

Hamiltonians (Lecture 25)

Mathematical model of Hamiltonians

selfadjoint matrix $H = H^\dagger$.

basic properties

- eigenvalues are real numbers
- eigenvectors for different eigenvalues are orthogonal.

$$\because H|\varphi\rangle = \lambda|\varphi\rangle, H|\psi\rangle = \mu|\psi\rangle$$

$$\Rightarrow \lambda^* \langle \varphi | \psi \rangle = \langle \varphi | H | \psi \rangle = \mu \langle \varphi | \psi \rangle, \lambda^* = \mu$$

physical interpretation: eigenvalues are (relative) energy levels of the system.

Schrödinger's equation: the system evolves according to the differential equation

$$i \frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

(here we model time by a continuous parameter t instead of discrete "steps")

Prop. Solution when H is independent of t is

$$|\psi(t)\rangle = e^{-itH} |\psi(0)\rangle.$$

Proof: we have $\frac{d}{dt} e^{tA} = A e^{tA}$ from

$$e^{tA} = \sum_{k=0}^{\infty} \frac{1}{k!} (tA)^k = I_n + tA + \frac{t^2}{2} A^2 + \dots$$

$$\text{So } \frac{d}{dt} e^{-itH} |\psi(0)\rangle = -iH e^{-itH} |\psi(0)\rangle$$

physical principle : states with lower energy are more stable ; particles can "emit" energy and transition to another state with lower energy spontaneously

→ we can try to cook up a Hamiltonian so that a solution to the given problem is encoded in the state with lowest energy (ground state)

• Encoding the 3-SAT problem

3-SAT problem ; setting : variables $x_0, \dots, x_{n-1}$ representing TRUE, FALSE (1, 0)

Boolean function $\varphi(x_0, \dots, x_{n-1})$ of the form

$$\varphi = C_0 \wedge \dots \wedge C_{m-1} = \text{AND}(C_0, \dots, C_{m-1})$$

s.t. each C_i is of the form $t_0 \vee t_1 \vee t_2 = \text{OR}(t_0, \dots)$

$$t_i = x_j \text{ or } \neg x_j (= \text{NOT}(x_j))$$

task : determine if $\varphi = \text{TRUE}$ has a solution

Ex. $\varphi = x_0 \wedge \neg x_1$ has sol. $x_0 = \text{TRUE}, x_1 = \text{FALSE}$

$\varphi = x_0 \wedge \neg x_0$ does not have a solution

Quantum scheme.

state space $(\mathbb{C}^2)^{\otimes n}$

Hamiltonian for $\varphi = C_0 \wedge \dots \wedge C_{m-1}$: $H = H_0 + \dots + H_{m-1}$

H_i acts on a -th, b -th and c -th qubit where

$$C_i = (x_a \text{ or } \neg x_a) \vee (x_b \text{ or } \neg x_b) \vee (x_c \text{ or } \neg x_c)$$

$$H_i = \sum (|z_0 z_1 z_2\rangle \langle z_0 z_1 z_2|) \text{ at } a, b, c$$

$x_a = z_0, x_b = z_1, x_c = z_2$ does not satisfy C_i

Idea: impose "penalty" energy for the cases that violate c_i
 (we must satisfy all c_i to satisfy φ)

So the eigenvectors of H are $(|z\rangle)_{z \in \{0,1\}^n}$
 eigenvalue for $|z\rangle$: $\#\{i : z \text{ violates } c_i\}$
 i.e. z s.t. $H|z\rangle = 0$ represents a solution to $\varphi = \text{TRUE}$.

- Trotterization (Trotter product formula, ^{lie-}T-Kato th'm)
 We often need to consider Hamiltonians of the form $H = \sum_{0 \leq i < m} H_i$ (many terms) and compute / estimate e^{itH}

Th'm $\exp(A+B) = \lim_{n \rightarrow \infty} (\exp(A/n) \exp(B/n))^n$

One (formal) argument: use the Baker-Campbell

- Hausdorff formula $e^X e^Y \sim \exp(X+Y + \frac{1}{2}[X,Y] + \dots)$

to $X = \frac{A}{n}$, $Y = \frac{B}{n}$, then $\exp(Z)^n = \exp(nZ)$

$\leadsto$ higher order terms $\frac{1}{2}[X,Y]$, $\frac{1}{12}[X,[X,Y]]$, etc.

give denominators n^k $k \geq 2$ that beat $\exp(Z)^n$

Cor. similar for $\exp(A_0 + \dots + A_{m-1})$

