Bad Honnef 1

Wednesday, 10 August 2022 08:59

# BAD HONNEF LECTURE 1

## "QUANTUM ALGORITHMIC TECHNIQUES"

PROBLEM: "imaginary time evolution"

First: real time evolution

~ Schrödinger's equation

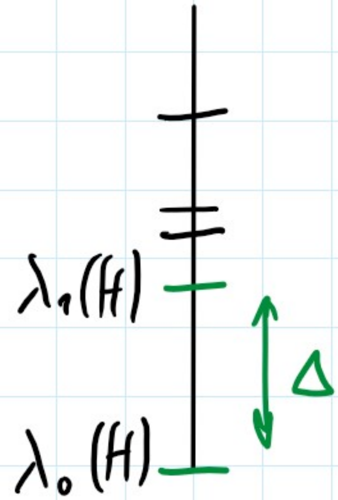
$$\partial_t |\psi_t\rangle = -i H |\psi_t\rangle, \; t \in \mathbb{R}$$

$$|\psi_0\rangle \longmapsto |\psi_t\rangle = e^{-iHt} |\psi_0\rangle$$

~ quantum dynamics

However, often interested in

**GROUND STATES**




? prepare ground state of Hamiltonian $H \geq 0$

↓

‖ imaginary time evolution

$$t \rightsquigarrow -it$$

$$e^{-iHt} \rightsquigarrow e^{-tH} = \sum e^{-t\lambda_j(H)} |v_j\rangle\langle v_j|$$

$$\approx |v_0\rangle\langle v_0| \text{ for } t \gg 1.$$

$$\simeq |v_0\rangle\langle v_0| \text{ for } t \gg \frac{1}{\Delta}.$$

So, given $|\psi_0\rangle$ with $\langle\psi_0|v_0\rangle \neq 0$,

$$e^{-tH}|\psi_0\rangle \to |v_0\rangle\langle v_0|\psi_0\rangle \sim |v_0\rangle.$$

? How to implement $e^{-tH}$ ?

↓

real time evolution

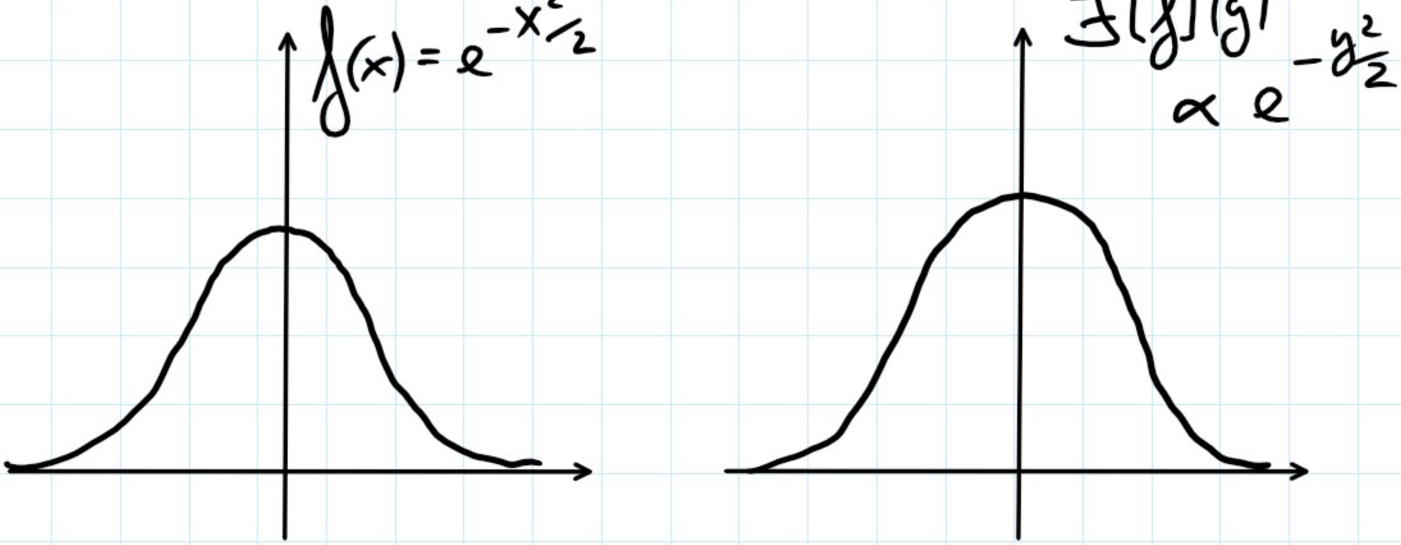
+

"linear combination of unitaries"

↳ uses elementary Fourier analysis

• uses elementary Fourier analysis

(or "Bose-Hubbard transform"):




i.e., $$e^{-\frac{x^2}{2}} = \frac{1}{\sqrt{2\pi}} \int dy \, e^{-y^2/2} \, e^{-ixy}$$

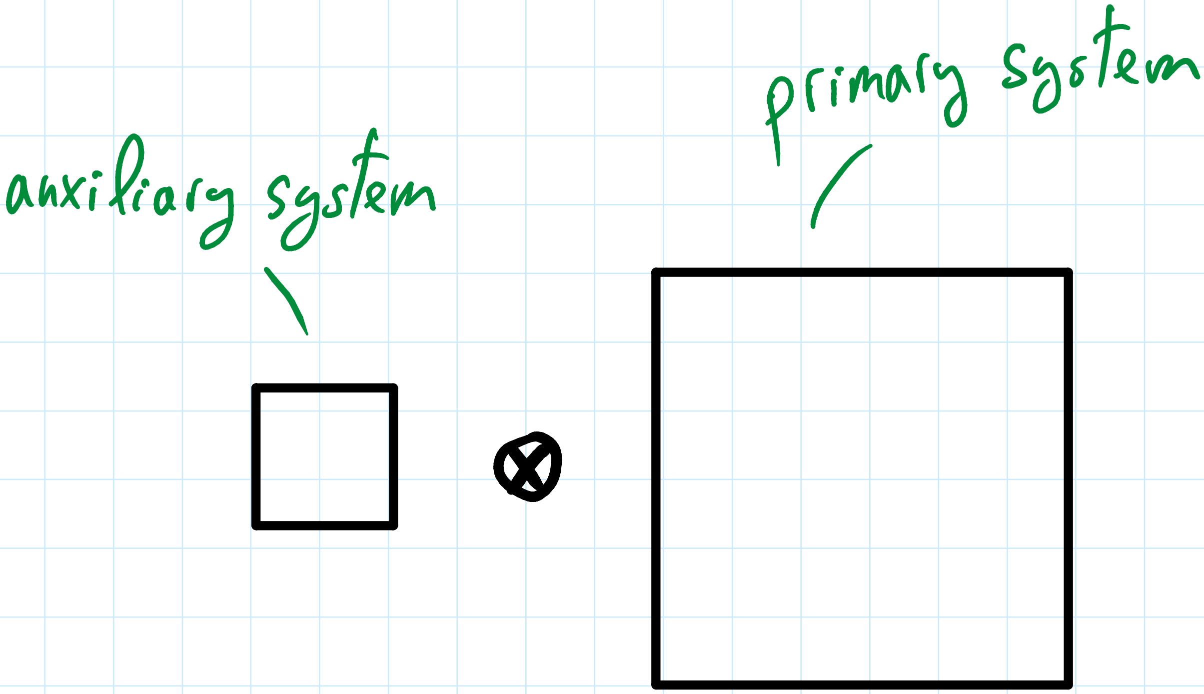
$x = \sqrt{2t}\,H$

$$e^{-tH^2} = \frac{1}{\sqrt{2\pi}} \int dy \, e^{-y^2/2} \, e^{-iy\sqrt{2t}\,H}$$

(imaginary, nonunitary) (real, unitary)

linear combination

* LINEAR COMBINATION OF UNITARIES:




state $\quad |N\rangle \otimes |\psi\rangle$

$$|N\rangle = \frac{1}{(2\pi)^{1/4}} \int dy\, e^{-y^2/4} |y\rangle = \text{"Gaussian state"}$$

Hamiltonian $\quad H' = \hat{y} \otimes H$

$$\hat{y} \sim \int dy\, y\, |y\rangle\langle y| = \text{"position operator"}$$

$$\int dy\, y\, |y\rangle\langle y| = \text{"position operator"}$$

$$\text{s.t. } e^{-itH'}\left(|y\rangle \otimes |\psi\rangle\right)$$

$$= |y\rangle \otimes \left(e^{-ityH}|\psi\rangle\right)$$

$\hookrightarrow$ $H'$ = "controlled"-$H$

<u>LEMMA:</u>

$$\left(|N\rangle\langle N| \otimes \mathbb{1}\right) e^{-i\sqrt{2t}H'}\left(|N\rangle \otimes |\psi\rangle\right)$$

$$= |N\rangle \otimes \left(e^{-tH^2}|\psi\rangle\right).$$

postselection after measurement $\{|N\rangle, |N^\perp\rangle, \ldots\}$, success probability $\| e^{-tH^2}|\psi\rangle \|_2^2$

Proof:

$$\frac{1}{(2\pi)^{\frac{1}{4}}}\int dy\, e^{-\frac{y^2}{4}}|\psi_0\rangle|y\rangle$$

$$(|N\rangle\langle N|\otimes \mathbb{1})\, e^{-i\sqrt{2t}\,H'}(|N\rangle\otimes|\psi\rangle)$$

$$= (|N\rangle\langle N|\otimes \mathbb{1})\,\frac{1}{(2\pi)^{\frac{1}{4}}}\int dy\, e^{-\frac{y^2}{4}}\, e^{-iy\sqrt{2t}\,H}\,|y\rangle|\psi\rangle$$

$$= |N\rangle\otimes\underbrace{\left(\frac{1}{\sqrt{2\pi}}\int dy\, e^{-\frac{y^2}{2}}\, e^{-iy\sqrt{2t}\,H}\,|\psi_0\rangle\right)}_{e^{-tH^2}|\psi_0\rangle}$$

$\square$

More general (and discrete):

if $\begin{cases} cU = \sum_t |t\rangle\langle t|\otimes U^t \\ |\ell\rangle = \sum \sqrt{\ell(t)}\,|t\rangle \end{cases}$

$$0 \quad \left\{ |f\rangle = \sum_{t} \sqrt{f(t)}\,|t\rangle \right.$$

then
$$\boxed{\begin{aligned}&(|f\rangle\langle f| \otimes \mathbb{1})\, cU\, |f\rangle|\psi\rangle \\ &\qquad = |f\rangle \Big( \sum f(t)\, U^{t} |\psi_0\rangle \Big).\end{aligned}}$$

$= \text{LCU}.$

(2ND) PROBLEM:

HAMILTONIAN SIMULATION

! quantum computers expected to be

DIGITAL

(discrete time, space)

gates qubits

(time)

? integrate continuous Schrödinger equation ?

$$|\psi_0\rangle \longrightarrow |\psi_t\rangle = e^{-iHt}|\psi_0\rangle$$

$\downarrow$

LCU ?

$$e^{-iHt} = \sum_{k=0}^{+\infty} \frac{(-it)^k}{k!} H^k$$

discrete,

$k=0$ $k$:

↳ discrete,
but nonunitary!

→ use "**BLOCK ENCODING**" of $H$,

($\|H\|_2 < 1$)

unitary $U = \begin{bmatrix} H & \cdot \\ \cdot & \cdot \end{bmatrix}$

$= |0\rangle\langle 0| \otimes H + \dots$

s.t. $(|0\rangle\langle 0| \otimes \mathbb{1})\, U\, |\psi\rangle|0\rangle$

$= |0\rangle\left(H|\psi\rangle\right)$

postselection,
success probability
$\|H|\psi\rangle\|_2^2$

$\| H|\psi\rangle \|_2$

$\rightarrow$ implements $H$!
What about $H^k$?

Let $U = \begin{bmatrix} H & R \\ L & D \end{bmatrix}$,

assume $U$ is "reflection":

$$U^2 = \mathbb{1} = \begin{bmatrix} \underbrace{H^2 + RL}_{=\mathbb{1}} & \underbrace{HR + RD}_{=0} \\ \underbrace{LH + DL}_{=0} & \underbrace{LR + D^2}_{=\mathbb{1}} \end{bmatrix}$$

Then

$$U \begin{bmatrix} \mathbb{1} & \\ & -\mathbb{1} \end{bmatrix} U = \begin{bmatrix} H & R \\ L & D \end{bmatrix} \begin{bmatrix} H & R \\ -L & -D \end{bmatrix}$$

$$U\begin{bmatrix} \mathbb{1} & \\ & -\mathbb{1}\end{bmatrix}U = \begin{bmatrix} H & R \\ L & D \end{bmatrix}\begin{bmatrix} H & R \\ -L & -D \end{bmatrix}$$

$$= \begin{bmatrix} H^2 - RL & HR - RD \\ LH - DL & LR - D^2 \end{bmatrix}$$

$$\overset{RL = \mathbb{1} - H^2}{=} \begin{bmatrix} 2H^2 - \mathbb{1} & \cdot \\ \cdot & \cdot \end{bmatrix}$$

So $\mathbb{1} = \begin{bmatrix} \mathbb{1} & \cdot \\ \cdot & \cdot \end{bmatrix}$, $\quad U = \begin{bmatrix} H & \cdot \\ \cdot & \cdot \end{bmatrix}$,

$$\begin{bmatrix} \mathbb{1} & \\ & -\mathbb{1}\end{bmatrix} U \begin{bmatrix} \mathbb{1} & \\ & -\mathbb{1}\end{bmatrix} U = \begin{bmatrix} 2H^2 - \mathbb{1} & \cdot \\ \cdot & \cdot \end{bmatrix}$$

<u>CLAIM:</u> (exercise?)

$$\left(\begin{bmatrix} \mathbb{1} & \\ & -\mathbb{1}\end{bmatrix} U\right)^k = \begin{bmatrix} T_k(H) & \cdot \\ \cdot & \cdot \end{bmatrix}$$

k-th Chebyshev poly
= basis for polynomials

Now, rewrite

$$\begin{bmatrix} e^{-itH} & \cdot \\ \cdot & \cdot \end{bmatrix} = \begin{bmatrix} \sum \alpha_k T_k(H) & \cdot \\ \cdot & \cdot \end{bmatrix}$$

$$= \sum \alpha_k \left( \begin{bmatrix} \mathbb{1} & \\ & -\mathbb{1} \end{bmatrix} U \right)^k$$

= LCU.

? How to obtain block encoding

$$U = \begin{bmatrix} H & \cdot \\ \cdot & \cdot \end{bmatrix}$$

$\longrightarrow$ exercise.