}(\rho_A) = \sum_i\sum_\mu \alpha^*_{i,\mu}\alpha_{i,\mu} = |\psi|^2 = 1$
  (iii)$\langle\psi|\rho_A|\psi\rangle \geq 0$ for all $|\psi\rangle \in A$ i.e. positive or null eigenvalues
- ⋆ Conseq., $\rho_A = \sum_j p_j|k\rangle\langle j|$ where $p_j \geq 0$ and $\sum p_j = 1$.
  $\langle O\rangle = \mathrm{Tr}(\rho_A O) = \sum_j p_j\langle j|O|j\rangle = \sum_{p_j}\langle O\rangle_{|j\rangle}$
- ⋆ If a density op. describes a pure state, then it is a projector ($\rho^2 = \rho$). If ρ is not pure then $\rho^2 \neq \rho$ and $\mathrm{Tr}[\rho^2] < 1$ (*purity* of a state).
- ⋆ **Evolution:** $\rho(t=0) = \sum_j \alpha_j|\psi_j(0)\rangle\langle\psi_j(0)|$ initial state
  $\Longrightarrow \rho(t) = \sum_j \alpha_j e^{-iHt}|\psi_j(0)\rangle\langle\psi_j(0)|e^{iHt} \Longrightarrow i\frac{\partial\rho}{\partial t} = [\hat{H}, \rho]$
- ⋆ Why is signaling impossible? No matter what is performed upon the other partitions, the reduced density matrix is unchanged. Because the statistics of local measurements are informed entirely by expected values of operators upon the reduced density matrix, they are also independent of operations on other partitions.

Identical multi-particle systems

- ⋆ $\mathbb{P}_{1,2}\psi(\boldsymbol{r_1}, \boldsymbol{r_2}) = \psi(\boldsymbol{r_2}, \boldsymbol{r_1}) = \pm\psi(\boldsymbol{r_1}, \boldsymbol{r_2})$ $\quad$ +1: bosons $\quad$ −1: fermions
- ⋆ $\mathbb{P}_{jk} = \mathbb{P}_{kj}$ $\qquad$ ⋆ $\mathbb{P}_{jk}^2 = \mathbb{I} \Leftrightarrow \mathbb{P}_{jk}^{-1} = \mathbb{P}_{jk}$ $\qquad$ ⋆ $\mathbb{P}_{jk} = \mathbb{P}_{jk}^\dagger$
- ⋆ $\langle\psi_{12}|O|\psi_{12}\rangle = \langle\psi_{12}|\mathbb{P}_{12}^\dagger O\mathbb{P}_{12}|\psi_{12}\rangle$ for all $\psi \Rightarrow [\mathbb{P}_{12}, O] = 0, [\mathbb{P}_{12}, H] = 0$
- ⋆ Possible basis states for a system of
  n bosons: $|\psi_{\boldsymbol{x}}\rangle = \mathcal{N}\sum_{\mathbb{P}\in S_n}\mathbb{P}|x_1, x_2, \ldots, x_n\rangle$ with $\mathcal{N} = \frac{1}{\sqrt{n!}\sqrt{\prod_k n_k!}}$
  n fermions $|\psi_{\boldsymbol{x}}\rangle = \frac{1}{\sqrt{n!}}\sum_{\mathbb{P}\in S_n}\mathrm{sign}(\mathbb{P})\mathbb{P}|x_1, x_2, \ldots, x_n\rangle$

Second Quantization

- ⋆ Kets indicate the number of times a wave function is involved:
  for Bosons $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \to |11\rangle$; $|\uparrow\uparrow\rangle \to |20\rangle$; $|\downarrow\downarrow\rangle \to |02\rangle$
  for Fermions $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \to |11\rangle$ (only possible values 0,1)
- ⋆ Creation and annihilation operators to increase or decrease the number of particles:
  Bosons: $\begin{cases}\hat{c}_i^\dagger|n_1, \cdots, n_i, \cdots\rangle = \sqrt{n_i+1}\,|n_1, \cdots, n_i+1, \cdots\rangle\\ \hat{c}_i|n_1, \cdots, n_i, \cdots\rangle = \sqrt{n_i}\,|n_1, \cdots, n_i-1, \cdots\rangle\end{cases}$
  $[\hat{c}_i, \hat{c}_j] = [\hat{c}_i^\dagger, \hat{c}_j^\dagger] = 0; \qquad [\hat{c}_i, \hat{c}_j^\dagger] = \delta_{ij}$
  Fermions: $\begin{cases}\hat{c}_i^\dagger|n_1, \cdots, n_i, \cdots\rangle = (-1)^{n_1+\cdots+n_i-1}(1-n_i)|n_1, \cdots, n_i+1, \cdots\rangle\\ \hat{c}_i|n_1, \cdots, n_i, \cdots\rangle = (-1)^{n_1+\cdots+n_i-1}n_i|n_1, \cdots, n_i-1, \cdots\rangle\end{cases}$
  $\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0; \qquad \{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}$

Perturbation Theory

- ⋆ $H = H_0 + \lambda V$, with $H_0|\phi_n\rangle = \epsilon_n|\phi_n\rangle$ known, $\lambda \in \mathbb{R}^+$.
- ⋆ $H|\psi_n\rangle = E_n|\psi_n\rangle$ eigenspectrum unknown. The solution in the limit of small λ is
  $|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \ldots$
  $E_n = \epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$
- ⋆ S.E.: $(H_0 + \lambda V)(|\phi_n\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \ldots) = (\epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots)(|\phi_n\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \ldots)$ must be satisfied at each order in λ

Non-degenerate Time-Indipendent Perturbation Theory

- ⋆ **Zero-th order** $H_0|\phi_n\rangle = \epsilon_n|\phi_n\rangle$ unperturbed eigenvalue problem
- ⋆ **1st order** $E_n^{(1)} = \langle\phi_n|V|\phi_n\rangle$; $\quad |\psi_n^1\rangle = \sum_{m\neq n}\frac{\langle\phi_m|V|\phi_n\rangle}{\epsilon_n - \epsilon_m}|\phi_m\rangle$
- ⋆ **2nd order** $E_n^{(2)} = \sum_{m\neq n}\frac{|\langle\phi_m|V|\phi_n\rangle|^2}{\epsilon_n - \epsilon_m}$; for approx. to be val. $|E_n^{(2)}| \ll |E_n^{(1)}|$
- ⋆ satisfied as long as $\frac{1}{\Delta}(\langle\phi_n|V^2|\phi_n\rangle - \langle\phi_n|V|\phi_n\rangle^2) \ll \langle\phi_n|V|\phi_n\rangle$,
  $\Delta = \min_m|\epsilon_n - \epsilon_m|$ or more restrictive: $\left|\frac{\langle\phi_m|V|\phi_n\rangle}{\epsilon_n - \epsilon_m}\right| \ll 1$

Degenerate Time-Indipendent Perturbation Theory

- ⋆ nth energy state has N-fold degeneracy $\Rightarrow H_0$ has energy ϵ_n with $\phi_{n_i}, i = 1\ldots N$
- ⋆ $\sum_j V_{ij}c_j = E_n^{(1)}c_i \Longleftrightarrow \hat{V}\boldsymbol{c} = E_n^{(1)}\boldsymbol{c} \qquad V_{ij} = \langle\phi_{n_i}|V|\phi_{n_j}\rangle$
  eigenvalue problem, must diagonalise V matrix (in the degenerate subspace only!)
- ⋆ The eigenvectors are the corrected eigenstates (to 0th order), the eigenvalues are the 1st order correction to energy. If eigenvalues are the same, degeneracy is not lifted.
- ⋆ E.g. $V = \begin{pmatrix}0 & \alpha & 0 & 0\\ \alpha & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix} \xrightarrow{\text{diag}} \alpha, \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\\ 0\\ 0\end{pmatrix}; -\alpha, \begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\\ 0\\ 0\end{pmatrix}; 0, \begin{pmatrix}0\\ 0\\ 1\\ 0\end{pmatrix}; 0, \begin{pmatrix}0\\ 0\\ 0\\ 1\end{pmatrix}$
  Thus $|0\rangle \to \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$; $\quad |1\rangle \to \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$; $\quad |2\rangle, |3\rangle$ unchanged
  The corrected eigenstates have an energy correction $E^{(1)}$ of $\alpha, -\alpha$, 0,0.

Time-Dependent Hamiltonians

- $\star$ $U(t,t_0) = \mathbb{I} + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2 \dots \int_{t_0}^{t} \mathrm{d}t_n T(H(t_1)\dots H(t_n))$ where $T[H(t_1)H(t_2)\dots H(t_n)] = H(t_{i_1})H(t_{i_2})\dots H(t_{i_n})$, $t_{i_1} \geq t_{i_2} \geq \dots$
- $\star$ Alternatively: $U(t,t_0) \approx \sum_j \exp(iH(t_j)\delta t)$ with an error of $|\int_{t_0}^{t} \mathrm{d}s H(s) - \delta t \sum_{r=1}^{n_t} H(t_0 + r\delta t)|^2$ (discretisation)

Interaction picture

- $\star$ Schrödinger picture: $i\frac{\partial}{\partial t}\left|\phi_S(t)\right\rangle = H(t)\left|\phi_S(t)\right\rangle, \quad O_S(t) = O_S$
- $\star$ Heisenberg picture: $O_H(t) = U_S(t,t_0)^\dagger O_S U_S(t,t_0), \quad \left|\phi_H(t)\right\rangle = \left|\phi_S(t_0)\right\rangle$
- $\star$ Interaction picture: $H(t) = H_H + V_S(t)$,
- $\star$ $O_I(t) = e^{iH_0(t-t_0)}O_S(t)e^{-iH_0(t-t_0)}$
- $\star$ $\left|\phi_I(t)\right\rangle = U_I(t,t_0)\left|\phi_I(t_0)\right\rangle, \quad U_I = e^{iH_0(t-t_0)}U_S(t,t_o)$
- $\star$ $\frac{\partial U_I}{\partial t} = -iV_I(t)U_I(t,t_0)$

Time-Dependent Perturbation Theory

- $\star$ $U_I(t,t_0) \approx \mathbb{I} - i\int_{t_0}^{t} \mathrm{d}t_1 V_I(t_1) + \dots$
- $\star$ The exact transition probability between two states is $|\langle\psi|\phi\rangle|^2$
- $\star$ $P_{i\to n}(t) = |\left\langle n|\phi_S(t)\right\rangle|^2 = |\left\langle n|U_I(t,t_0)|i\right\rangle|^2 =$ $= \left|-i\int_{t_0}^{t}\mathrm{d}t_1 e^{i(E_n-E_i)(t-t_0)}\left\langle n|V(t_1,t_0)|i\right\rangle\right|^2$ general expression of transition probabilities between eigenstates $|i\rangle$ and $|n\rangle$ of H_0. Note: if $V=0$ then a system in an eigenstate stays in an aigenstate.
- $\star$ For a constant potential $P_{i\to n}(t) \overset{t\to\infty}{=} 2\omega t\,|\langle n|V|i\rangle|^2\,\delta(E_n - E_i)$ $\frac{\partial}{\partial t}P_{i\to n}(t) = 2\pi\,|\langle n|V|i\rangle|^2\,\delta(E_n - E_i)$

Variational method

- $\star$ $\dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$ Variational principle
- $\star$ The idea is to come up with a parameterised guess for the state $|\psi\rangle$, and then we use the variational principle to find the parameter values that minimize ψ. It generalises to excited states ($\langle\phi_0|\psi\rangle = 0$) by replacing E_0 with E_1.
- $\star$ Steps: compute $\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = E(a)$ then minimise E with respect to the parameter.

Particle in a box

- $\star$ $V(x) = \begin{cases} 0 & \text{if}|x| \leq L/2 \\ \infty & \text{else} \end{cases} \qquad \phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos(\frac{n\pi}{L}x) & n \text{ odd} \\ \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x) & n \text{ even} \end{cases}$
- $\star$ $E_n = n^2\frac{\pi^2\hbar^2}{2mL^2}$

Harmonic oscillator

- $\star$ $H = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega(\hat{N} + \frac{1}{2}), \quad \hat{N} = \hat{a}^\dagger\hat{a}$ $\quad\star$ $\hat{p}^2 = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$
- $\star$ $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)$
- $\star$ $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \quad \hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a})$
- $\star$ $[\hat{x},\hat{p}] = i\hbar, \quad [\hat{a},\hat{a}^\dagger] = 1, \quad [\hat{N},\hat{a}] = -\hat{a}, \quad [\hat{N},\hat{a}^\dagger] = \hat{a}^\dagger$
- $\star$ $\phi_0(x) = \left(\frac{m\omega}{\phi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)$
- $\star$ $\phi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n\phi_0 = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega x^2}{2\hbar}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$ with $H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}(e^{-z^2})$
- $\star$ $\hat{H}\phi_n = E_n\phi_n = \hbar\omega(n + \frac{1}{2})\phi_n$
- $\star$ $\hat{a}^\dagger\phi_n = \sqrt{n+1}\phi_{n+1} \quad \hat{a}\phi_n = \sqrt{n}\phi_{n-1}$

Hermitian and unitary operators

- $\star$ Hermitian operator: $M = M^\dagger \longrightarrow$ diagonalisable with real eigenvalues, linear
- $\star$ Unitary operators: $UU^\dagger = U^\dagger U = \mathbb{I} \longrightarrow \langle\psi|U^\dagger U|\psi\rangle = \mathbb{I}$ and linear

Tensor product

- $\star$ $\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} a\alpha & a\beta & b\alpha & b\beta \end{pmatrix}^T$
- $\star$ $A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{pmatrix}$ $\quad\star$ $A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$
- $\star$ $R(g)^{\otimes k} = R(g) \otimes \dots \otimes R(g)$ $\quad\star$ $\bigoplus_k R(g) = (R \bigoplus \dots \bigoplus R)(g)$
- $\star$ $f(\hat{A} \otimes \hat{B})\left|a\right\rangle\left|\phi\right\rangle = \left|a\right\rangle \otimes f(a\hat{B})\left|\phi\right\rangle$

Different basis

Trigonometry

- $\star$ $\cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$ $\quad\star$ $\sin(2a) = 2\sin a\cos a$
- $\star$ $\sin(a+b) = \sin(a)\cos(b) + \cos(a)\sin(b)$ $\quad\star$ $\cos(2a) = \cos^2 a - \sin^2 a$
- $\star$ $2\sin(a)\sin(b) = \cos(a-b) - \cos(a+b)$ $\quad\star$ $\sin(a/2) = \pm\sqrt{(1-\cos(a))/2}$
- $\star$ $2\cos(a)\cos(b) = \cos(a+b) + \cos(a-b)$ $\quad\star$ $\cos(a/2) = \pm\sqrt{(1+\cos(a))/2}$
- $\star$ $2\cos(a)\sin(b) = \sin(a+b) - \sin(a-b)$ $\quad\star$ $\sin^2 a = (1-\cos 2a)/2$
- $\star$ $\cos(a) + \cos(b) = 2\cos((a+b)/2)\cos((a-b)/2)$ $\quad\star$ $\cos^2 a = (1+\cos 2a)/2$
- $\star$ $\sin(a) + \sin(b) = 2\sin((a+b)/2)\cos((a-b)/2)$
- $\star$ $\cos(a) - \cos(b) = -2\sin((a+b/2)\sin((a-b/2)$

ciao

Group Theory

- **Group**: Set G equipped with operation $*$ such that
  - G closed under $*$, i.e. if $a, b \in G$ then $a * b \in G$
  - Associative: $\forall a, b, c \in G$ one has $(a * b) * c = a * (b * c)$
  - Has identity, i.e an element e such that $e * a = a \forall a \in G$
  - Has inverse, i.e. $\forall a \in G$ it exists $b \in G$ such that $b * a = a * b = e$. $(b = a^{-1})$
- Any unitary that leaves a property invariant forms a grop with * matrix multiplic.
- **Finite group**: A group that contains a finite number of elements (the group *order*).
- Order 1 group (the only one, trivial group):

$*$	e
e	e

- Order 2: parity group

$*$	e	a
e	e	a
a	a	e

- The unique order 3 group is the cyclic $\mathbb{Z}_3$ group

$*$	e	a	b
e	e	a	b
a	a	b	e
b	b	e	a

- Order 4 has cyclic and symmetry of a rectangle
- Order 6 has cyclic group $\mathbb{Z}_6$ and the C3v group (on the right)

$*$	e	a	a^2	b	c	d
e	e	a	a^2	b	c	d
a	a	a^2	e	c	d	b
a^2	a^2	e	a	d	b	c
b	b	d	c	e	a^2	a
c	c	b	d	a	e	a^2
d	d	c	b	a^2	a	e

- The general cyclic group $\mathbb{Z}_n$ $(a^n = 1)$ is

$*$	e	a^1	a^2	$\dots$	a^{n-1}
$*$	e	a^1	a^2	$\dots$	a^{n-1}
a^1	a^1	a^2	a^3	$\dots$	e
a^2	a^2	a^3	a^4	$\dots$	a^1
$\vdots$					
a^{n-1}	a^{n-1}	e	a^1	$\dots$	a^{n-2}

- Symmetric permutation group S_n (all possible permutations of n objects)
  e.g. $S_3 = \{I, \text{SWAP}_{12}, \text{SWAP}_{13}, \text{SWAP}_{23}, \text{CYCLE}_{123}, \text{CYCLE}_{321}\}$ isomorphic to C3v
- **Lie group**: a continous group that depends analytically on some continous parameters λ. Examples: Real d-dimensional rotations $SO(d)$, the orthogonal group $O(d)$, the unitary group $U(d)$, the special unitary group $SU(d)$
- **Abelian group**: $a * b = b * a \ \forall a, b \in G$
- **Subgroup**: a subset H of the group G is a subgroup of G if and only if it is nonempty and itself forms a group. If it is neither the identity or G itself then it is a *proper* subgroup. Lagrange Theorem: the order of H divides the order og G. Thus if the order of a group is prime there is only one possible group
- **Group homomorphism**: an application from $(G, *)$ to $(G, **)$ such that $\forall x, y \in G \quad f(x * y) = f(x) ** f(y)$. An isomorphism sets a one-to-one correspondance.

Representations

- A representation R of a group G on a vector space V is a group homomorphism from G to a set of matrices that act on a vector space V. The dimension of a representation R is defined to be the dimension of the vector state V, i.e., $\dim(R) = \dim(V)$.
- All groups allow trivial representation $\forall g \in G,\ R(g) = \mathbb{I}$
- The *regular* representation is obtained by reordering the Caylei table so that only e fills the diagonal, then to every element assign the matrix obtained by replacing 1 in the positions where the element is in the table and 0 everywhere else.
- **Equivalent** reps are related by a similarity transformation $R'(g) = SR(g)S^{-1}$
- If R_1 and R_2 are two representations for G, then $R_1(g) \otimes R_2(g)$ is also a rep
- The direct sum $R_1 \oplus R_2$ is a rep of G acting on $V_1 \oplus V_2$
  $(R_1 \oplus R_2)(g) = \begin{pmatrix} R_1(g) & 0 \\ 0 & R_2(g) \end{pmatrix}$
- Let U_g be a rep of G and H an Hermitian operator such that $[U_g, H] = 0 \ \forall g$. Then H and U_g are simultaneously block diagonalised (in the same basis).
  E.g. $U_g \otimes U_g$, the tensor product representation of $SU(2)$, commutes with SWAP and has therefore a symmetric $(d = 3)$ and an asymmetric $(d = 1)$ invariant subspace.
- **Reducible representation**: a rep $R(g)$ of G over a vector space V is reducible if there exists an invariant subspace, i.e. if there exists a non-trivial subspace W of V such that for all $|w\rangle \in W$ we have $R(g)|w\rangle \in W$ for any g.
- **Completely reducible rep**: if it splits into a direct sum of irreducible reps
- **Schur's 1st lemma**: Let $R_1(g)$ and $R_(g)$ be two non-equivalent irreducible reps of G, acting on vector spaces V_1, V_2. If there is a matrix A such that
  $AR_1(g) = R_2(g)A \ \forall g \quad$ then $A = 0$.
  Equivalently, if you can find A different than 0 that satisfies the eq., then the reps are reducible.
- **Schur's 2nd lemma**: Let R be an irreducible rep of G. If $AR(g) = R(g)A \ \forall g \in G$ then $A = \lambda\mathbb{I}$ for some $\lambda \in \mathbb{C}$
- **Burnside's lemma**: for a finite group of order h there are only a finite number n of irreducible representations $a = 1 \dots n$ of dimension l_a and $\sum_{a=1}^n l_a^2 = h$
- In a group G, two elements g and g' are **equivalent** if there exists another element f such that $g' = f^{-1}gf$. This divides G in conjugacy classes.
- For a finite group, the number of (non-equiv.) irreps is equal to the number of conjugacy classes
- All irreducible reps of Abelian groups are scalar $(d = 1)$. An Abelian group of order n has n conjugacy classes and thus n irreducible reps.
- **Grand Orthogonality Theorem**: Let R_a and R_b be two non-equiv. unitary irreducible reps of a finite group G of order N. Let n_a and n_b be the dimensions of the vector space for R_a and R_b. Then
  $\sum_{g \in G} \frac{n_a}{N} \left[R_a(g)^\dagger\right]_{jk} [R_b(g)]_{lm} = \delta_{ab}\delta_{jm}\delta_{lk}$
  - if $a \neq b$ then $\sum_{g \in G} \left[R_a(g)^\dagger\right]_{jk} [R_b(g)]_{lm} = 0$ for all i, j, k, l
  - if $a = b$ then $\sum_{g \in G} \left[R_a(g)^\dagger\right]_{jk} [R_a(g)]_{lm} = 0$ if $j \neq m$ and/or $l \neq k$
  - if $a = b$ and $j = m$ and $l = k$ then $\sum_{g \in G} \left[R_a(g)^\dagger\right]_{jk} [R_a(g)]_{jk} = \dfrac{N}{n_a}$
- A finite group can only have a finite number of inequivalent irreducible representations. Specifically, the **maximum number of possible irreps** is given by the order of the group. Proof: irreps give us 'vectors of matrices' in a vector space of dimension $|G|$ and the theorem says they must be orthogonal. But there are at most $|G|$ orthogonal vectors in a vector space of dimension $|G|$
- **Group averaging**: if d is the dim. of vector space of rep and U_g is an irreducible representation then $\langle X \rangle_G = \frac{1}{N} \sum_g U_g X U_g^\dagger = \frac{1}{d} \text{Tr}[X]\mathbb{I}$
- Proof: $\frac{1}{N} \sum_g U_g X U_g^\dagger = \frac{1}{N} \sum_g \left(\sum_{l,m} [U_g]_{lm} |l\rangle\langle m|\right) X \left(\sum_{k,j} [U_g^\dagger]_{kj} |k\rangle\langle j|\right)$
  $= \frac{1}{N} \sum_g \sum_{lmkj} [U_g]_{lm} X_{mk} [U^\dagger]_{kj} |l\rangle\langle j|$ then apply orthogonality
  $= \frac{1}{n_a} \sum_{lmkj} \delta_{lj}\delta_{mk} X_{mk} |l\rangle\langle j|$
- $\langle X \rangle_G = \int_G d\mu(g) U_x(g) X U_x(g)^\dagger = \frac{1}{d} \text{Tr}[X]\mathbb{I}$ for continous groups
- For reducible representations U_g we have
  $\langle X \rangle_G = \frac{1}{N} \sum_g U_g X U_g^\dagger = \sum_x \dfrac{\text{Tr}[\Pi_x X]}{d_x} \Pi_x = \bigoplus_x \dfrac{\text{Tr}[\Pi_x X]}{d_x} \mathbb{I}_x$
- In a representation R, all elements which are in the same conjugacy class have the same trace. Proof: $\text{Tr}(R(u^{-1}yu)) = \text{Tr}(R(u)R(u^{-1})R(y)) = \text{Tr}R(y)$
- **Petit Orthogonality Theorem**: Let R_a and R_b be two non-equiv. unitary irreducible reps of a finite group of order N, then $\sum_{g \in G} \chi_a^*(g)\chi_b(g) = N\delta_{a,b}$
  where $\chi_R(g) = \text{Tr}[R(g)]$, or equiv. $\sum_{\mu=1}^{N_c} \eta_\mu \chi_a^*(g)\chi_b(g) = N\delta_{a,b}$ with η_μ the nb of elements in class μ and N_c total nb of conjugacy classes
- The set of all traces $\{\chi_R(g)\}$ is the **character** of representation R. Two irreps are equivalent iff they have the same character. Proof by contradiction with Petit.
- Trace of all reps within a conj. class are the same $\rightarrow \chi_R(C_\mu) = \sum_a b_a \chi_a(C_\mu)$
- Assuming a decomposition in irreps $R(g) = \bigoplus_{a,x} R_{a,x}(g)$ for $x = 1 \dots b_a$, the degeneracy of conjugacy class a is $b_a = \frac{1}{N} \sum_\mu \eta_\mu \chi_a^*(C_\mu)\chi_R(C_\mu)$ NOT CLEAR
- A necessary and sufficient condition for a representation R to be an irrep is that $\sum_{\mu=1}^{N_c} \eta_\mu |\chi(C_\mu)|^2 = N$. Proof: decompose trace and use Petit.

Lie Algebras

- Rotation through infinitesimal angle $R(\theta) = \mathbb{I} + A$ and as $R^T R = \mathbb{I}$ we must have $A^T = -A$

Irreducible representations of C3v

⋆ Trivial ⋆ 2D irrep

$$R(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} R(c_+) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} R(c_+) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

$$R(\sigma) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} R(\sigma') = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} R(\sigma'') = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

⋆ $R(e) = 1, R(c_+) = 1, R(c_-) = 1, R(\sigma) = -1, R(\sigma') = -1, R(\sigma'') = -1$