
# Quantum Computation and Simulation with NISQ devices

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# (g) Loschmidt Amplitude

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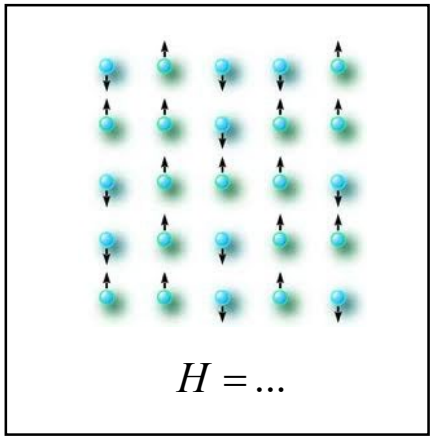
Easy to simulate

$$\langle \Psi_1 | e^{-iHt} | \Psi_0 \rangle$$

Easy to meaure

Easy to prepare



# (g) Loschmidt Amplitude

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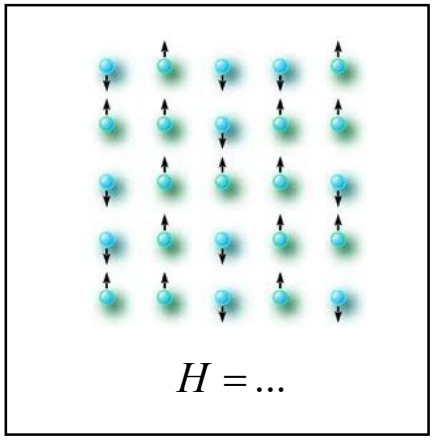
$$\langle \Psi_1 | e^{-iHt} | \Psi_0 \rangle$$




- Example:

$|\Psi_0\rangle = |p\rangle$ product state

$|\Psi_1\rangle = |p\rangle$

$\langle p | e^{-iHt} | p \rangle$

return amplitude

- Example:

$|\Psi_0\rangle = U|p\rangle$

$|\Psi_1\rangle = U|p\rangle$

$U$ is a low depth circuit

$\langle p | U^\dagger e^{-iHt} U | p \rangle$

return amplitude

- Example:

$|\Psi_0\rangle = U|p\rangle$

$|\Psi_1\rangle = \sigma_x^1 e^{-iHt'} U|p\rangle$

$\langle \Psi_0 | U^\dagger e^{-iHt'} \sigma_x^1 e^{-iHt} U | \Psi_0 \rangle$

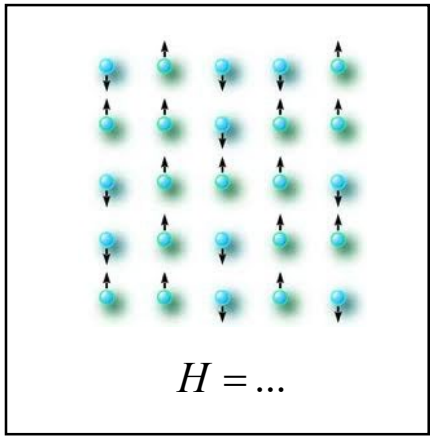
# (g) Loschmidt Amplitude



$$\langle \Psi_1 | e^{-iHt} | \Psi_0 \rangle = r(t)\, e^{i\phi(t)}$$

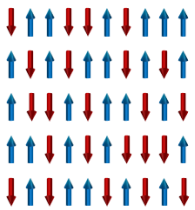
$$r(t) = \left| \langle \Psi_1 | e^{-iHt} | \Psi_0 \rangle \right|$$

- $r(t)$ is easy in practice
- $\phi(t)$ is difficult in practice



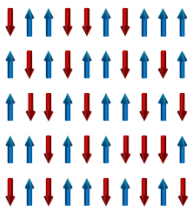

- Example: $\langle p | e^{-iHt} | p \rangle$

Prepare state p:



Evolve with $H$

Measure



# OUTLINE

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- Quantum algorithm for finite temperature / energy

  Sirui Lu, Mari Carmen Bañuls, JIC, PRXQuantum (2021)

  - Microcanonical
  - Canonical: Hybrid Quantum Monte Carlo + Quantum simulation

- Measuring the generalized Loschmidt amplitude

  - Review: Hadamard test

    Cleve, Ekert, Macchiavello, Mosca PRSL (1998)
  - Sequential

    Sirui Lu, Mari Carmen Bañuls, JIC, PRXQuantum (2021)
  - Complex analysis

    Yilun Yang, Arthur Christianen, Mari Carmen Bañuls, Dominik S. Wild, JIC, arxiv: 2308.10796
  - Comparison

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# QUANTUM SIMULATION:
# Dynamics and Zero Temperature

# Quantum Many-body Problems

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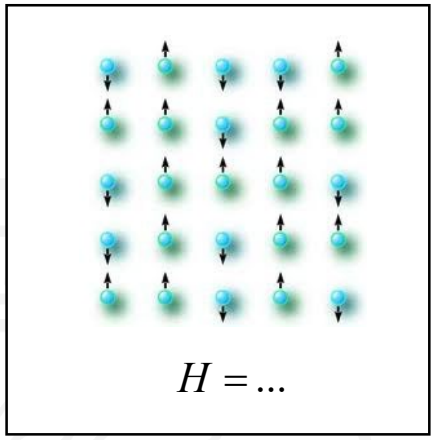



Quantum Simulation:

(NISQ)

- DIGITAL
- ANALOG

# Dynamics

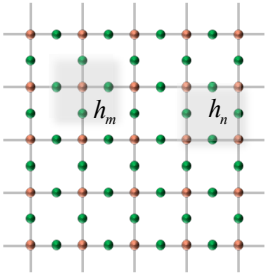


- We want to compute $\langle \Psi | O | \Psi \rangle$

  up to some precision $\varepsilon$

$$|\Psi\rangle = e^{-iHt} |\Psi_0\rangle$$

easy to prepare,
eg, product state




- Prepare the state $\Psi$ and measure $O$:

  Lloyd, Science (1996)

  - Digital Q Computers: Trotterization

$$e^{-iHt} = \left(e^{-iHt/M}\right)^M \approx \left(e^{-ih_1 t/M} \ldots e^{-ih_N t/M}\right)^M$$

- Efficient:

$$\tau \approx \left(N \,||\, h \,||\, t\right)^2 / \varepsilon^2$$

# Ground State (T=0)



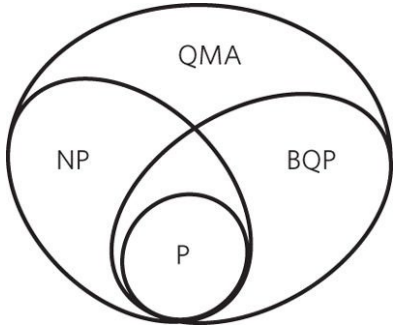
- We want to compute $\langle \Psi_0 | O | \Psi_0 \rangle$ ground state

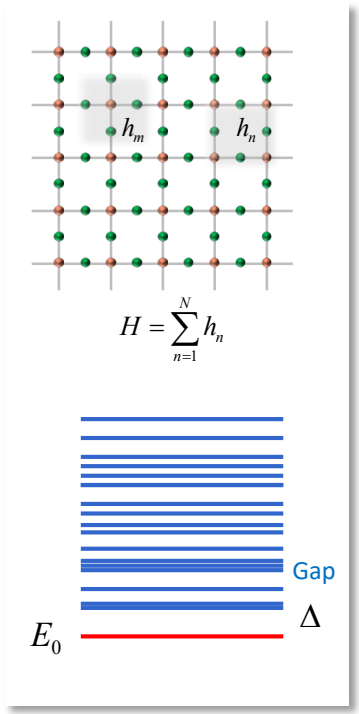
  up to some precision $\varepsilon$

- Difficult:

  Kempe, Kitaev, Regev, SIAM 5, 1070 (2006)

$$\tau \approx 2^{\alpha N}$$



# Ground State (T=0)
## Heuristic Quantum Algorithms

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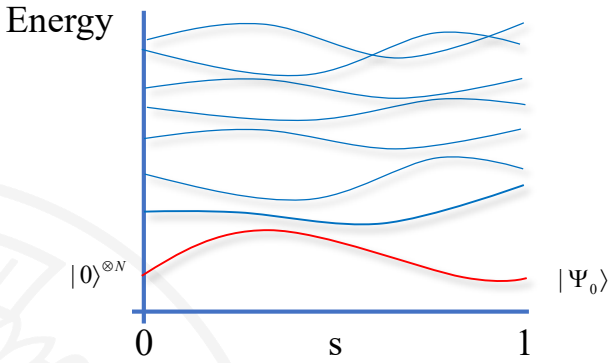
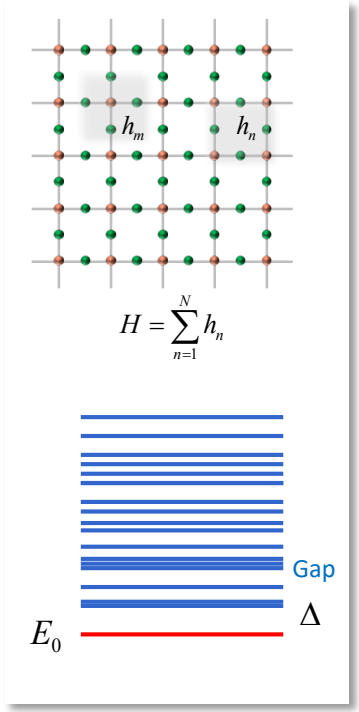
- Adiabatic algorithm

See, eg, Farhi, Goldstone, Gutmann, Sipser, Science (2001)

$$H(0)=\sum_{n=1}^{N}\sigma_z^n \qquad H(s) \qquad H(1)=\sum_{n=1}^{N}h_n$$




„slow“ change of s




- Computational time: $\tau \sim N\delta^{-3}\varepsilon^{-1}$

  Jansen, Ruskai, Seiler, JMP (2007) $\qquad \delta=\min_t \Delta(t)$

- Typical physics problems: $\delta=\text{const}$ or $\delta=1/N^{\alpha}$

For many physics problems, adiabatic is efficient and can be used with analog devices

# Ground State (T=0)
## Heuristic Quantum Algorithms

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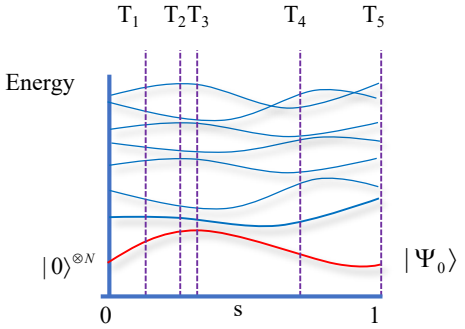
- **Variational algorithms**

  Farhi, Goldstone, Gutmann, arXiv:1411.4028
  A. Peruzzo et al Nat. Comm. (2014)

$$|\Psi(p)\rangle = U_m(p_m)...U_1(p_1)\,|0\rangle^{\otimes N}$$

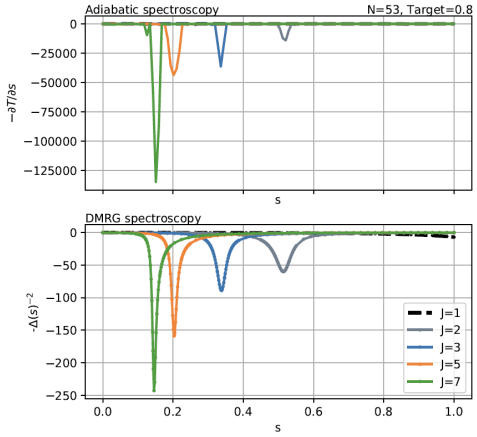
- **Variational-adiabatic algorithm**

  Schiffer, Tura, JIC, PRXq (2021)

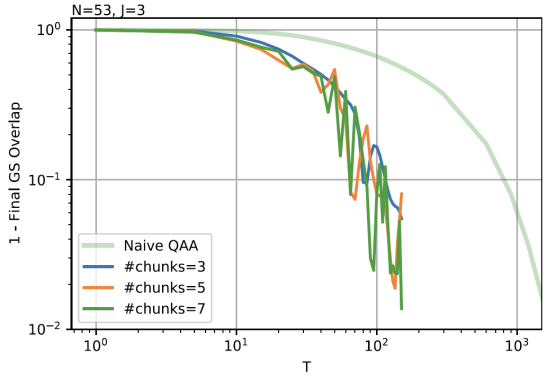



$$H = \sum_{j=1}^{N} J\sigma_i^z\sigma_{i+1}^z + h\sigma_i^x + g\sigma_i^z$$

Adiabatic spectroscopy




VAQA



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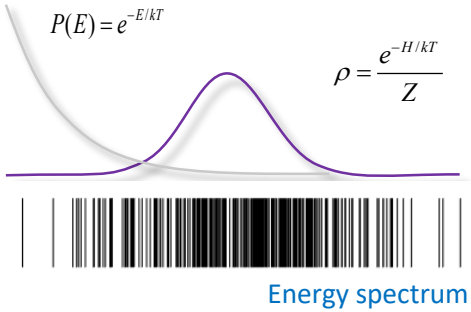
# QUANTUM SIMULATION:
## Finite energies / temperatures

- We want to compute $\langle O \rangle = \mathrm{tr}(\rho O)$

## Microcanonical


## Canonical

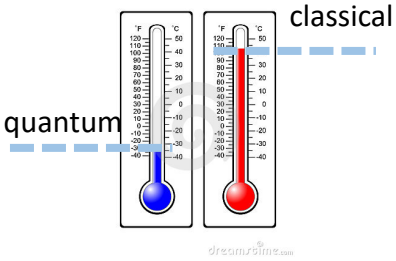



- Exponential, in general:

Kempe, Kitaev, Regev, SIAM 5, 1070 (2006)

Temme et al, Nature 471, 87 (2011)
Mota et al, Nat. Phys. 16, 205 (2020)
Cohn et al, arXiv:1812.03607
and many other….

- There may be an advantage




\+ physics problems

# Density of States

(local Hamiltonians)

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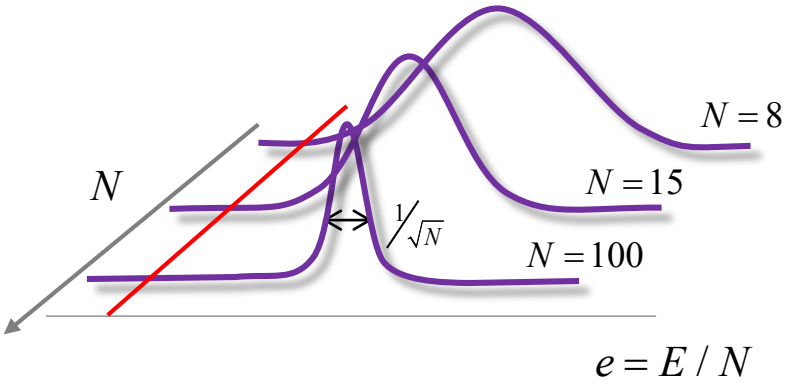


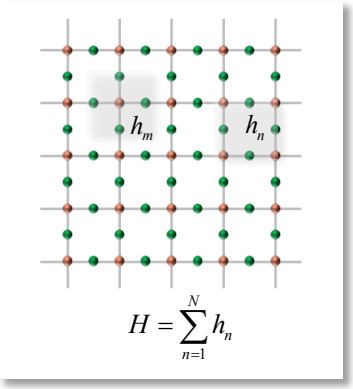


## Strategy 1:

- Prepare state: $e^{-H/2T} \,|\, r\rangle$ — random (product state)
- Sample $r$: $\sum_r \langle r \,|\, e^{-H/2T} O e^{-H/2T} \,|\, r\rangle = \mathrm{tr}(e^{-H/t} O)$

Quantum circuit?

Normalization

# Density of States

(local Hamiltonians)

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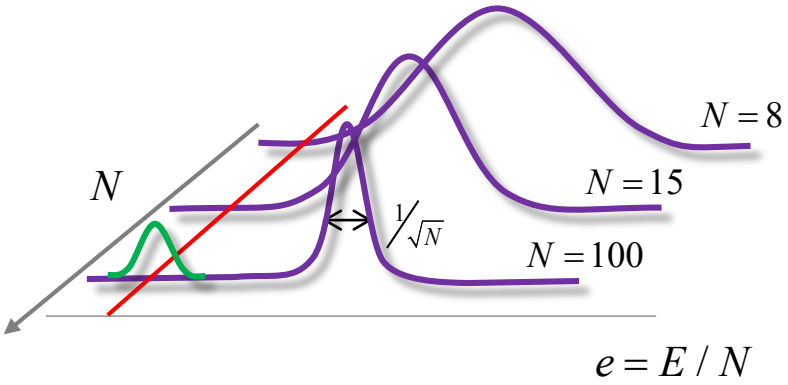


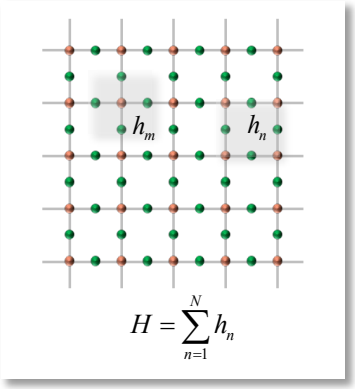


## Strategy 2:

- Prepare a state with the right energy: $|\Psi_0\rangle$
- Measure O: $\langle\Psi_0|O|\Psi_0\rangle$

It will not be an eigenstate

Wrong result

Should have a low variance $\delta = \dfrac{1}{poly(N)}$

# Finite Energy

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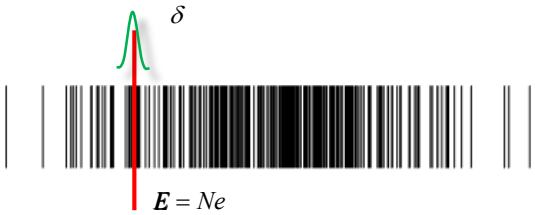
## PROBLEM:




## Formulation (not precise):

- Fix the energy density: $e$
- Take an observable: $O$
- Compute $\langle \Psi | O | \Psi \rangle$

  For some $\Psi$ with $\langle \Psi | H | \Psi \rangle = E$

  $\langle \Psi | (H - E)^2 | \Psi \rangle = \delta$

  with some prescribed precision, $\varepsilon$ and variance $\delta$

  **How does the computational time scale with $N$?**

  and $\varepsilon$ and $\delta$?

*For physically relevant problems, $\delta = 1/\,poly(N)$

Dymarsky, Liu (2019).

# Finite Energy:
## Classical Algorithms

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### Finite energies: Tensor networks (in 1D)

Banuls, Huse, JIC (2020)

- To compute expectation values of a state with a variance $\delta$

$$\tau \sim \min \left[\exp(1/\delta), \exp(N)\right]$$

- To obtain relevant information, we need $\delta \sim 1/\,poly(N)$

⇒ Classical algorithms require exponential time

# Finite Energy:
## Quantum Algorithm

Lu, Banuls, JIC, PRXq (2021)

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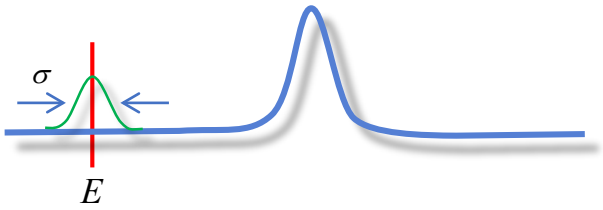
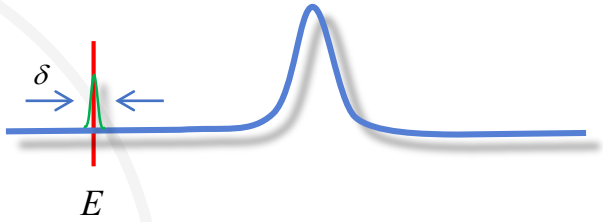
**1.** Take a state that is easy to prepare




restriction

**2.** Apply a spectral filter to decrease the variance




$$|\Psi\rangle = G_\delta(H)\,|p\rangle$$

$$G_\delta(H) = e^{-(H-E)^2/\delta^2} = \sum c_m e^{iEt_m} e^{-iHt_m}$$

**3.** Do not create the state:

Time series: Somma et al (2002)

$$\langle O\rangle = \frac{\langle\Psi|O|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

Use the quantum simulator to obtain quantities needed to compute the observables

$$a(t) = \langle p|e^{-iHt}|p\rangle$$

$$b(t_n,t_m) = \langle p|e^{iHt_n} O e^{-iHt_m}|p\rangle$$

# INITIALIZATION

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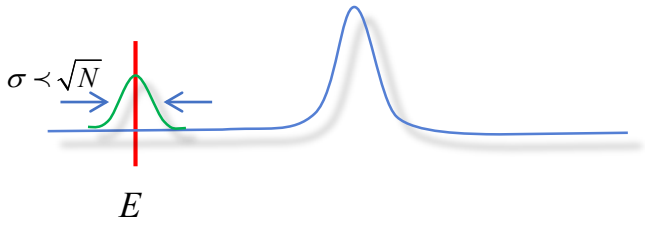
**1.** Take a state that is easy to prepare

- For instance, a product state $|p\rangle = |p_1, p_2, \ldots\rangle$ with $E = \langle p | H | p \rangle$

$$|p\rangle = \sum_n \alpha_n |e_n\rangle$$




- This is always possible for some $e \geq e_{\min}$

➡ restriction

- For lower energies, use adiabatic or other algorithm

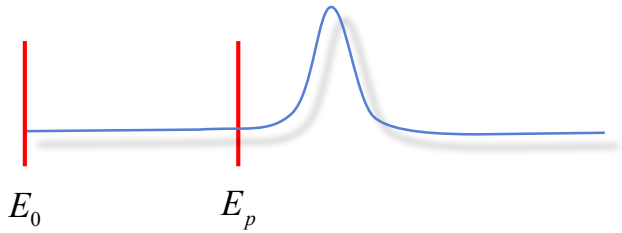
# INITIALIZATION



What is the minimal energy?

- In general, $E_0/9$

  Lieb, Bravy, Anshu, Gosset, König, …




- For nearest-neighbor interactions: $E_0/3$

- By blocking $\log^{1/d}(N)$, we can get $E_0(1-k/\log^{1/d}(N))$ and prepare the state efficiently

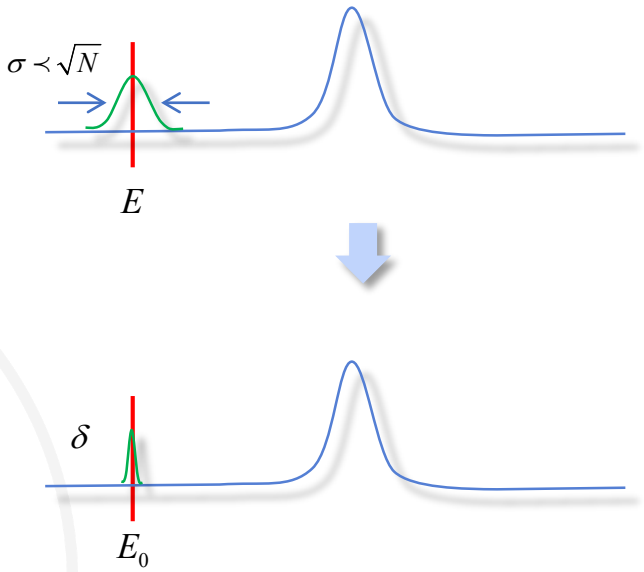
- The energy variance will be too big

# SPECTRAL FILTER



## **2.** Apply a spectral filter to decrease the variance

- Apply an operator: $|\Psi\rangle = G_\delta(H)\,|p\rangle$




Gaussian filter

$$G_\delta(H) = e^{-(H-E)^2/2\delta^2}$$

Fourier transform

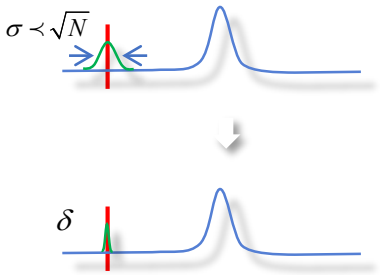
$$G_\delta(H) = \sum c_m e^{iEt_m} e^{-iHt_m}$$

evolution operator

The procedure creates the state $|\Psi\rangle = \sum_m c_m(t) e^{-iHt_m}\,|p\rangle$

# FINITE ENERGY






$$|\Psi\rangle = \sum_{m=1}^{M} c_m(t) e^{-iHt_m} |p\rangle$$

## REMARKS:

- Number of terms: scale as $1/\delta$
- Maximum time:
- The state is not normalized. Probabilistic method
- The state is highly entangled

# MEASUREMENTS



**3.** Do not create the state:

- We want to compute $\langle O \rangle = \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | \Psi \rangle}$ with $| \Psi \rangle = \sum_m c_m(t_m) e^{-iHt_m} | p \rangle$

- Express it explictely: $\langle O \rangle = \ldots$

$$a(t) = \langle p | e^{-iHt} | p \rangle$$

$$b(t_n, t_m) = \langle p | e^{iHt_n} O e^{-iHt_m} | p \rangle$$

**(g) Loschmidt Amplitudes**

- Measure $a(t_n)$ and $b(t_n, t_m)$

compute $\langle O \rangle$ with a classical computer

# Finite Energy:
## Summary

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### PROBLEM:

$\langle e | O | e \rangle$


### EFFICIENCY:

- Time: $\tau = \mathrm{poly}(N, 1/\delta, 1/\varepsilon)$
- Efficient to physical properties: $\delta \prec 1/\ poly(N)$

- Can be used with both analog and NISQ devices

as long as one can measure generalized Loschmidt Amplitudes

# FINITE TEMPERATURE

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## PROBLEM

Finite temperature

$$\rho = \frac{e^{-H/kT}}{Z}$$

More precise formulation:

- Fix the temperature: $T$
- Take an observable: $O$
- Compute $\langle O \rangle = \mathrm{tr}(\rho O)$

  with some prescribed precision, ε

  where $\rho = \frac{e^{-H/kT}}{Z}$

- How does the computational time scale with $N$?

  and ε and $T$?

- Heuristic algorithm that overcomes the sign problem

# QUANTUM MONTE CARLO

## Classical algorithm

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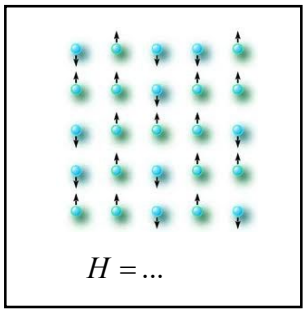
### THERMAL EQUILIBRIUM:




$$\rho = \frac{e^{-H/kT}}{\mathrm{tr}\left[e^{-H/kT}\right]}$$

- Sample configuration $n$ with probability $P_n$

$$\mathrm{tr}(O\rho) = \frac{\sum_n \langle n | e^{-H/T} | n \rangle \, O_n}{\sum_n \langle n | e^{-H/T} | n \rangle} = \frac{\sum_n P_n \, O_n}{\sum_n P_n}$$

- We need to compute $P_n = \langle n | e^{-H/T} | n \rangle$

  This is a many-body calculation

- Approximate

$$P_n = \sum_{n_1, n_2, \ldots, n_M} Q_{n,n_1} Q_{n_1,n_2} \ldots$$

- If $Q_{n,m} \geq 0$ , then we can sample $n_1, n_2, \ldots$ with a Metropolis algorithm

- Heuristics: $\tau \prec \frac{f(N)}{\varepsilon^2}$

# QUANTUM MONTE CARLO

## Classical algorithm

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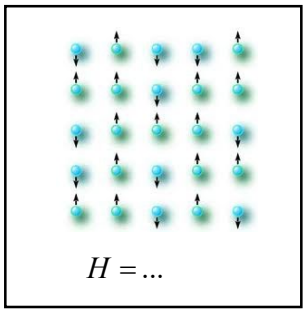
### THERMAL EQUILIBRIUM:




- Sample configuration $n$ with probability $P_n$

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- We need to compute $P_n = \langle n | e^{-H/T} | n \rangle$

  This is a many-body calculation

- Approximate

$$P_n = \sum_{n_1, n_2, \ldots, n_M} Q_{n,n_1} Q_{n_1,n_2} \ldots$$

SIGN PROBLEM: This is not possible, in general

With sign problem, the computational time is exponential

# FINITE TEMPERATURE
## Sampling

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Use the quantum simulator to sample and avoid the sign problem

- Observables:

$$\langle O\rangle = \frac{\mathrm{tr}(Oe^{-H/T})}{\mathrm{tr}(e^{-H/T})} = \lim_{\delta\to 0}\frac{\int dE e^{-E/T}\mathrm{tr}\left[G_\delta(E)O\right]}{\int dE e^{-E/T}\mathrm{tr}\left[G_\delta(E)\right]}$$

where $G_\delta(E) = e^{-(H-E)/2\delta^2}$ is the Gaussian filter we used before

- Discretize:

$$\langle O\rangle \approx \frac{\sum_E\sum_p P_p(E)\langle\Psi_p|O|\Psi_p\rangle}{\sum_E\sum_p P_p(E)}$$

sum over product states and energies

- $P_p$ and $\langle\Psi_p|O|\Psi_p\rangle$ can be computed if we know $a(t_n), b(t_n,t_m)$
- We can compute the sums using (classical) Monte-Carlo

Use the Quantum simulator as a subroutine

# FINITE TEMPERATURE
## Sampling

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- No sign problem: we use the simulator to compute probabilities
- More measurements because of sampling
- Heuristic since sampling may take long to converge

Can be used with both analog and NISQ devices

as long as one can measure generalized Lochschmidt Amplitudes

# Generalized Loschmidt Amplitude

# Hadamard Test

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Cleve, Ekert, Macchiavello, Mosca PRSL (1998)

- Goal: Retrieve $\langle \Psi_1 | e^{-iHt} | \Psi_0 \rangle = r(t)\, e^{i\phi(t)}$

$$|\Psi_0\rangle \otimes \left( e^{i\varphi} |0\rangle_a + |1\rangle_a \right)$$

Conditional preparation

$$e^{i\varphi} |\Psi_0\rangle \otimes |0\rangle_a + |\Psi_1\rangle \otimes |1\rangle_a$$

Conditional dynamics

$$\widehat{H} = H \otimes |0\rangle_a \langle 0|$$

$$e^{i\varphi} e^{-iHt} |\Psi_0\rangle \otimes |0\rangle_a + |\Psi_1\rangle \otimes |1\rangle_a$$

Measure ancilla

$$\langle \sigma_x \rangle_a = \frac{1}{2} \left[ 1 + \mathrm{Re}\left( e^{i\varphi} \langle \Psi_1 | e^{-iHt} | \Psi_0 \rangle \right) \right]$$

- Requires non-local interactions
- Can be made local by using several ancillas in a GHZ state

$$|\Psi_0\rangle \otimes \left( e^{i\varphi} |000\ldots0\rangle_a + |111\ldots1\rangle_a \right)$$

# Sequential Method

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Sirui Lu, Mari Carmen Bañuls, JIC, PRXQuantum (2021)

- Goal: Retrieve $\langle p | e^{-iHt} | p \rangle = r(t)\, e^{i\phi(t)}$ where $| p \rangle = | p_1, p_2, ... \rangle$ is a product state
  - Assume there is a reference state: $\langle aa...a | e^{-iHt} | aa...a \rangle = r_0 e^{i\phi_0}$ Can be computed (classically)
    - Eg: $| aa...a \rangle$ is an eigenstate
    - This can be implemented with three-level systems
  - Measure $\left| \langle ba...a | e^{-iHt} | b...a \rangle \right|^2$ with $| b \rangle = \begin{cases} | b \rangle = | a \rangle \pm | p_1 \rangle \\ | b \rangle = | p_1 \rangle \end{cases}$
  - With those outcomes, and knowing $r_0$ and $\phi_0$, compute $\langle p_1 a...a | e^{-iHt} | p_1 a...a \rangle$
  - Continue in the same way with $\langle p_1 p_2 ...a | e^{-iHt} | p_1 p_2 ...a \rangle$

$$\langle p_1 p_2 ... p_n | e^{-iHt} | p_1 p_2 ... p_n \rangle$$

# Sequential Method

Sirui Lu, Mari Carmen Bañuls, JIC, PRXQuantum (2021)

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- Advantages:
  - No ancillas, local
  - one only has to measure the absolute values

$$\left|\langle p_1 b \ldots a \,|\, e^{-iHt} \,|\, p_1 b \ldots a \rangle\right|^2$$

  - one only has to prepare product states

$$\left|\langle p_1 b \ldots a \,|\, e^{-iHt} \,|\, p_1 b \ldots a \rangle\right|^2$$

- Drawback: Errors accumulate

# Complex Analysis Method

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Yilun Yang, Arthur Christianen, Mari Carmen Bañuls, Dominik S. Wild, JIC, arxiv: 2308.10796

- Goal: Retrieve $\langle p | e^{-iHt} | p \rangle = r(t)\, e^{i\phi(t)}$ where $| p \rangle = | p_1, p_2, \ldots \rangle$ is a product state

  - Analytical extension $G(z) = \langle p | e^{-iHz} | p \rangle = r(z)\, e^{i\phi(z)}$

    $$z = t + i\beta$$

    - The real and imaginary part of $G(z)$ are related
    - Are the modulus and the phase connected?

$$\frac{\partial}{\partial t}\phi(z) = \frac{\partial}{\partial \beta}\log\left[r(z)\right] \quad \Rightarrow \quad \phi(t_2) - \phi(t_1) = \int_{t_1}^{t_2} \frac{\partial}{\partial \beta}\ln\left[r(z)\right]\Big|_{\beta=0} dt$$

- Approximate

$$\frac{\partial}{\partial \beta}\ln\left[r(z)\right]\Big|_{\beta=0} \approx \frac{\ln r(t-ih) - \ln r(t+ih)}{h} \qquad \text{for } h \text{ small}$$

- Measure

$$r(t \pm ih) = \left|\langle p | e^{-iHt} e^{\pm hH} | p \rangle\right| = q\left|\langle p | e^{-iHt} | \varphi \rangle\right|$$

can be computed classically

can be easily prepared

# Complex Analysis Method



- Advantages:
  - No ancillas, local
  - one only has to measure the absolute values

$$r(t \pm ih) = \left| \langle p \mid e^{-iHt} e^{\pm hH} \mid p \rangle \right| = q \left| \langle p \mid e^{-iHt} \mid \varphi \rangle \right|$$

one only has to prepare product states and apply a low depth circuit

  - There is a simple error-mitigation method

Yilun Yang, Arthur Christianen, Sandra Coll-Vinent, Vadim Smelyanskiy, Mari Carmen Bañuls, Thomas E. O'Brien, Dominik S. Wild, JIC, arXiv: 2303.08461

- Drawback: Errors accumulate

# Complex Analysis Method
## Illustration: Ising chain

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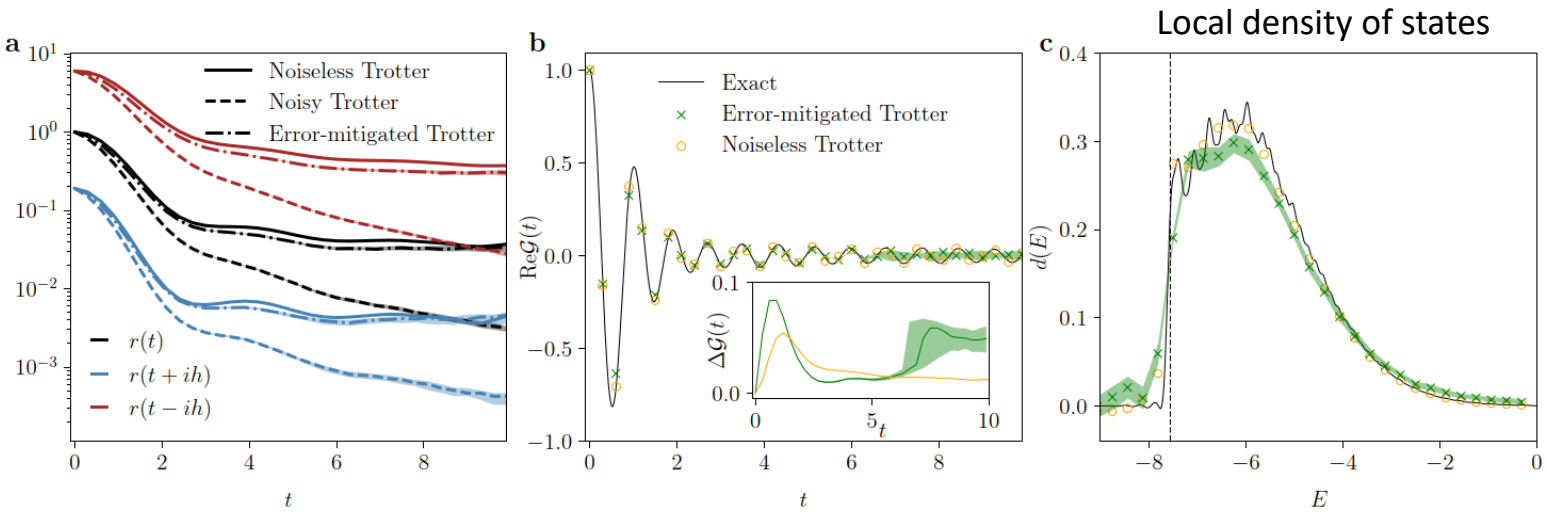
$N = 24$ spins

Initial state: $|p\rangle = |000...0\rangle$

Trotter step: $\tau = h = 0.3$




Dashed lines: error after each gate with a probability $0.003$

Simulation of 100 experiments using $10^6$ measurements

# Comparison

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| Method | Circuit Depth | # measurements |
|---|---|---|
| Hadamard test | $\mathcal{O}(t^{1+\frac{1}{p}} N^{1+\frac{1}{d}+\frac{1}{p}} / \epsilon^{\frac{1}{p}})$ | $\mathcal{O}(1/\epsilon^2)$ |
| Sequential interferometry | $\mathcal{O}(r^{\frac{1}{p}} t^{1+\frac{1}{p}} N^{\frac{2}{p}} / \epsilon^{\frac{1}{p}})$ | $\mathcal{O}(\tilde{I}^2 r^2 N^2 / \epsilon^2)$ |
| This work | $\mathcal{O}(r^{\frac{1}{p}} t^{1+\frac{2}{p}} N^{\frac{1}{p}} / \epsilon^{\frac{1}{p}})$ | $\mathcal{O}\left(I^2 r^3 t^3 N / \epsilon^3\right)$ |

$d$: spatial dimension

$\varepsilon$: prescribed error in $G(t)$

$I$: constants that depend on $G(t)$

$p$: Trotter order

$N$: Number of qubits

- Quantum simulation is (arguably) the most suitable application of quantum computers

- Currently, analog and NISQ quantum computers are very well suited for quantum simulation

- There exists a variety of quantum algorithms for dynamics and thremal equilibrium

  - Generalize Loschmidt Amplitudes play important role in those and other algorithms

- One can avoid Hadamard Tests which may have practical advantages

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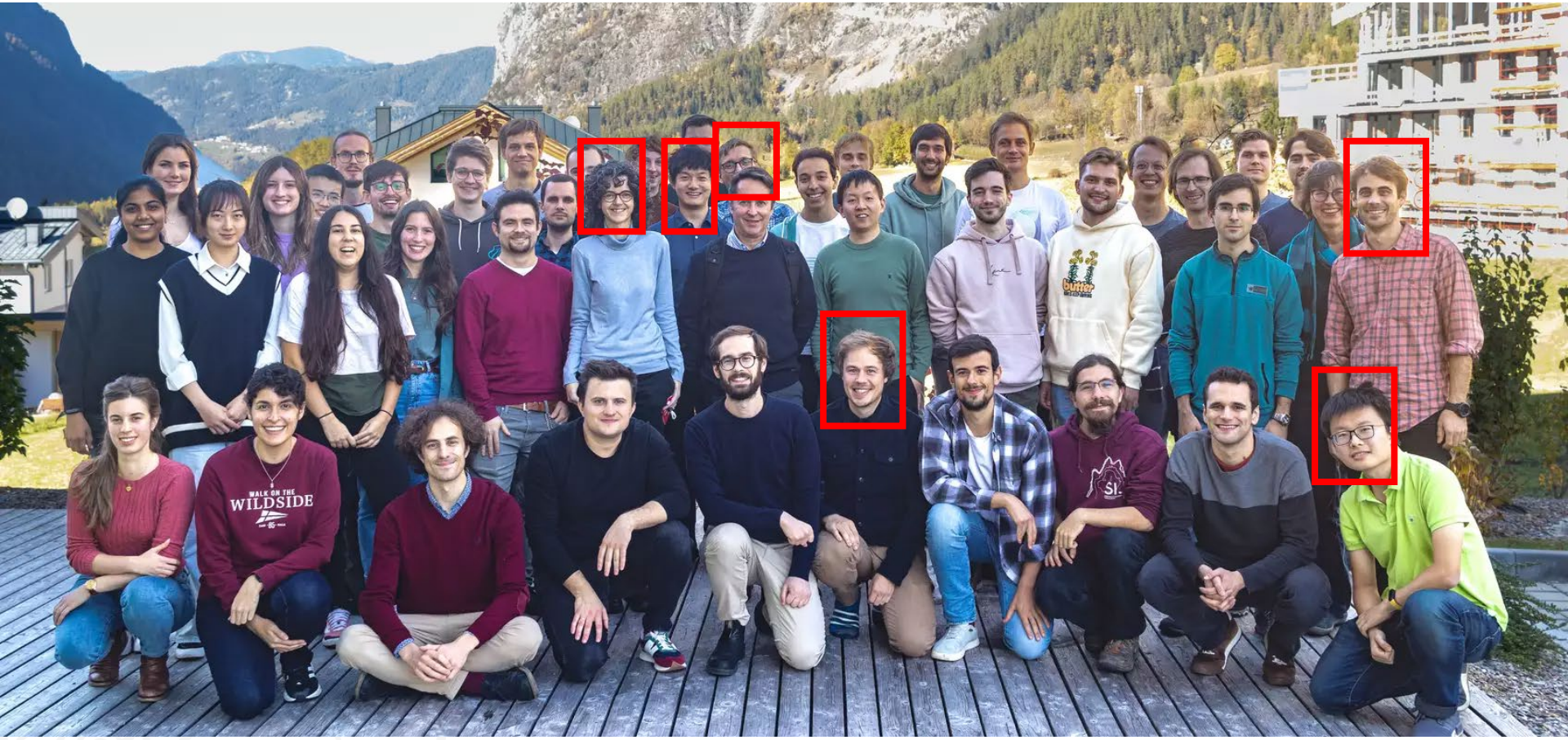


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