2.5.3. Quantum counting algorithm

How quickly can we determine the number of target states in Grover's algorithm, i.e. marked states, r, to an $N=2^n$ data base search problem, if r is not known in advance.

Classical search $\sim \mathrm{O}(N)$

Quantum search $\sim \mathrm{O}(\sqrt{N})$

(Grover iteration + phase estimation algorithm)

⇩ applications

1) Quantum search, even if the number of solutions is unknown
2) NP-complete SAT (satisfiability) problems
   (= existence of a solution to a search problem)

Quantum algorithm:

$|a\rangle, |b\rangle$: the two eigenvectors of the Grover iteration

$\hat{Q} = -\hat{I}_\gamma \hat{U}^{-1} \hat{I}_\tau \hat{U}$ in the space spanned by

$|\alpha\rangle$(non-solution state) and $|\beta\rangle$(solution state).

$\theta = \sin^{-1}\left(2U_{\tau\gamma}\right)$: the angle of rotation determined by $\hat{Q}$

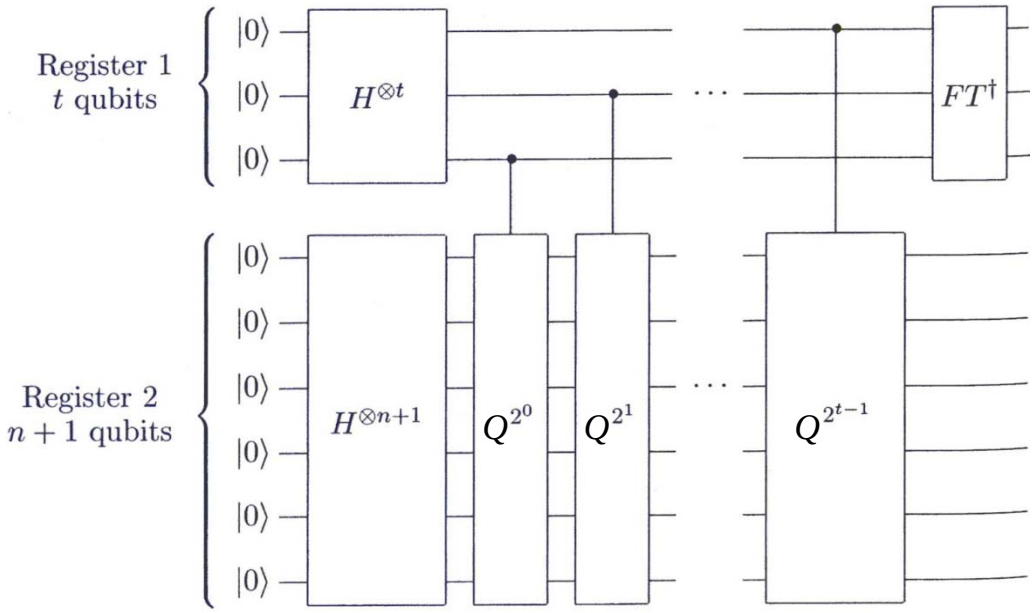
⇩

$$\hat{Q} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{matrix} |\alpha\rangle \\ |\beta\rangle \end{matrix}$$

basis

⇩

Corresponding eigenvalues $e^{i\theta}$ and $e^{i(2\pi-\theta)}$



Step 1: initialization

$|0\rangle_1 |0\rangle_2$ ← $n+1$ qubits ⇨ enough to implement the Grover iteration ($2N=2^{n+1}$ expanded search space)

$t \equiv m + \log\left(2 + \frac{1}{2\varepsilon}\right)$ qubits ⇨ estimate θ to m bits of accuracy with a probability of success $\geq 1 - \varepsilon$.

Step 2: Walsch-Hadamard transform on the first and second register

$$\xrightarrow{\hat{H}_1 \otimes \hat{H}_2} \frac{1}{\sqrt{2^t}} \sum_{x=0}^{2^t-1} |x\rangle_1 \otimes \frac{1}{\sqrt{2^{n+1}}} \sum_{y=0}^{2^{n+1}-1} |y\rangle_2$$

Linear superposition of $|a\rangle$ and $|b\rangle$

$C_a |a\rangle + C_b |b\rangle$

⇨ The above circuit provides an estimate of θ and 2π- θ.

Step 3: Controlled – Q^{2^j} operation

$$\xrightarrow{C-\hat{Q}^{2^j}} \frac{1}{\sqrt{2^t}} \sum_{x=0}^{2^t-1} |x\rangle_1 \left(e^{2\pi i x\theta} C_a |a\rangle_2 + e^{2\pi i x(2\pi-\theta)} C_b |b\rangle_2 \right)$$

Step 4: inverse Fourier transform on the first register

$$\xrightarrow{\hat{F}_1^{-1}} C_a \left|\tilde{\theta}\right\rangle_1 \left|a\right\rangle_2 + C_b \left|2\pi - \tilde{\theta}\right\rangle_1 \left|b\right\rangle_2$$

equivalent

Step 5: projective measurement of the first register

$\longrightarrow$ estimate of θ with an accuracy of $|\Delta\theta| \le 2^{-m}$ with probability of success $1-\varepsilon$

$\longrightarrow$ estimate r through $\sin^2\frac{\theta}{2} = \frac{r}{2N}$

How large an error, Δr , in this estimate?

$$\frac{|\Delta r|}{2N} = \left|\sin^2\left(\frac{\theta+\Delta\theta}{2}\right) - \sin^2\left(\frac{\theta}{2}\right)\right|$$

$$= \left|\left[\sin\left(\frac{\theta+\Delta\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)\right]\left[\sin\left(\frac{\theta+\Delta\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)\right]\right|$$

$$< \left(2\sin\left(\frac{\theta}{2}\right) + \frac{|\Delta|}{2}\right)\frac{|\Delta\theta|}{2}$$

$\sin\frac{\theta}{2} = \sqrt{\frac{r}{2N}}$ $\qquad$ $|\Delta\theta| < 2^{-m}$

$$|\Delta r| \le \left(\sqrt{2rN} + \frac{N}{2^{m+1}}\right)2^{-m}$$

$$m = \left\lceil \frac{n}{2} \right\rceil + 1,\ \varepsilon = 1/6 \quad \rightarrow \quad t = \left\lceil \frac{n}{2} \right\rceil + 3$$

$$|\Delta r| < \sqrt{\frac{r}{2}} + \frac{1}{4} \sim O\left(\sqrt{r}\right) \qquad O\left(\sqrt{N} = 2^{\frac{n}{2}}\right)$$

Grover iterations

allowable angle error and reasonable success probability

Number of required iterations:

$$R \sim \frac{\pi}{4}\sqrt{\frac{N}{r}}$$

Angle error:

$$\frac{\pi}{4}\left(1+\frac{|\Delta\theta|}{\theta}\right)\sim\frac{3}{8}\pi$$

$$\left(\mathrm{m}=\frac{n}{2}+1\right)$$

Success probability:

$$\cos^2\left(\frac{3}{8}\pi\right)\sim 0.15$$

If $r=0$ (no solution), $|\Delta r| = 1/4$ so that the algorithm produces the estimate $r=0$ with the probability >*5/6*.

$\Rightarrow$ NP-complete SAT problems

Example: 3-SAT (satisfiability) problem

Find if the following Boolean function can be satisfied or not.

$$f(x)=(x_1 \vee x_2 \vee \overline{x}_3)\wedge(\overline{x}_4 \vee x_5 \vee x_3)\wedge\cdots\cdots=1$$

$\Downarrow$

$$t=\left|f^{-1}(1)\right|\geq 1 \text{ or zero ?}$$ (Solution exists or not)

Classical brute-force algorithm requires $\sim \mathrm{O}\left(\mathrm{poly}(n)2^n\right)$

Grover algorithm requires $\sim \mathrm{O}\left(\mathrm{poly}(n)\sqrt{2^n}\right)$

This is bad news for quantum computing. The essential reason for the difficulty of NP-complete problems is that their search space has essentially no structure. The best possible method for solving such a problem is to adopt a Grover search method. This means that NP-complete problems cannot be solved by quantum computers (except for a square-root speed up) since the Grover algorithm is Known to be optimum.

2.6 Quantum simulation

- Digital quantum simulation:
  A quantum computer solves a physical (many body) problem.
- Analog Quantum simulation:
  An artificial and controllable quantum system simulates a real physical system under study.

In order to calculate thermodynamical properties of a many body system, an ensemble quantum computer, in which many independent microscopic quantum computers execute the same operation and produce a macroscopic readout signal, is more efficient than a standard quantum computer consisting of a qubit system.

2.6.1. Spin-lattice systems

System Hamiltonian $\hat{\mathcal{H}}\ (\sigma_1, \sigma_2, \cdots \sigma_n) \Rightarrow$ magnetic ordering (phase transition)

Helmholtz free energy per spin

$$F = -\frac{k_B T}{n} \ln Z = -\frac{k_B T}{n} \ln\left(\sum_m e^{-\beta E_m} \right)$$

$$\beta = \frac{1}{k_B T} \quad : \text{temperature parameter}$$

$$Z = \sum_m e^{-\beta E_m} \approx \int_{-\infty}^{\infty} \rho(E) e^{-\beta E} dE \quad : \text{thermodynamic partition function}$$

$\Downarrow$

m : eigenstate index

$\rho(E)$: energy density of states

thermodynamic properties (magnetization, specific-heat, magnetic susceptibility ·····) can be easily calculated by the free energy F once it is known.

A brute-force approach to enumerate the eigen-energies $\{E_m\}$ of $\hat{\mathcal{H}}$ is difficult, because the number of eigenstates grows exponentially with the number of spins in the lattice.

cf. quantum Monte Carlo methods
(sign problem: D.P. Landau and K. Binder, A Guide to Monte Carlo Simulation in Statistical Physics (Cambridge Univ. Press, Cambridge, 2000))

The following quantum algorithms are based on

$$f(t)=\int_{-\infty}^{\infty}\rho(E)e^{-iEt}dE=\sum_m e^{-iE_m t}=Tr\left(e^{-i\hat{\mathcal{H}}t}\right)$$

Fourier transform of $\rho(E)$ $(\hbar=1)$

trace of the time evolution operator $\hat{U}(t)$

$$|f(t)|\le 2^n \Rightarrow g(t)\equiv\frac{f(t)}{2^n}=\frac{1}{2^n}Tr\left(e^{-i\hat{\mathcal{H}}t}\right)$$

# of eigenstates $|g(t)|\le 1$

flow of computational step:

$$\{t_l\}\longrightarrow g(t_l)\longrightarrow\rho(E)\longrightarrow Z$$

discrete times — inverse Fourier transform — simple integration

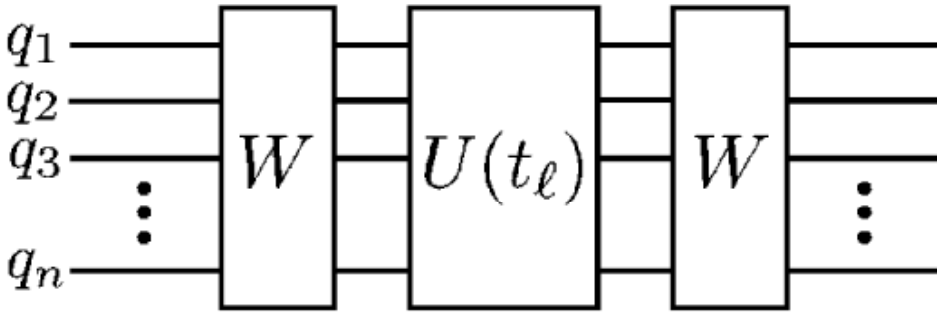
quantum computation — classical computation

2.6.2 Ising model

$$\hat{\mathcal{H}} = -J_z \sum_{\{ij\}} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} - \sum_i h_i \hat{\sigma}_z^{(i)}$$: diagonal in computational basis

example: hetero-spin network with dipolar coupling under dc magnetic field

Simple configuration (failure case)



Step 1: $|0\rangle \xrightarrow{\hat{W}} \frac{1}{\sqrt{2^n}} \sum_{m=0}^{2^n-1} |m\rangle$

$|0\rangle_1 |0\rangle_2 \cdots |0\rangle_n = |\uparrow\rangle_1 |\uparrow\rangle_2 \cdots |\uparrow\rangle_n$

example: $|0\rangle_1 |1\rangle_2 \cdots |0\rangle_n = |\uparrow\rangle_1 |\downarrow\rangle_2 \cdots |\uparrow\rangle_n$ ← eigenstate of $\hat{\mathcal{H}}$

eigen-energy

Step 2: $\frac{1}{\sqrt{2^n}}\sum_{m=0}^{2^n-1}|m\rangle \xrightarrow{\hat{U}(t_l)} \frac{1}{\sqrt{2^n}}\sum_{m=0}^{2^n-1} e^{-iE_m t_l}|m\rangle$

This step can be implemented as a sequence of single qubit and two-qubit gates, where the number of gates is a polynomial function of *n*. For Ising model in which the Hamiltonian consists of commuting pair-wise interactions, this decomposition is elementary. For the case of non-commuting terms, Trotter-Suzuki expansion can be employed.

Step 3: $\frac{1}{\sqrt{2^n}}\sum_{m=0}^{2^n-1} e^{-iE_m t_l}|m\rangle \xrightarrow{\hat{W}} \underbrace{\frac{1}{2^n}\sum_{m=0}^{2^n-1} e^{-iE_m t_l}}_{\frac{1}{2^n}Tr\left(e^{-i\hat{\mathcal{H}}t_l}\right)}|0\rangle + \text{orthogonal components}\ \sum_{m'=1}^{2^n-1} c_{m'}|m'\rangle$

$\Downarrow \qquad\qquad g(t_l)$

An unbiased estimator for $|g(t_l)|$ can be obtained by repeating the algorithm many times and counting the number of times all qubits are found in the logical $|0\rangle$ state. This probability is equal to $|g(t_l)|^2$. If an ensemble of identical microscopic quantum computers executes the same algorithm, the ensemble measurements for all qubits reveal $|g(t_l)|$ by only one computation:

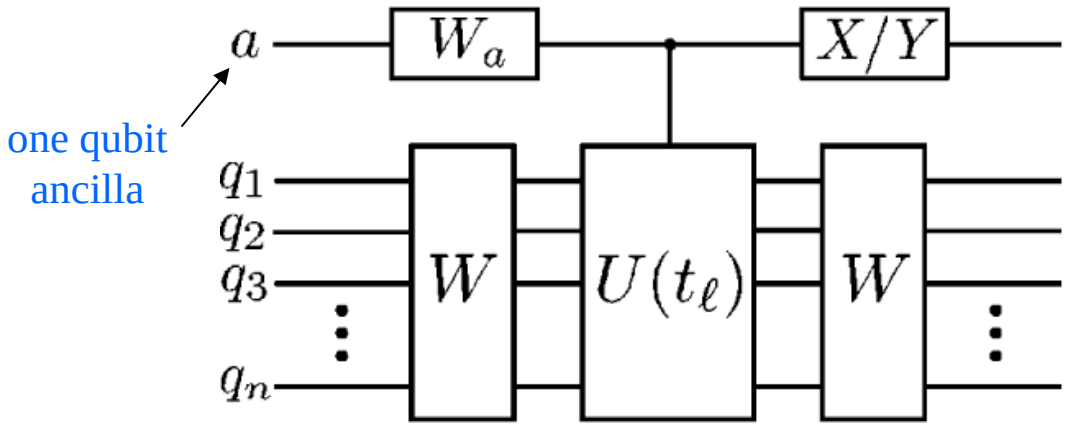
$\Downarrow$

However, $|g(t_l)|$ is insufficient to reconstruct $\rho(E)$. We need $\mathrm{Re}(g(t_l))$ and $\mathrm{Im}(g(t_l))$.

$\Downarrow$

failure

Modified configuration (successful case)



Step 1: $|0\rangle_a|0\rangle_q \xrightarrow{\hat{W}_a,\hat{W}} \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)_a \otimes \frac{1}{\sqrt{2^n}}\sum_{m=0}^{2^n-1}|m\rangle_q$

Step 2:

$$\xrightarrow{C\text{-}\hat{U}(t_l)} \frac{1}{\sqrt{2}}\left[|0\rangle_a \otimes \frac{1}{\sqrt{2^n}}\sum_{m=0}^{2^n-1} e^{-iE_m t_l}|m\rangle_q + |1\rangle_a \otimes \frac{1}{\sqrt{2^n}}\sum_{m=0}^{2^n-1}|m\rangle_q\right]$$

Step 3:

$$\xrightarrow[\hat{W}]{\hat{R}_x} \frac{1}{2}\left\{(i|0\rangle+|1\rangle)_a \otimes \frac{1}{2^n}\left[Tr\left(e^{-i\hat{\mathcal{H}}t_l}\right)|0\rangle_q + \cdots\right]\right.$$

$$\left. + (|0\rangle + i|1\rangle)_a \otimes |0\rangle_q\right\}$$

$$= \left[\frac{1+ig(t_l)}{2}\right]|0\rangle_a|0\rangle_q + i\left[\frac{1-ig(t_l)}{2}\right]|1\rangle_a|0\rangle_q + \text{orthogonal components}$$

$\hat{R}_x$: rotation about x-axis by 90° $\quad \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix}\begin{matrix}|0\rangle \\ |1\rangle\end{matrix}$

Step 3':

$$\xrightarrow[\hat{W}]{\hat{R}_y} \frac{1}{2}\left\{ \left(|0\rangle + |1\rangle\right)_a \otimes \frac{1}{2^n}\left[Tr\left(e^{-i\hat{\mathcal{H}}_l}\right)|0\rangle_q + \cdots \right] \right.$$

$$\left. + \left(|0\rangle - |1\rangle\right)_a \otimes |0\rangle_q \right\}$$

$$= \left[\frac{1+g(t_l)}{2}\right]|0\rangle_a|0\rangle_q - \left[\frac{1-g(t_l)}{2}\right]|1\rangle_a|0\rangle_q + \text{orthogonal components}$$

$\hat{R}_y$: rotation about *y*-axis by 90° $\quad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{matrix}|0\rangle \\ |1\rangle\end{matrix}$

$$\Pr(X,0,0) = \left|\frac{1+ig(t_l)}{2}\right|^2$$

$$\Pr(X,1,0) = \left|\frac{1-ig(t_l)}{2}\right|^2$$

$$\Pr(Y,0,0) = \left|\frac{1+g(t_l)}{2}\right|^2$$

$$\Pr(Y,1,0) = \left|\frac{1-g(t_l)}{2}\right|^2$$

$$\mathrm{Re}\left[g(t_l)\right] = \Pr(Y,0,0) - \Pr(Y,1,0)$$

$$\mathrm{Im}\left[g(t_l)\right] = \Pr(X,1,0) - \Pr(X,0,0)$$

success

2.6.3 General spin Hamiltonian

Heisenberg model:

$$\hat{\mathcal{H}} = \sum_{\{i,j\}} J_{ij} \hat{\sigma}^{(i)} \cdot \hat{\sigma}^{(j)} - \sum_i h_i \hat{\sigma}_z^{(i)}$$

example: electron spin network with exchange coupling

XXZ model:

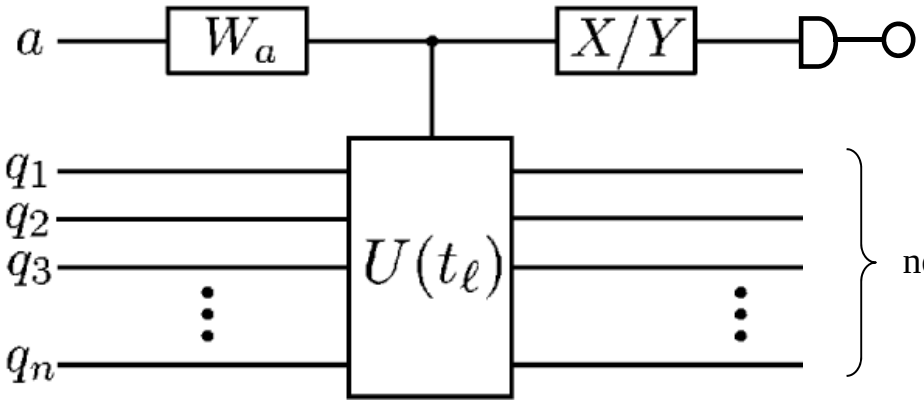
$$\hat{\mathcal{H}} = \sum_{\{i,j\}} J_x \left[\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} + \hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \right] + J_z \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} - \sum_i h_i \hat{\sigma}_z^{(i)}$$

example: electron/nuclear homo-spin network with dipolar coupling

⇩

Hamiltonians are not diagonal in the computational basis.

E. Knill and R. Laflamme, Phys. Rev. Lett. 81, 5672 (1998)



no need to measure!

The ancilla qubit is initialized in $|0\rangle_a$ state, while the remaining n qubits are in a fully mixed state:

$$\hat{\rho} = \frac{1}{2}\left(\hat{I}^{(a)} + \hat{\sigma}_z^{(a)}\right) \otimes \frac{1}{2^n} \hat{I}^{(q_1)} \hat{I}^{(q_2)} \cdots \hat{I}^{(q_n)}$$

$$\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\left[|0\rangle\langle 0| + |1\rangle\langle 1|\right]$$

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 0|$$

$$\sum_l |\psi_l\rangle\langle\psi_l| = \hat{I}$$: decomposition of unity

orthonormal set of states for $q_1 \cdots q_n$

⇩

We can choose the eigen-states of $\hat{\mathcal{H}}$ as $\{|\psi_l\rangle\}$

⇩

The initial density matrix can be considered as an incoherent mixture of the eigen-states of $\hat{\mathcal{H}}$.

We choose the eigenstates of the given Hamiltonian $\hat{\mathcal{H}}$ as $\{|\psi_l\rangle\}$. Even though we do not know explicitly $\{|\psi_l\rangle\}$, the initial density matrix $\frac{1}{2^n}\hat{I}^{(q_1)}\hat{I}^{(q_2)}\cdots\hat{I}^{(q_n)}$ can be considered as an incoherent mixture of eigenstates for any Hamiltonian.

$$\hat{R}_x \rightarrow \left\langle \hat{\sigma}_z^{(a)} \right\rangle = \mathrm{Im}\left[g(t_l)\right]$$

$$\hat{R}_y \rightarrow \left\langle \hat{\sigma}_z^{(a)} \right\rangle = \mathrm{Re}\left[g(t_l)\right]$$

ensemble averaged result

The required accuracy for measuring $\hat{\sigma}_z^{(a)}$ scales exponentially ($\Delta\sigma_z^{(a)} \sim 1/2^n$) as the problem size.

$f(t) = 2^n \cdot g(t)$ ⇨ # of molecules $\sim 10^{24}$ ⇨ $n = 40$ spins

The computational time scales polynomially with the problem size, $\sim O(n^2)$.

C.P. Master et al., Phys. Rev. A 67, 032311 (2003)

2.6.4 Jordan-Wigner transformation

In order to simulate a many-fermion system, we need a mapping between the algebra of fermionic system and the algebra of spin- $\frac{1}{2}$ system.

$$\left\{\hat{a}_j, \hat{a}_k^+\right\}_+ = \delta_{jk}, \quad \left\{\hat{a}_j, \hat{a}_k\right\}_+ = \left\{\hat{a}_j^+, \hat{a}_k^+\right\}_+ = 0$$

⇩ mapping onto spin-operators (isomorphism)

$$\hat{a}_j \to \left(\prod_{l=1}^{j-1} -\hat{\sigma}_z^{(l)}\right)\hat{\sigma}_-^{(j)} = (-1)^{j-1}\,\hat{\sigma}_z^1\hat{\sigma}_z^2\cdots\hat{\sigma}_z^{j-1}\hat{\sigma}_-^j$$

$$\hat{a}_j^+ \to \left(\prod -\hat{\sigma}_z^{(l)}\right)\hat{\sigma}_+^{(j)} = (-1)^{j-1}\,\hat{\sigma}_z^1\hat{\sigma}_z^2\cdots\hat{\sigma}_z^{j-1}\hat{\sigma}_+^j$$

example: 1-D spinless fermions

● ● ····· ● ·····

1 2 j

$$\hat{\mathcal{H}} = -t\sum_j\left(\hat{a}_{j+1}^+\hat{a}_j + \hat{a}_j^+\hat{a}_{j+1}\right) + U\sum_j \hat{n}_j\hat{n}_{j+1}$$

tunneling ⇩ mutual Coulomb interaction

$$\hat{\mathcal{H}} = -2t\sum_j\left(\hat{\sigma}_x^{(j)}\hat{\sigma}_x^{(j+1)} + \hat{\sigma}_y^{(j)}\hat{\sigma}_y^{(j+1)}\right) + 4U\sum_j\hat{\sigma}_z^{(j)}\hat{\sigma}_z^{(j+1)} + U_0$$

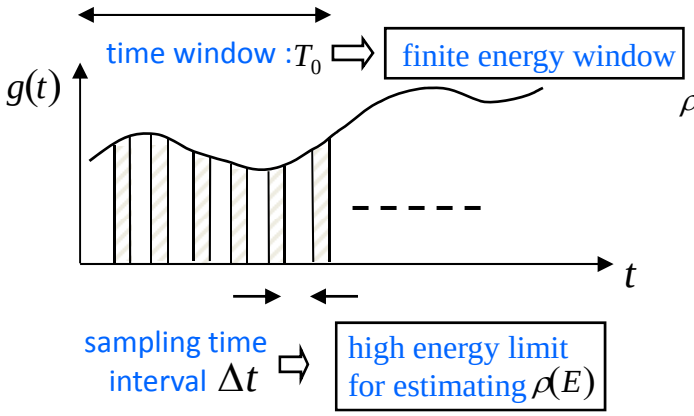
: anisotropic Heisenberg (XXZ) model

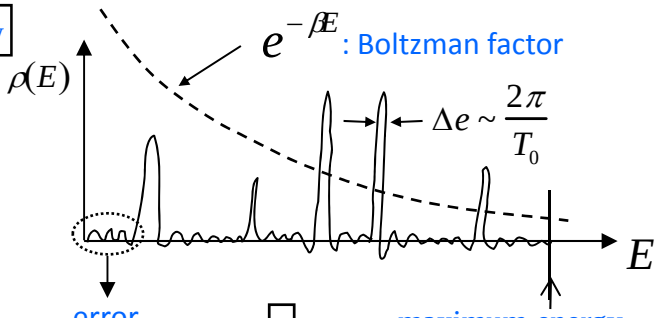
⇩

Ensemble quantum algorithm using mixed state qubits

2.6.5 Efficiency of the ensemble quantum algorithm

How many samples of $g(t)$ do we need to accurately calculate Z ?



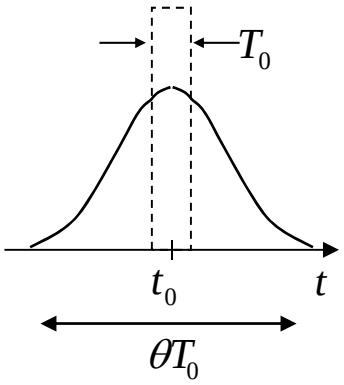


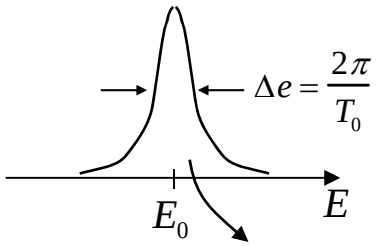
broadening function $b(E) = \frac{1}{\Delta e}\sin c\left(\frac{\pi E}{\Delta e}\right)$

$\Delta e = \frac{2\pi}{T_0}$: energy resolution

$Z = \int \rho(E) e^{-\beta E} dE$ has an error due to low-energy side lobes

Rectangular time window





envelope falls off $\left(\frac{\Delta e}{\Delta E}\right)^{\theta}$

Gaussian time window

$b_\theta(E) = \alpha_\theta \left[\sin c\left(\frac{\pi \Delta E}{\Delta e}\right)\right]^{\theta}$

The error can be minimized by small Δe and large θ, but the number of iterations $N = \frac{\theta T_0}{\Delta t}$ increases. How does N scale with the number of spins n?

The total time scale polynomially with the number of spins ($\sim O(n^2)$).