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

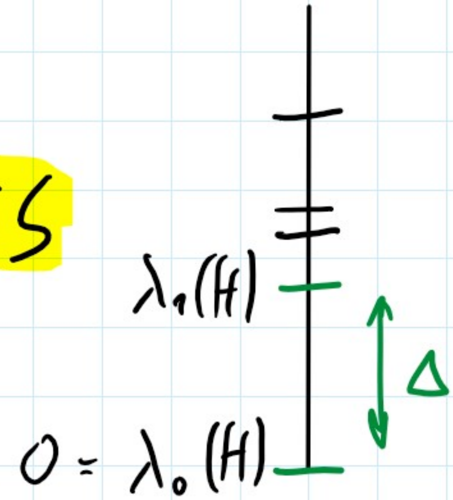
$$\partial_t |\psi_t\rangle = -i H |\psi_t\rangle, \; t \in \mathbb{R}$$

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

~ quantum dynamics

However, often interested in

GROUND STATES



? prepare ground state of Hamiltonian H

$\downarrow$

‖ imaginary time evolution

$$t \rightsquigarrow -it \qquad H = \sum \lambda_j(H)\, |v_j\rangle\langle v_j|$$

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

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

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

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

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

? How to implement e^{-tH} ?

↓

real time evolution

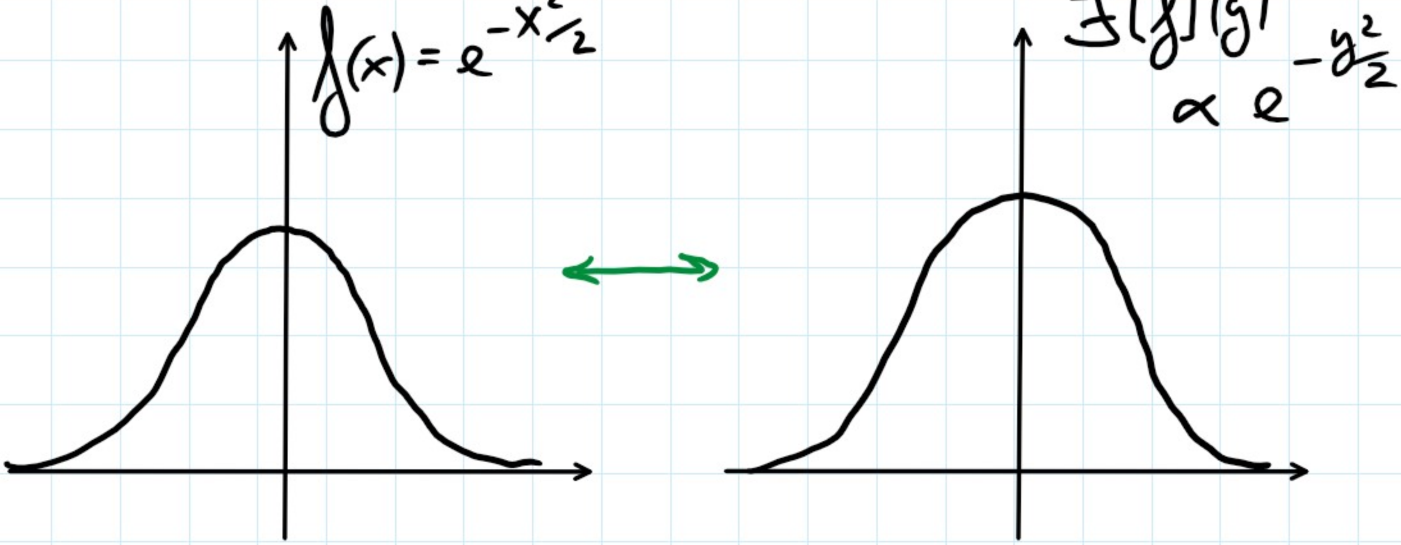
+

"linear combination of unitaries"

↳ uses elementary Fourier analysis

• uses elementary Fourier analysis

(or "Hubbard-Stratonovich transform"):



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

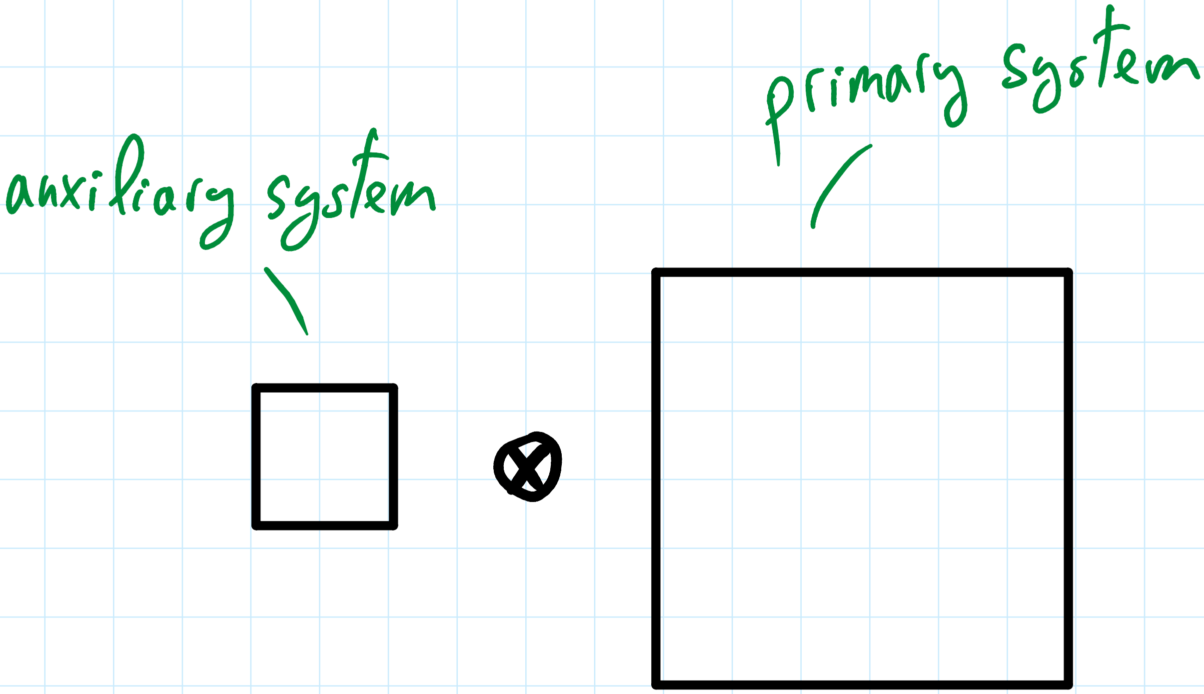
$x = \sqrt{2t}\, H$

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

(imaginary, nonunitary) (real, unitary)

linear combination

* LINEAR COMBINATION OF UNITARIES:



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

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

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

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

$\int dy\, y\, |y\rangle\langle y|$ = "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 $\{|N\rangle, |N^\perp\rangle, \dots\}$, success probability $\| e^{-tH^2}|\psi\rangle\|_2^2$

Proof:

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

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

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

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

$\square$

More general (and discrete):

if
$$\begin{cases} cU = \sum_t |t\rangle\langle t|\otimes U^t \\ |\ell\rangle = \sum_t \sqrt{\ell(t)}\,|t\rangle \qquad \left(\ell(t)\geq 0,\ \sum \ell(t)=1\right) \end{cases}$$

$\cdot\, 0 \quad \left\{ |f\rangle = \sum_t \sqrt{f(t)}\, |t\rangle \right.$ $\quad (f(t) \geq 0,\ \sum f(t) = 1)$

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

$= \mathrm{LCU}.$

(2ND) PROBLEM:

HAMILTONIAN SIMULATION

! quantum computers expected to be

DIGITAL

(discrete time, space)

gates qubits

? integrate continuous (time) 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

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

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

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

$RL = \mathbb{1}-H^2$

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

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

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

$$= \sum \alpha_k \Big(\underbrace{\begin{bmatrix} \mathbb{1} & \\ & -\mathbb{1} \end{bmatrix} U}_{\text{"easy" to implement}} \Big)^k$$

$= LCU.$

? How to obtain block encoding

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

$\longrightarrow$ exercise.