How to compute using quantum walks

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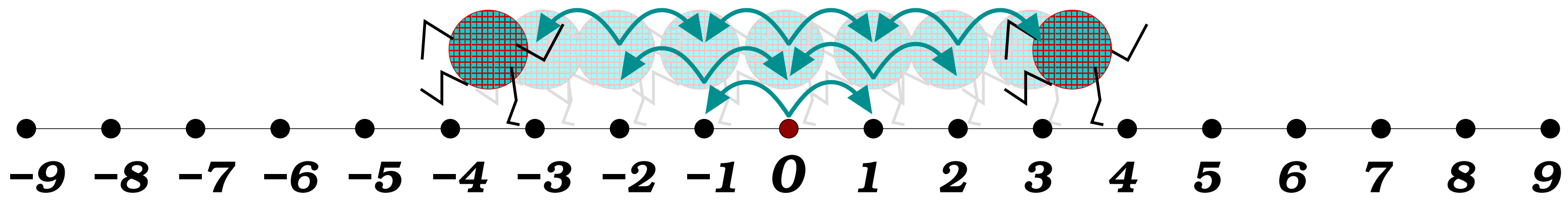
Quantum Simulation and Quantum Walks

CIRM *20th January 2020*

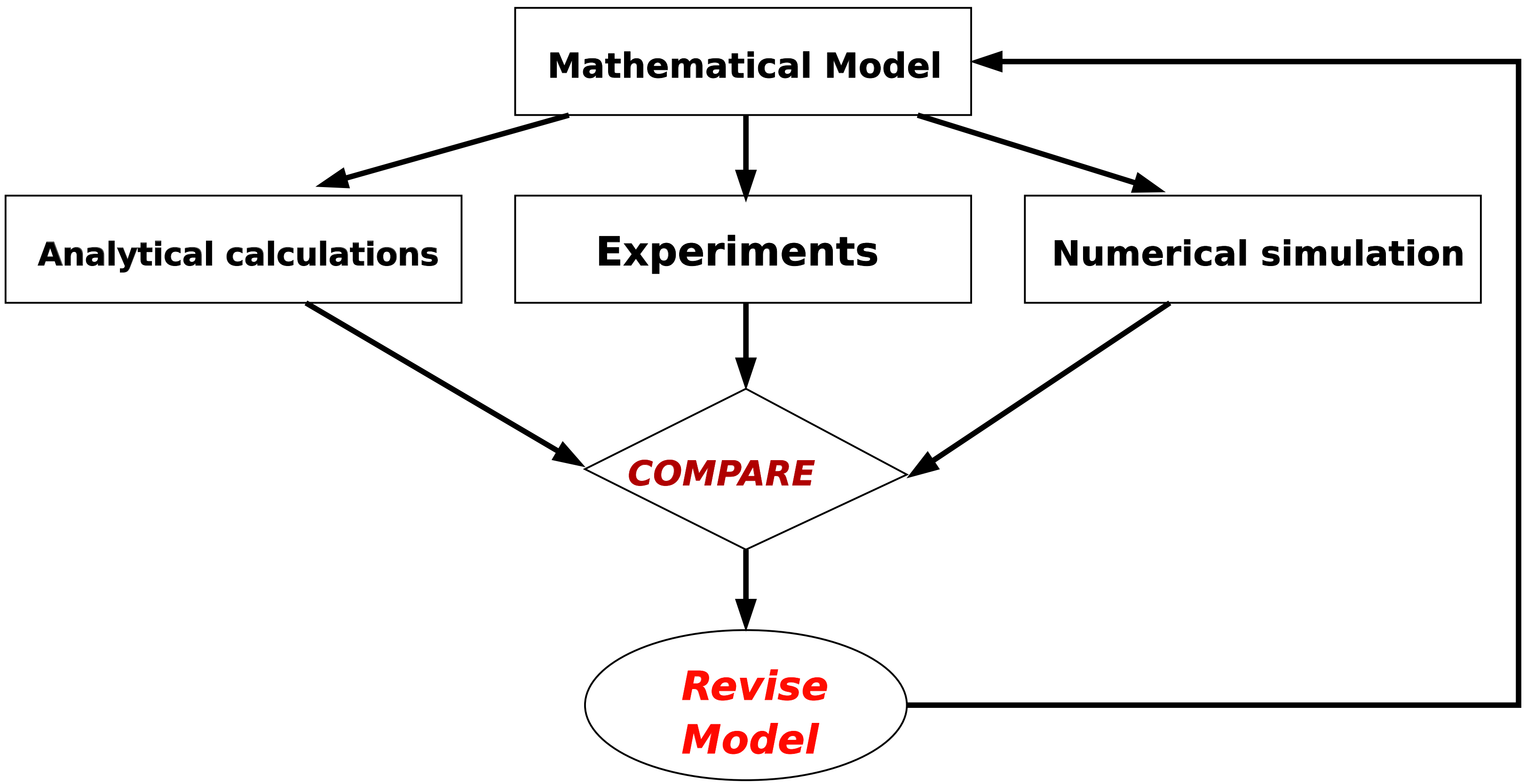
Overview

- modeling vs simulation?
- abstraction/representation framework
- solving classical problems with quantum walks
- searching and spin glasses
- universal quantum walk computing
- summary and outlook



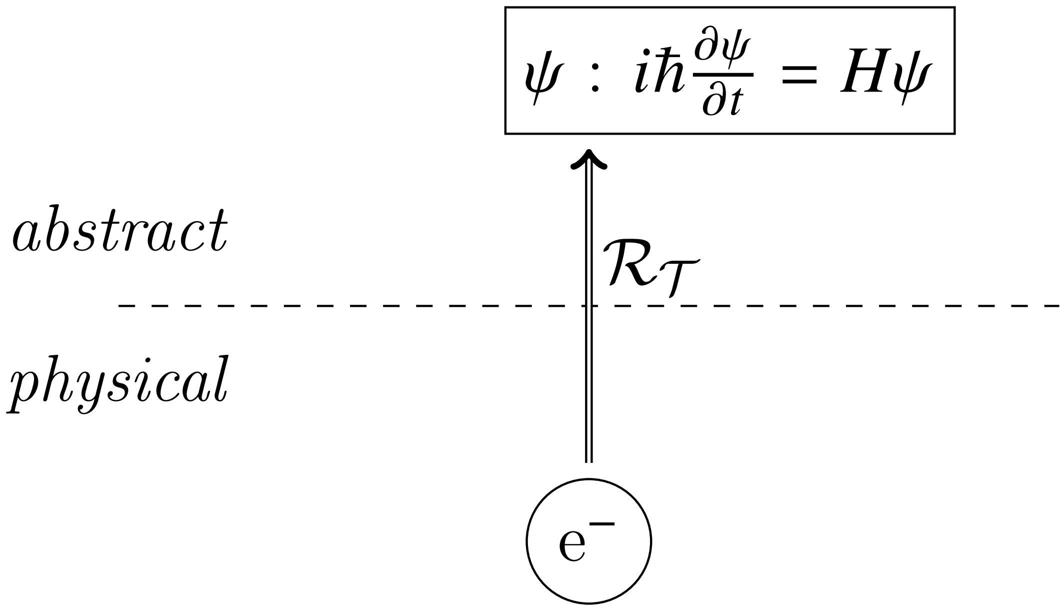
numerical simulation...

★ we simulate mathematical models, not physical systems:



computational physics tests our models when can't calculate analytically...

representation relation in physics:

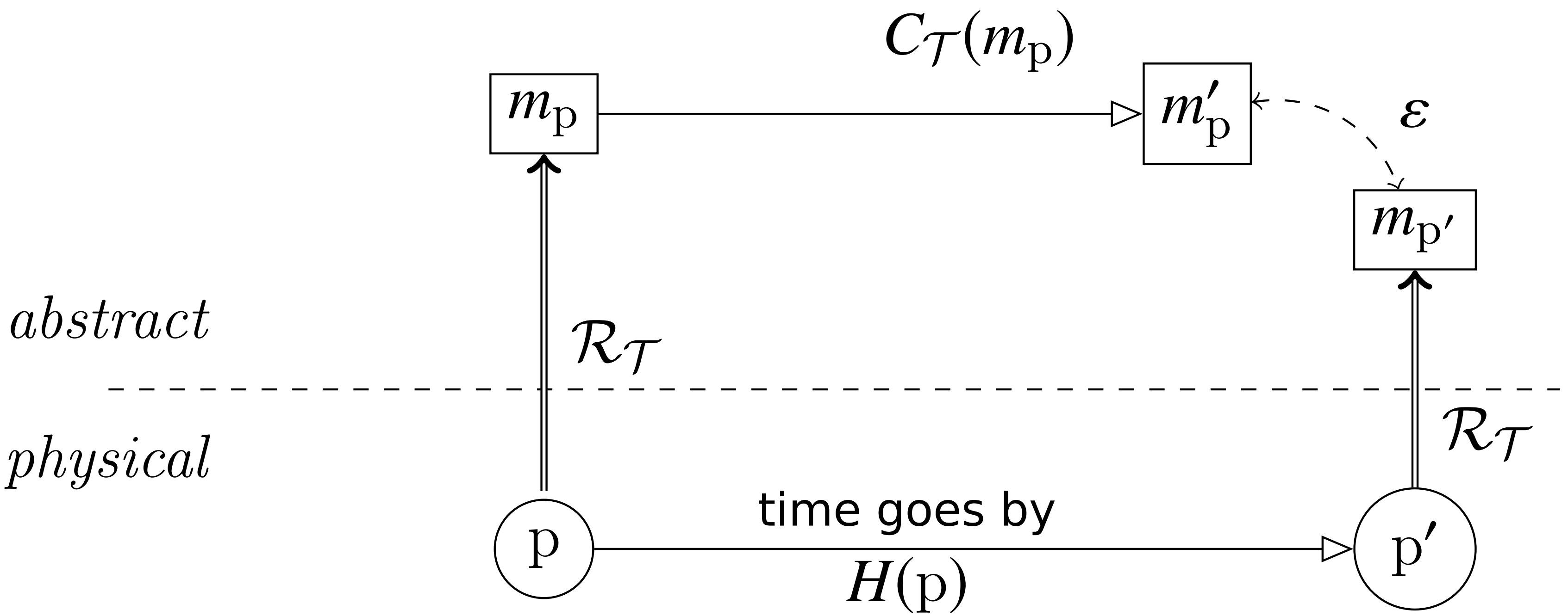


spaces of $abstract$ and $physical$ objects (here, an electron and a wave-function) with a representation relation (modelling) $\mathcal{R}_\mathcal{T}$ mediating between the spaces

$\mathcal{R}$ is theory dependent, so write $\mathcal{R}_\mathcal{T}$ for theory $\mathcal{T}$

★ *could represent electron as point charge if doing electrostatics . . .*

science



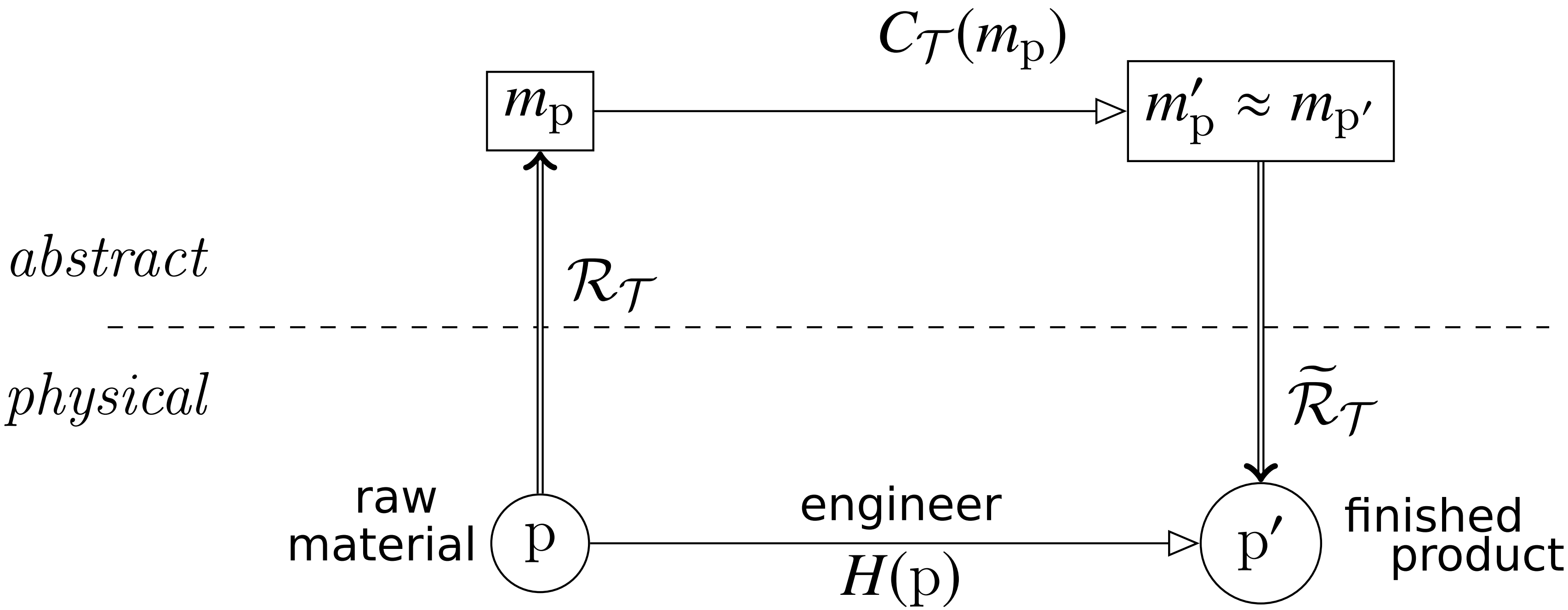
– physical system p evolves under $H(\mathrm{p})$ to p'

– theory m_{p} calculated $C_{\mathcal{T}}(m_{\mathrm{p}})$ to obtain m'_{p}

– "good" theory agrees with observation to within $\varepsilon : |m'_{\mathrm{p}} - m_{\mathrm{p}'}| < \varepsilon$

technology

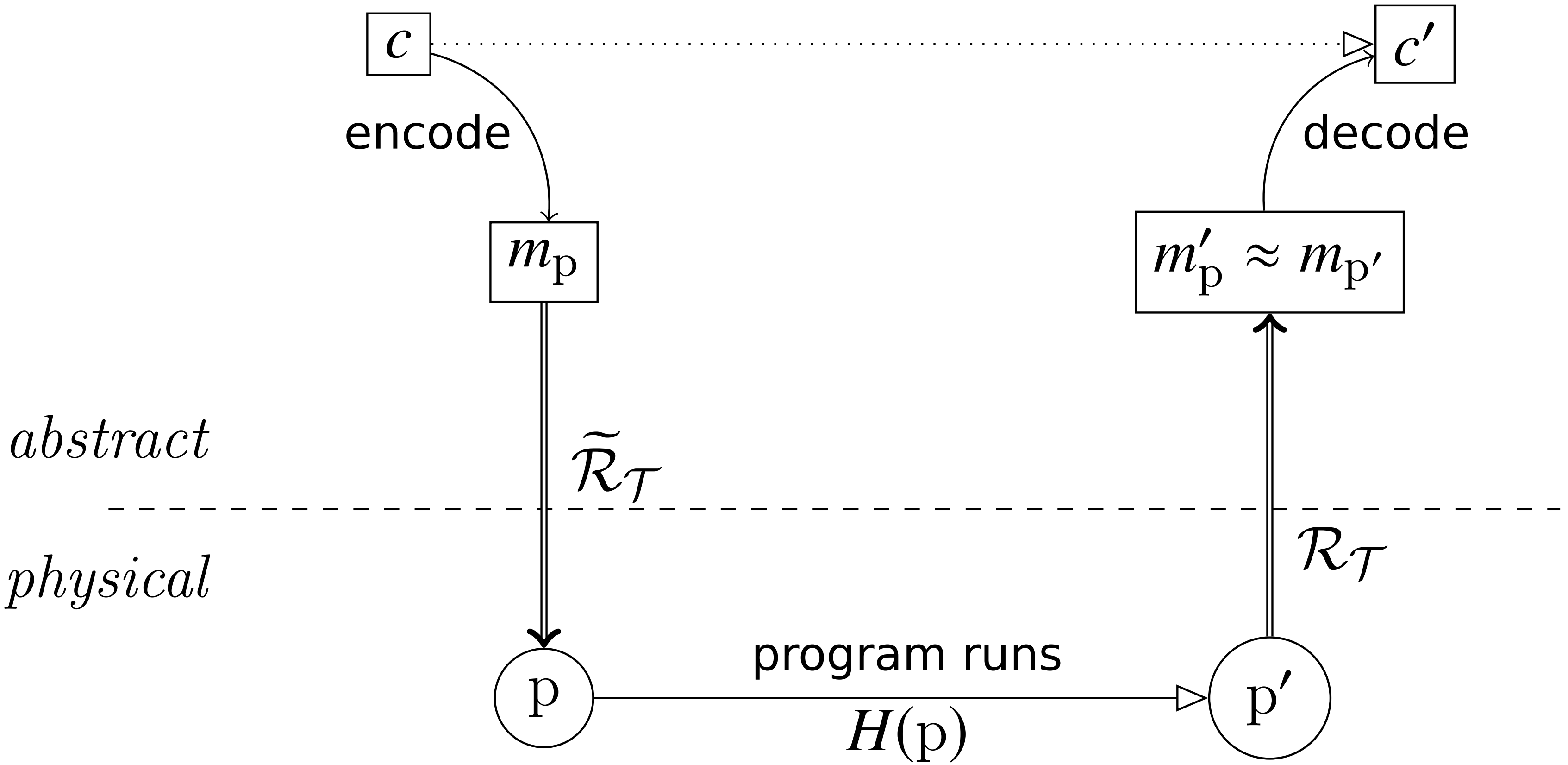
technology is making things we designed, here making a p'



p, $\mathcal{T}$ and H such that we can engineer a physical system to our specifications m'_{p} – effectively inverting $\mathcal{R}_{\mathcal{T}} \longrightarrow \widetilde{\mathcal{R}}_{\mathcal{T}}$
– an instantiation representation relation

computing

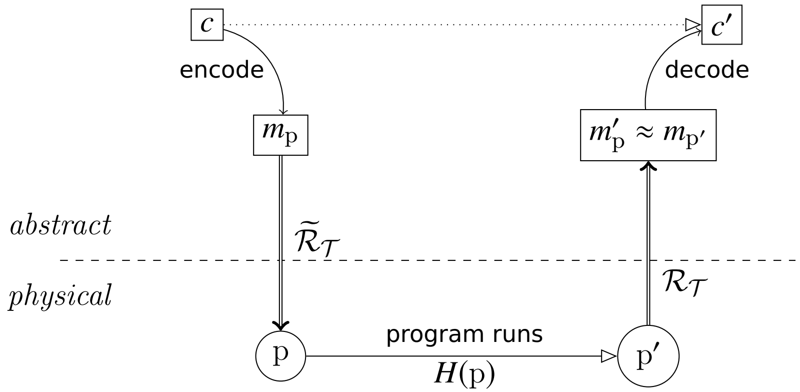
among many things, we engineer computers



computing: use a physical computer p to calculate abstract problem c encode c into model m_p, instantiate $\widetilde{\mathcal{R}}_\mathcal{T}$ into p, run, decode output

requirements for computing

computing is a high level process...



- computations have outputs (else can replace computer with brick...)
- representational entity ("owns" the computation)

  [Stepney/VK "The role of the representational entity..." 219–231 UCNC 2019 & Nat. Comp. 2020]

abstract is instantiated in the representational entity

(does not need to be human – Horsman/VK/Stepney/Young Abstraction and representation in living organisms: when does a biological system compute? in: Representation and reality: Humans, Animals and Machines. Gordana Dodig-Crnkovic and Raffaela Giovagnoli, Editors. Springer 2016)

GOAL: increase computing power . . .

★ *current computers already very powerful*
– two barriers to more computing power:

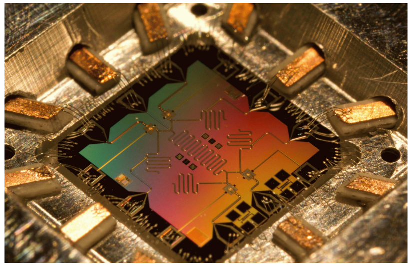
1. silicon chip technology reaching limits
2. energy consumption far from optimal:
   – *resource limits; global warming*

[lots of room to improve on energy consumption

– see, e.g., SpiNNaker project for other ways to use Si]

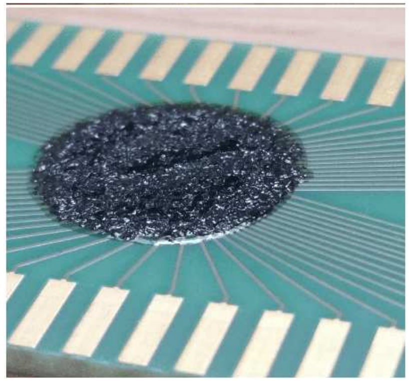
note these are related: can't cool Si chips any faster

beyond silicon . . .

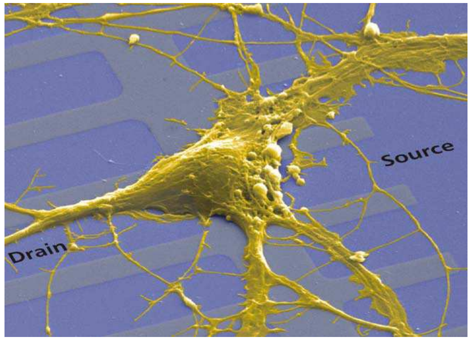


quantum: IBM 5 qubit

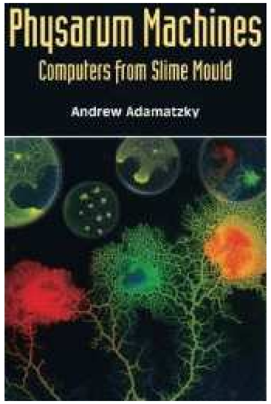
BZ reaction chemical

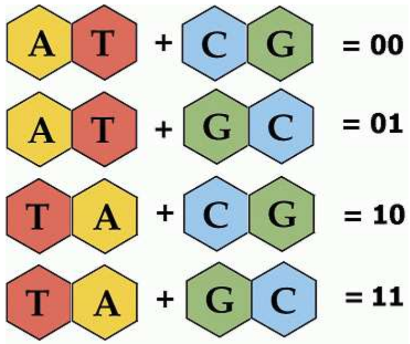


reservoir computer



rat neuron on silicon





encoding for DNA computer

★ future computing is diversifying ★

⇒ *need to co-design algorithms with hardware* ⇐

hybrid computers . . .

practice: co-processors:

conventional:

- graphics cards
- ASIC application-specific integrated circuit
- FPGA field-programmable gate array

unconventional: control + substrate:

- quantum
- NMR
- reservoir
- slime mould

★ hybrid computational systems are the norm ★

theory: single paradigm:

- classical – Turing Machine
- analog – Shannon's GPAC
- quantum – gate model, QTM, CV, MBQC, QW, AQC, . . .
- linear optics (Bosons) `[Aaronson/Arkhipov STOC 2011 ECCC TRI-10 170]`

quantum computing

$$\text{input} \longrightarrow \boxed{\text{encode}} \longrightarrow |\psi_{in}\rangle \longrightarrow \hat{U} \longrightarrow |\psi_{out}\rangle \longrightarrow \boxed{\text{decode}} \longrightarrow \text{result}$$

$\hat{U}$ is unitary evolution (or more generally, open system/environment)
– can be gate sequence, or engineer Hamiltonian $\hat{H}(t)$ such that

$$|\psi_{out}\rangle = \mathcal{T} \exp\{-i/\hbar \int dt \ \hat{H}(t)\} \, |\psi_{in}\rangle$$

★ covers most of quantum information processing . . .
. . . including communications, where aim is *result=input*

$\boxed{\text{encode}}$ – arbitrary choices:

using spin-down $|\downarrow\rangle \equiv 0$ instead of spin-up $|\uparrow\rangle \equiv 0$ makes no difference
$\rightarrow$ provided $\boxed{\text{encode}}$ and $\boxed{\text{decode}}$ done consistently

quantum information processing

quantum information is built on the idea that:

quantum logic allows greater **EFFICIENCY** than **classical logic**

classical	**quantum**
bits, 0 or 1	qubits, $\alpha\,\lvert 0\rangle + \beta\,\lvert 1\rangle$
yes or no, binary decisions	yes and no, superpositions
HEADS or TAILS, random numbers	random measurement outcomes

$\Rightarrow$ quantum gives different computation from classical: how different?

- **computability** – what can be computed?
- **complexity** – how efficiently can it be computed?

$\Rightarrow$ quantum **computability** is the same as classical
complexity differs: some problems can be computed more **EFFICIENTLY**

quantum advantage?

how to translate quantum logic into better computing devices?

depends on definition of **EFFICIENCY**

- *in theory: polynomial scaling with system size*
- *in practice: produces answers on human timescales*

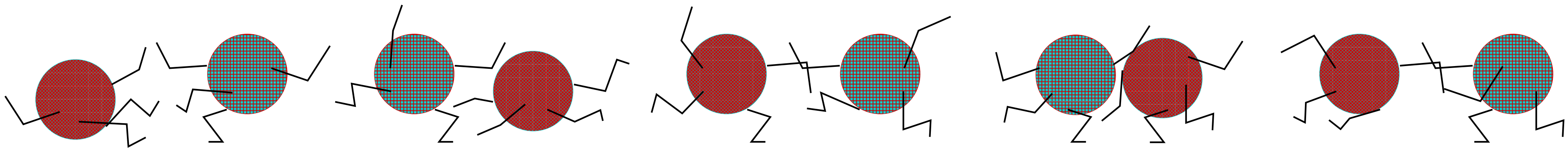
roughly speaking:

quadratic speed up exploits quantum coherence, interference effects

exponential speed up exploits parallelism in quantum superposition

★ comparison of real physical devices, not of mathematical theories

⇒ complexity theory alone won't tell you whether useful in practice



encoding matters . . .

. . . it determines the physical resources required:

Number	*Unary*	*Binary*
0		0
1	•	1
2	••	10
3	• • •	11
4	• • ••	100
...	...	...
2x4	• • ••	1000
=8	• • ••	
...	...	...
N	$N \times \bullet$	$\log_2 N$ bits

Read out:

Unary: measurements with N outcomes

Binary: $\log_2 N$ measurements with 2 outcomes each

$\longrightarrow$ exponentially better for precision

[Ekert & Jozsa PTRSA 356 1769-82 (1998)]

$\longrightarrow$ exponential reduction in memory

[does not have to be binary: Blume-Kohout, Caves, I. Deutsch, Found. Phys. 32 1641-1670 (2002)]

★ floating point: 0.1234567×10^{89} even more efficient, trade precision/memory ★

encoding problems into qubit Hamiltonians

+ computational basis state $|j\rangle = |q_0 q_1 \dots q_k \dots q_{n-1}\rangle$ with $q_k \in \{0,1\}$
+ superposition of all basis states:

$$|\psi_0\rangle = 2^{-n/2} \sum_{j=0}^{2^n-1} |j\rangle = (|0\rangle + |1\rangle)^{\otimes n}$$

encode problem into n-qubit Hamiltonian $\hat{H}_p$

such that solution is lowest energy state (ground state)

example: find state $|m\rangle$ then $\hat{H}_p = \mathbb{1} - |m\rangle\langle m|$

$$\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

example: three qubits, exactly one must be $|1\rangle$

$$\hat{H}_p = (\mathbb{1} - \hat{Z}_1 - \hat{Z}_2 - \hat{Z}_3)^2$$

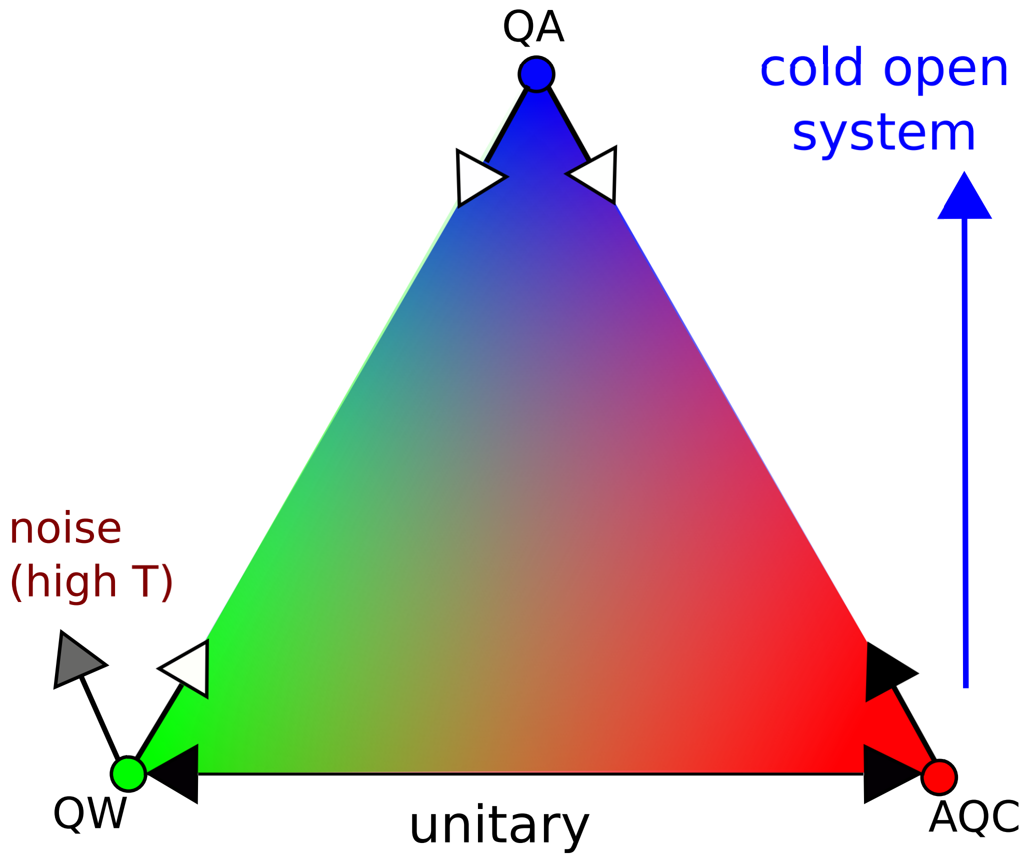
$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Pauli-Z operator: $\hat{Z}|0\rangle = |0\rangle$ and $\hat{Z}|1\rangle = -|1\rangle$

continuous-time quantum computing

family of computational models:

- **discrete** – qubits for efficient encoding
- **continuous time** evolution with engineered Hamiltonian
- coupling to low temp bath – open system effects **cooling**



exploits natural properties of quantum systems

adiabatic quantum computing

given $\hat{H}_p$ [Farhi et al, quant-ph/0001106]

initialise in ground state $|\psi_{\text{init}}\rangle$ of simpler Hamiltonian $\hat{H}_0$ – easy to prepare –

transform adiabatically:

$$\hat{H}(t) = [1 - s(t)]\hat{H}_0 + s(t)\hat{H}_p$$

with *annealing parameter* $s(t = 0) = 0$ and $s(t = t_f) = 1$

$s(t)$ monotonically increasing, function of size of problem space $N = 2^n$ and the *accuracy parameter* ϵ determined by adiabatic condition,

$$\frac{\left|\left\langle \frac{d\hat{H}}{dt} \right\rangle_{1,0}\right|}{(E_1 - E_0)^2} \equiv \epsilon \ll 1, \qquad (1)$$

0 and 1 refer to the ground and excited states, and $\left|\left\langle \frac{d\hat{H}}{dt} \right\rangle_{1,0}\right| \equiv \langle E_1| \frac{d\hat{H}}{dt} |E_0\rangle$

closer ϵ is to zero – the more completely the system will stay in the ground state and the longer the computation will take

continuous time quantum walk

[Farhi & Gutmann, PRA 58, 915-928 (1998); exponential speed up: Childs et al STOC 2003; universal for QC: Childs PRL 102, 180501 2009]

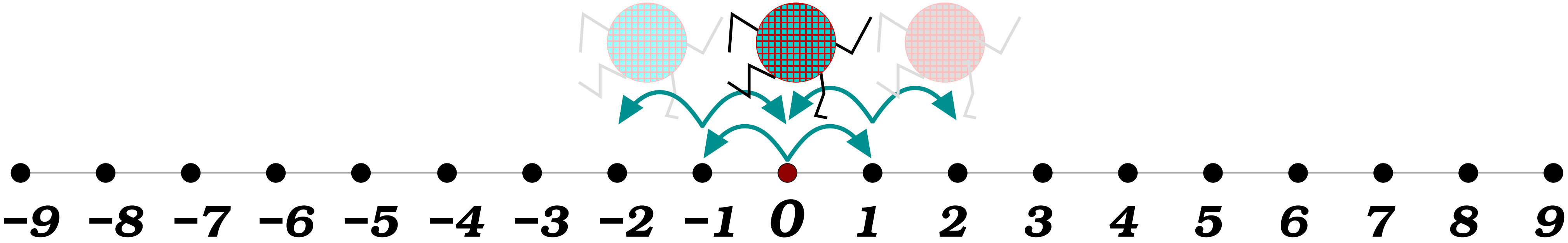
A – adjacency matrix of graph ($A_{jk} = 1$ iff $\exists$ an edge between sites j and k)

Laplacian: $\mathrm{L} = \mathrm{A} - \mathrm{D}$, where D is diagonal matrix $D_{jj} = deg(j)$, the degree of site j of graph [irrelevant global phase for regular graphs]

Hamiltonian of the quantum walk: $\hat{H}_w = -\gamma \mathrm{L}$

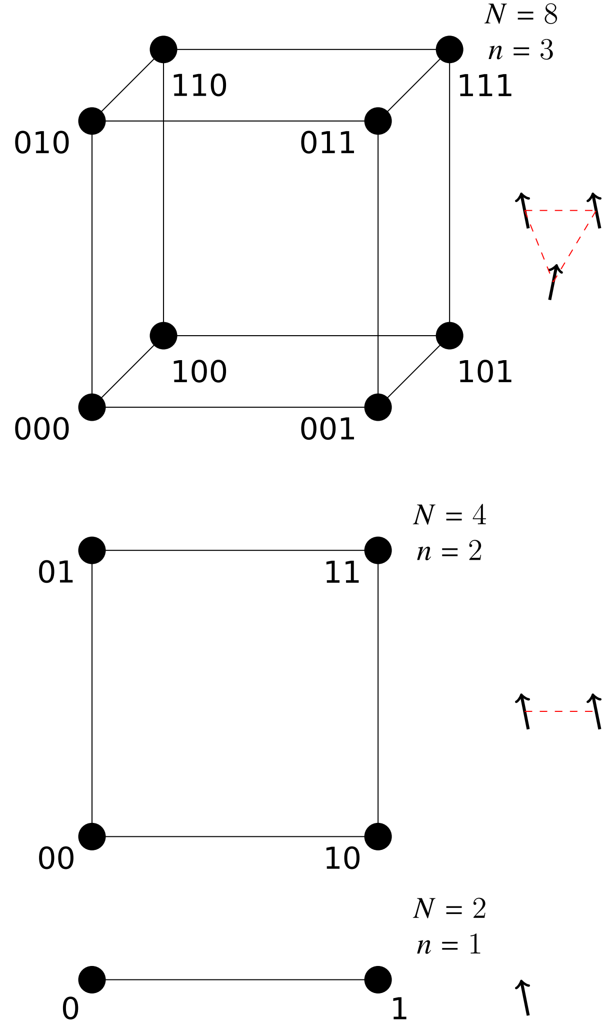
γ = transition rate (prob of moving to connected site per unit time)

$\boxed{\text{quantum walk is } \psi(t) = \exp\{-i\hat{H}_w t\}\psi(0) \text{ then measure at time } t = t_f}$



encoded hypercubes for quantum walks

n qubits encode 2^n vertices:



for a hypercube graph, $\hat{H}_h = \gamma \left(n\mathbb{1} - \sum_j \hat{X}_j \right)$

where j is the qubit label: $j = 0 \ldots n-1$

Pauli-X operator $\hat{X}_j$
bit-flips qubit j $\quad 0 \leftrightarrow 1$

$\longrightarrow$ this moves the position of the quantum walker along an edge of the hypercube

continuous-time quantum search

find the marked state:
the problem Hamiltonian

$$\hat{H}_p = \hat{H}_m = \mathbb{1} - |m\rangle\langle m|$$

– makes $|m\rangle$ lower energy –
★ use the hypercube Hamiltonian $\hat{H}_h$ for the easy Hamiltonian/initial state
– ground state is superposition over all states $|\psi(t=0)\rangle = \{(|0\rangle + |1\rangle)/\sqrt{2}\}^{\otimes n}$

in Pauli operators:

$$\hat{H}_m = \mathbb{1} - \frac{1}{2^n}\prod_{j=1}^{n}(\mathbb{1} + q_j \hat{Z}_j),$$

where $q_j \in \{-1, 1\}$ defines bitstring corresponding to m for $-1 \equiv 0$ to convert to bits; for gadgets to implement this:

Dodds/VK/Adams/Chancellor arχiv:1812.07885

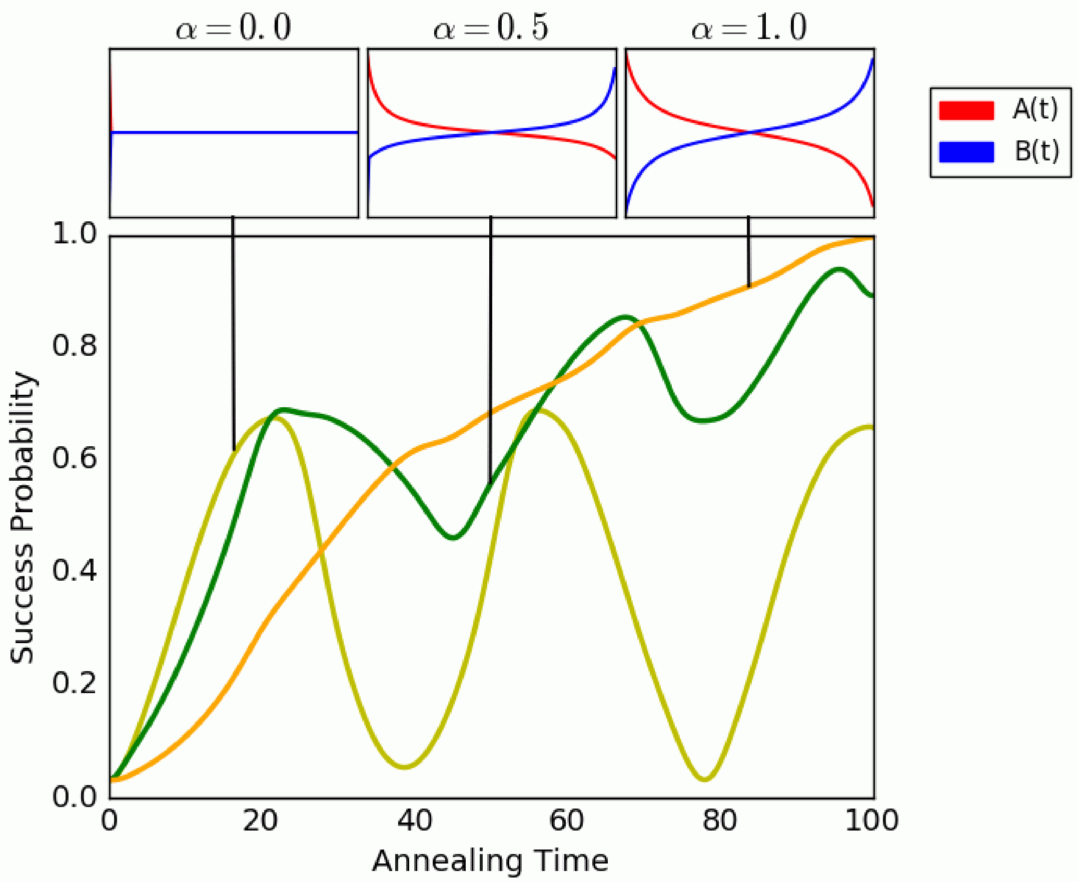
$$\hat{H}(t) = A(t)\hat{H}_h + B(t)\hat{H}_m$$

apply time-evolution

$$|\psi(t_f)\rangle = \mathcal{T}\exp\{-i\int dt\ \hat{H}(t)\}\,|\psi(t=0)\rangle$$

measure after suitable time $t_f \propto \sqrt{N}$ to obtain quantum speed up

hybrid continuous-time quantum search algorithms



interpolate between QW ($\alpha = 0$) and AQC ($\alpha = 1$)

$$\hat{H}(\alpha, t) = A(\alpha, t)\hat{H}_h + B(\alpha, t)\hat{H}_m$$

$$\hat{H}_{QW} = \gamma\hat{H}_h + \hat{H}_m$$

$$\hat{H}_{AQC} = [1 - s(t)]\hat{H}_h + s(t)\hat{H}_m$$

$\rightarrow$ need γ and $s(t)$ . . .

[James Morley's work (UCL CDT)

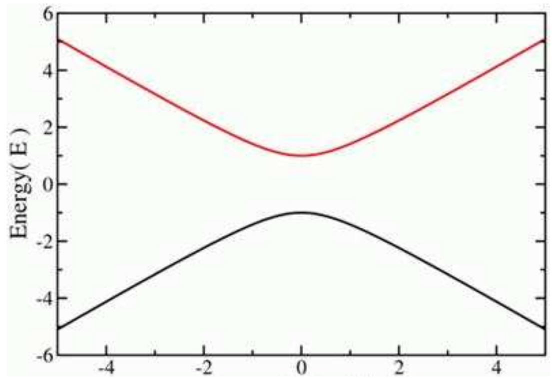
PRA 99, 022339 (2019)

arχiv:1709.00371]

single avoided crossing model

continuous-time quantum seach algorithms all solved analytically
– for large N limit reduces to a 2-dim subspace (single qubit) – for AQC

$$\hat{H}^{(\mathrm{AC})}(s) = (1-s)\hat{H}_0^{(\mathrm{AC})} + s\hat{H}_p^{(\mathrm{AC})}$$
$$= (1-s)\left\{\frac{1}{2}(\mathbb{1}+\hat{Z}) - g_{\mathrm{min}}\hat{X}\right\} + s\frac{1}{2}(\mathbb{1}-\hat{Z})$$



with $g_{\mathrm{min}} = N^{-1/2}$ solving the eigensystem gives

$$E_1 - E_0 = g^{(\mathrm{AC})}(s) = \{(1-2s)^2 + 4g_{\mathrm{min}}^2(1-s)^2\}^{\frac{1}{2}}$$

apply method of Roland+Cerf (2002) to obtain optimal $s(t)$ as solution of

$$\frac{ds}{dt} = \frac{\epsilon[g^{(\mathrm{AC})}(s)]^2}{\left|\left\langle \frac{d\hat{H}_{\mathrm{AC}}}{ds}\right\rangle_{0,1}\right|} = (1-2s)^2 + 4g_{\mathrm{min}}^2(1-s)^2$$

in limit $g_{\mathrm{min}} \ll 1$

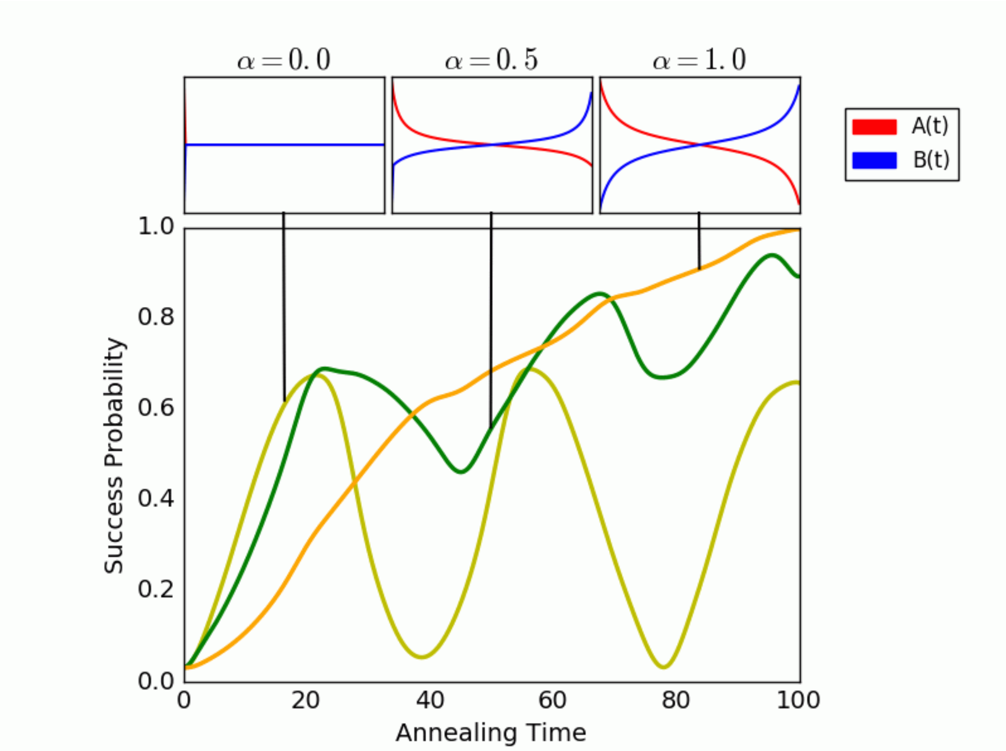
$$s(t) \simeq \frac{1}{2}\left\{1 - g_{\mathrm{min}}\cot\left[g_{\mathrm{min}}(2\epsilon t + 1)\right]\right\}$$

single avoided crossing model

for quantum walk, $\gamma \equiv s = 1/2$ and model reduces to Rabi flops

$$\hat{H}(\gamma) = \frac{1}{2}(\mathbb{1} - g_{\text{min}}\hat{X})$$

interpolate between QW $(\alpha = 0)$ and AQC $(\alpha = 1)$ where $\beta = 1/(1+\gamma)$



$$\hat{H}(\alpha,t) = A(\alpha,t)\hat{H}_h + B(\alpha,t)\hat{H}_m$$

$$\hat{H}_{QW} = \gamma\hat{H}_h + \hat{H}_m$$

$$\hat{H}_{AQC} = [1 - s(t)]\hat{H}_h + s(t)\hat{H}_m$$

$$A(\alpha,t) = \frac{1 - s(\tau)}{\alpha + (1-\alpha)\frac{(1-s(t))}{(1-\beta)}}$$

$$B(\alpha,t) = \frac{s(t)}{\alpha + (1-\alpha)\frac{s(t)}{\beta}}$$

[James Morley’s work (UCL CDT)]

more realistic problems

Sherrington Kirkpatrick spin glasses: frustrated spin systems

★ NP-hard for finding ground state *i.e., expect polynomial speed up*

★ more like realistic hard optimisation problems

$$\hat{H}_p = -\sum_{j=0}^{n=1}\sum_{k=j+1}^{n-1}\frac{J_{jk}+J_{kj}}{2}\hat{Z}_j\hat{Z}_k - \sum_{j=0}^{n=1} h_j\hat{Z}_j$$

J_{jk}, h_j drawn from Gaussian distributions with mean $= 0$ (hardest)

- AQC can find ground states faster than guessing

  [e.g., Martin-Mayor/Hen Sci Rep 5, 15324 (2015); arXiv:1502.02494]

$$\hat{H}(t) = (1 - s(t))\hat{H}_w + s(t)\hat{H}_p$$

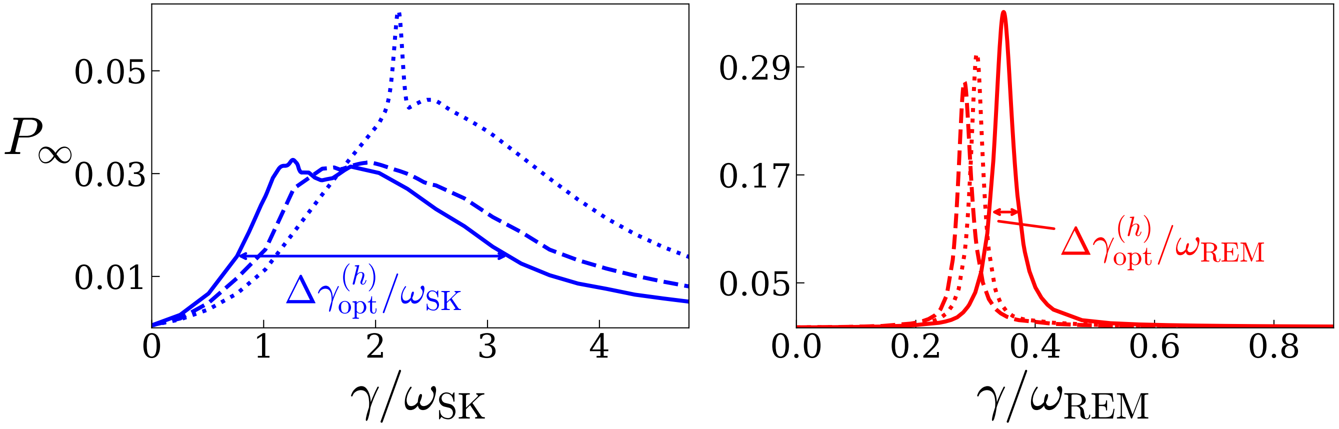
- *what about continuous-time quantum walks?*

$$\hat{H}(t) = \gamma\hat{H}_w + \hat{H}_p$$

- compare with a random energy model (REM)

SK spin glass optimal gamma

need to choose γ i.e., the relative weight of Hamiltonian components:



$$\hat{H}(t) = \gamma \hat{H}_w + \hat{H}_p$$

SK has broad peak compared with narrow peak for random energy model (REM)

11 qubit examples [Adam Callison's work (Imperial CDT) arχiv:1903.05003]

P_∞ = long time success probability of finding the ground state (easy to calculate)

SK spin glass QW dynamics

8 qubit example:

top: time evolution of ground state prob

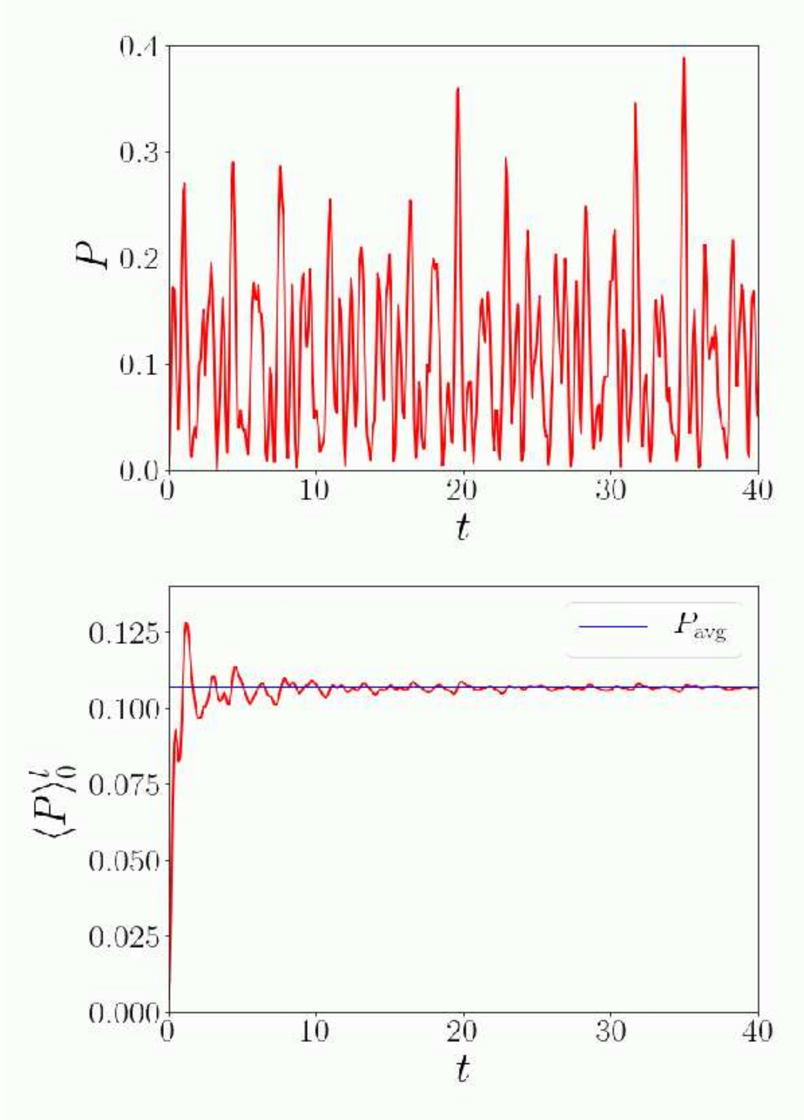
bottom: time-averaged ground state prob

measure at random time to sample time-averaged probability

$$\bar{P}(t,\Delta t) = \frac{1}{\Delta t}\int_{t}^{t+\Delta t} dt P(t)$$

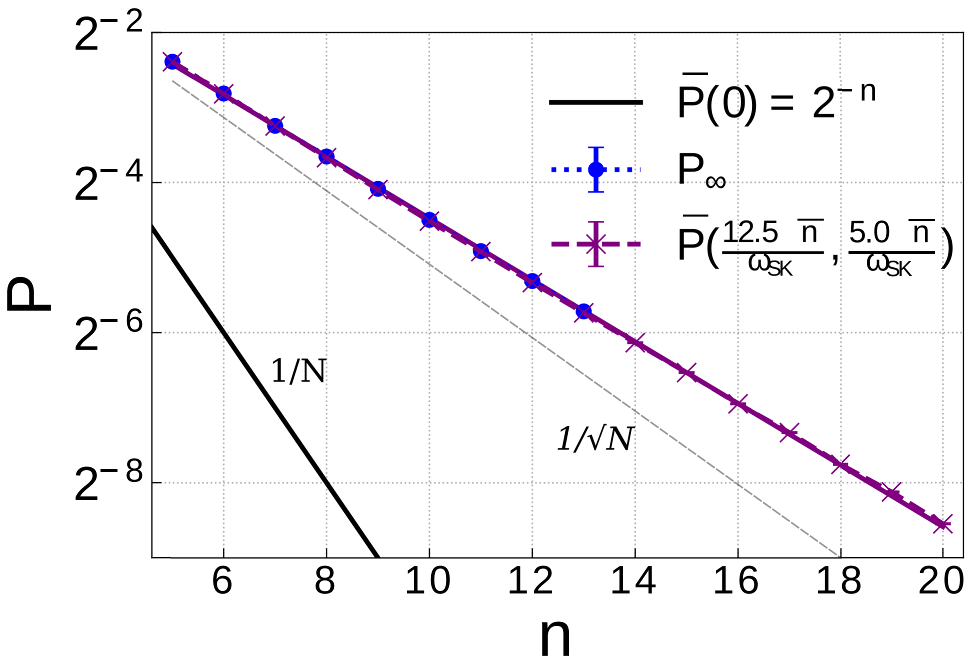
(time scaling better than $O(\log N)$, numerically $n^{0.75}$)

[Adam Callison (Imperial CDT) arχiv:1903.05003]

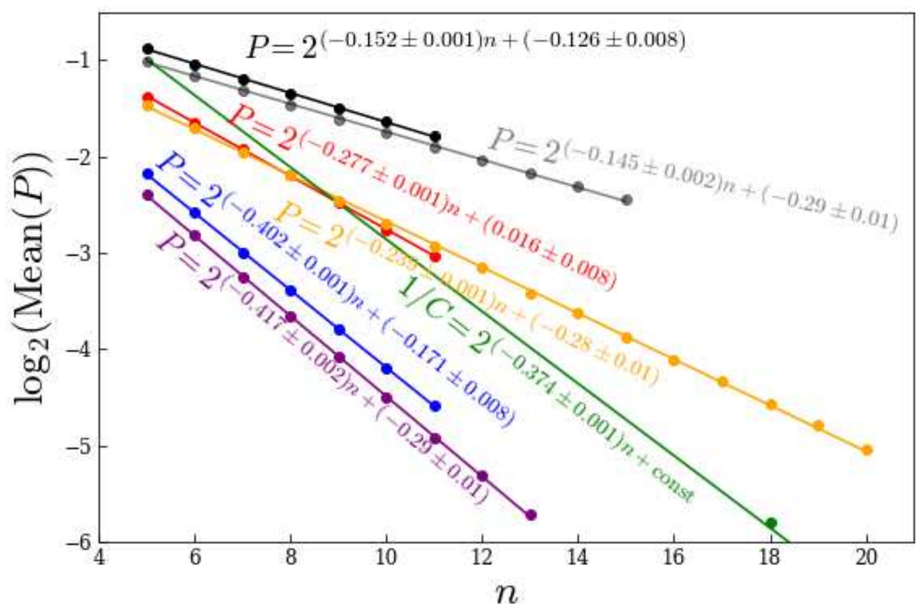


SK spin glass results

success probability scaling for heuristic γ based on energy scales



(average over 10 000 random instances)

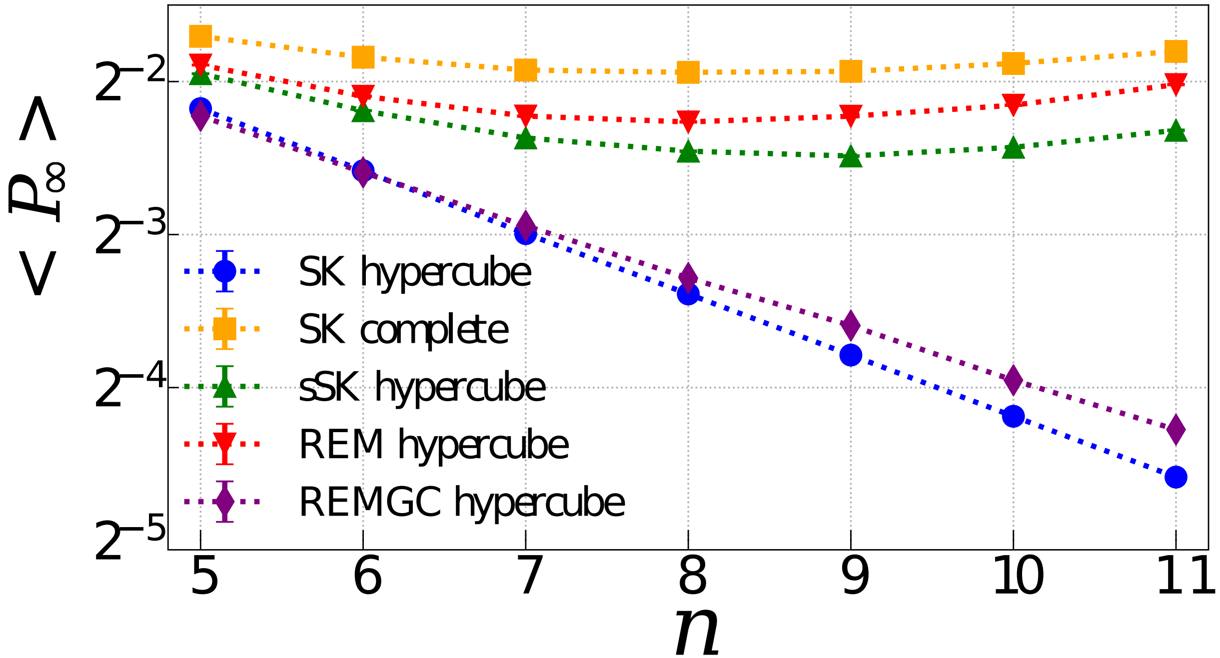


don't need to solve problem to set parameters, heuristic does well

P $\sim N^{-0.41}$ for short run times [Callison/Chancellor/Mintert/VK arχiv:1903.05003 & NJP]

cf P $\sim N^{-0.5}$ for search, i.e., ★ better than search ★

SK spin glass structure



$\longleftarrow$ need to know γ precisely = not practical?

+ add pairwise corrs to REM
– remove corrs from SK
– remove corrs from $\hat{H}_w$

$\Rightarrow$ pairwise correlations matched with hypercube QW Hamiltonian work best

$$\hat{H}_{SK} = -\sum_{j=0}^{n-1}\sum_{k=j+1}^{n-1}\frac{J_{jk}+J_{kj}}{2}\hat{Z}_j\hat{Z}_k - \sum_{j=0}^{n-1} h_j\hat{Z}_j \qquad \hat{H}_h = 1\!\!1 - \frac{1}{n}\sum_{j=0}^{n=1}\hat{X}_j$$

real problems have correlations

★ match problem encoding to algorithm ★

[Callison/Chancellor/Mintert/VK arχiv:1903.05003 & NJP]

Quantum walks are universal for quantum computing

[Childs PRL 102 18051 arχiv:0806.1972]

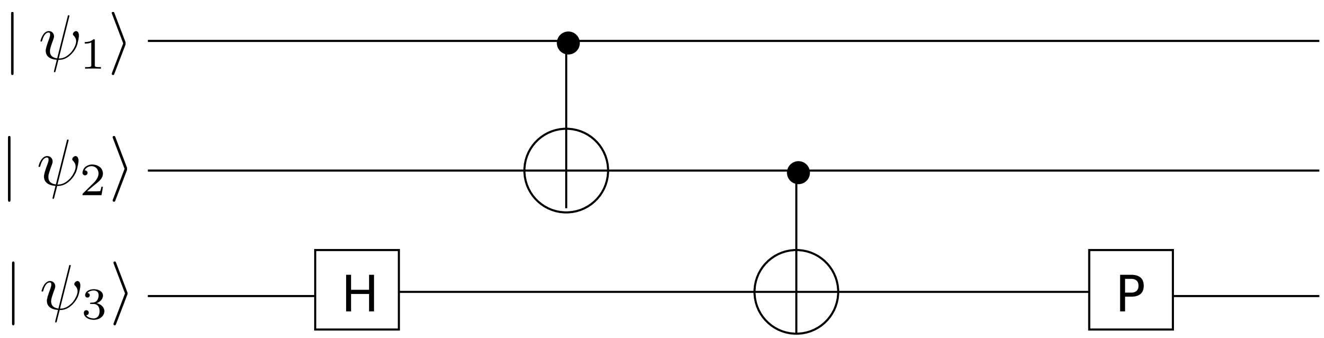
[Lovett/Cooper/Everitt/Trevers/VK PRA 81 042330 arχiv:0910.1024]

...about proving can implement QW efficiently on a quantum computer
...has nothing to do with physical implementation of quantum walks

key phrase from Childs' paper: "any sufficiently sparse graph"
i.e., graph has a description that is logarithmic in the number of sites

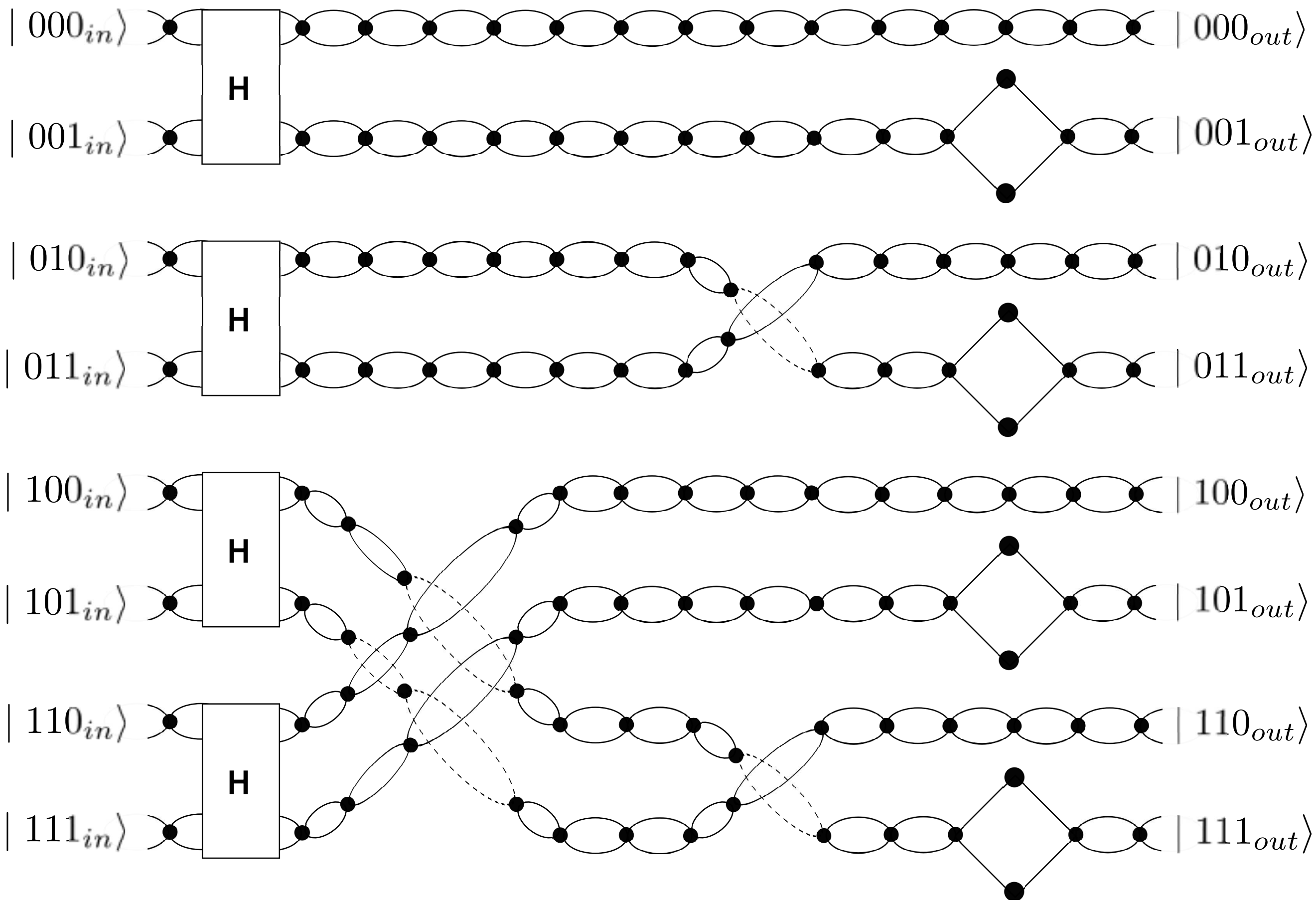
Childs' results characterise which Hamiltonians are efficient to simulate on a quantum computer [Berry et al. Comm. Math. Phys. 270 359 (2007)]

this gate model circuit:



Quantum walk gates

...becomes this quantum walk graph *(thanks to Neil Lovett for figure)*



exponential number of sites is compensated for by binary encoding and superposition

Multiple quantum walkers

★ quantum walkers that **interact** at the same or neighbouring sites
– *like a spin lattice with many excitations delocalised over the lattice*
– special case of quantum cellular automata

QCA are universal for quantum computing
– Quantum Cellular Automata overview: [Wiesner arχiv:0808.0679]

– continuous-time quantum walk construction of universal quantum computation [Childs+Gosset+Webb Science 339, 791 2013] m walkers on L locations $\longrightarrow$ full Hilbert space is L^m
⋆ experiments: atoms in optical lattice [Karski et al Science 325 174 (2009)]
★ multiple **non-interacting** walkers = particle statistics:

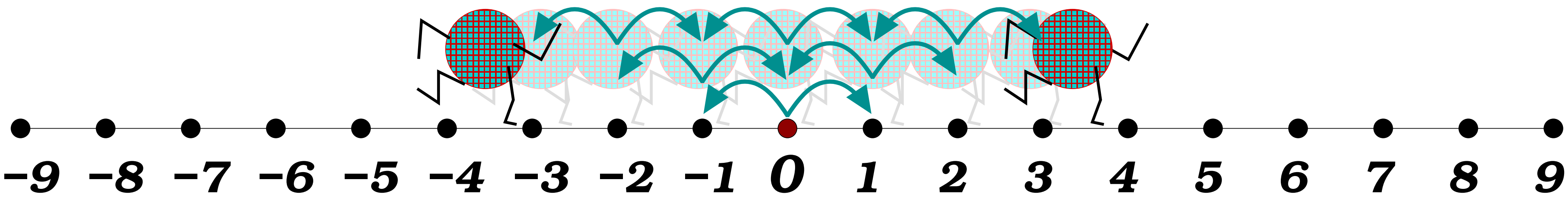
- bosons, intermediate between classical and quantum computing
  Aaronsons+ Arkhipov arχiv:1011.3245
- fermions, only two at once if start on same site – simulate with entanglement
  Sansoni et al arχiv:1106.5713

CTQW computation summary

1. quantum walks can find spin glass ground states
   – *quantum speed up (polynomial, better than Grover's search)*
   – Callison/Chancellor/Mintert/VK arχiv:1903.05003 / NJP 21 123022 2019

2. **continuous-time quantum computing** for simulation and computation
   – Morley/Chancellor/Bose/VK arχiv:1709.00371 / PRA 99 022339 2019 search

3. **abstraction/representation theory** framework
   – Horsman/Stepney/Wagner/VK Proc. Roy. Soc. A 470(2169):20140182
   – Horsman/Stepney/VK Communications of the ACM 60:8 31-34 2017
   – Stepney/VK "The role of the representational entity..." 219–231 UCNC 2019



what next?

- QW on more problems e.g. MAX2SAT
  – *(Adam Callison with Lewis Light & Puya Mirkarimi)*
- adapt Ashley Montanaro's branch and bound speed up to continous-time
  – *optimal algorithm for spin glass ground state problem*
  – *(Adam Callison with Zoë Bertrand & Max Fentenstein)*
- cooling/open system effects – single avoided crossing model/search problem
  – *(Jim Cresser & Steve Barnett (Glasgow); Parth Patel)*