Optimization and physics: the hardness of a problem and annealing strategies to solve it

# JQI Summer School Lecture on July 27<sup>th</sup>, 2018

Tobias Grass (JQI)

### Vacations coming :-)

# In 1954: Write a breakthrough paper! (linear programming algorithm)

Reprinted from JOURNAL OF THE OPERATIONS RESEARCH SOCIETY OF AMERICA Vol. 2, No. 4, November, 1954 Printed in U.S.A.

SOLUTION OF A LARGE-SCALE TRAVELING-SALESMAN PROBLEM\*

> G. DANTZIG, R. FULKERSON, AND S. JOHNSON The Rand Corporation, Santa Monica, California (Received August 9, 1954)

It is shown that a certain tour of 49 cities, one in each of the 48 states and Washington, D. C., has the shortest road distance.



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# In 2018: Ask Siri!



Description

Even the best algorithms fail (i.e. take too long) when the problem size gets bigger

World record:

85,900 connections Took 136 cpu-years to calculate Design of computer chip





**NP-hard:** Problems at least as hard as NP-complete problems, but not necessarily in NP

**NP-complete:** "Hardest" problems in NP (to which any NP problem can be mapped in polynomial time)

**NP**: Decision problems whose positive answer can be *verified* on a deterministic computer in polynomial time, that is equivalent to,

decision problems which can be solved on a non**deterministic** computer in polynomial time.

**P**: Decision problems solvable on a deterministic computer in polynomial time

Open problem:

 $NP \supseteq P$  or NP = P?

(Note the 1 million dollar reward for a proof!)

#### Examples for NP-hard problems:

- Traveling salesperson
- Number partitioning
- Exact cover
- Spin glasses
  - . . .

Journal of Physics A: Mathematical and General

Journal of Physics A: Mathematical and General > Volume 15 > Number 10

On the computational complexity of Ising spin glass models

F Barahona Show affiliations

F Barahona 1982 J. Phys. A: Math. Gen. 15 3241. doi:10.1088/0305-4470/15/10/028

# 1) Simulated annealing:

- Cooling a problem to its solution
- Example: traveling salesperson problem
- 2) Quantum annealing:
  - Quantum time evolution to the solution
  - Examples: Spin models, exact Cover
  - Adiabatic theorem, limitations, and workarounds
  - Physical implementations (D-Wave, ions)
  - 3) Phases of a computational problem:

Statistical physics analysis applied to the number partitioning problem

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#### **Statistical physics:**

- Macroscopic behavior can be understood without knowing microscopic state
- Likelihood of a microscopic state *j* is controlled by Boltzmann factors:  $p_j = e^{-\frac{E_j}{k_B T}}$
- Thermal averages:  $\langle O \rangle_T = \frac{1}{\mathcal{Z}} \sum_j e^{-\frac{E_j}{k_B T}} \langle j | O | j \rangle$

#### **Statistical physics:**

- Macroscopic behavior does not depend on the microscopic state
- Likelihood of a microscopic state *j* is controlled by Boltzmann factors:  $p_j = e^{-\frac{E_j}{k_BT}}$

• Thermal averages: 
$$\langle O \rangle_T = \frac{1}{\mathcal{Z}} \sum_j e^{-\frac{E_j}{k_B T}} \langle j | O | j \rangle$$

#### Metropolis sampling to evaluate average:

- (1) Start with a random microscopic state *j*, and evaluate its energy  $E_j$
- (2) Follow some (well chosen) rules to modify the state, leading to a new state k with energy  $E_k$
- (3) If  $E_k \leq E_j$ : Always accept new configuration:  $p_{j \to k} = 1$ Else: Accept with probability  $p_{j \to k} = e^{-\frac{(E_k - E_j)}{k_B T}}$
- $\blacktriangleright \quad \text{Detailed balance:} \quad p_j \ p_{j \to k} = p_k \ p_{k \to j}$
- Ergodicity: path between any pair of configurations?







# Simulated annealing

#### Intuition:

• Heating and slow cooling can reduce defects in a material

#### Implementation:

- Use Metropolis algorithm for sampling in configuration space
- Energy ↔ Cost function
- Temperature as control parameter:
  - High temperature: explore gross "energy" landscape
  - Lower temperature: force the algorithm into good solution



13 May 1983, Volume 220, Number 4598

# Optimization by Simulated Annealing

S. Kirkpatrick, C. D. Gelatt, Jr., M. P. Vecchi

# SCIENCE

Annealing, as implemented by the Metropolis procedure, differs from iterative improvement in that the procedure need not get stuck since transitions out of a local optimum are always possible at nonzero temperature. A second and more important feature is that a sort of adaptive divide-and-conquer occurs. Gross features of the eventual state of the system appear at higher temperatures; fine details develop at lower temperatures. This will be discussed with specific examples.

## Simulated annealing in the traveling salesperson problem

#### Example: 400 cities in 9 clusters

- High-T: find an efficient way to connect clusters
- Low-T: optimize connection within each cluster



Fig. 9. Results at four temperatures for a clustered 400-city traveling salesman problem. The points are uniformly distributed in nine regions. (a) T = 1.2,  $\alpha = 2.0567$ ; (b) T = 0.8,  $\alpha = 1.515$ ; (c) T = 0.4,  $\alpha = 1.055$ ; (d) T = 0.0,  $\alpha = 0.7839$ .

# Simulated annealing in the traveling salesperson problem

#### Example: 400 cities in 9 clusters

- High-*T*: find an efficient way to connect clusters
- Low-T: optimize connection within each cluster

Simulated annealing typically performs well in finding a good solution, but it usually fails to give the best solution.



Fig. 9. Results at four temperatures for a clustered 400-city traveling salesman problem. The points are uniformly distributed in nine regions. (a) T = 1.2,  $\alpha = 2.0567$ ; (b) T = 0.8,  $\alpha = 1.515$ ; (c) T = 0.4,  $\alpha = 1.055$ ; (d) T = 0.0,  $\alpha = 0.7839$ .

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Statistical physics analysis applied to the number partitioning problem

PHYSICAL REVIEW E

VOLUME 58, NUMBER 5

NOVEMBER 1998

#### Quantum annealing in the transverse Ising model

Tadashi Kadowaki and Hidetoshi Nishimori Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551, Japan (Received 30 April 1998)

	Simulated annealing (SA)	Quantum annealing (QA)
Dynamics	Master equation	Schroedinger equation
	$\frac{\mathrm{d}}{\mathrm{d}t}P_i(t) = \mathcal{L}_{ij}(t)P_j(t)$	$i\hbar\partial_t\Psi(t) = \mathcal{H}(t)\Psi(t)$
Driving force	Thermal fluctuations	Quantum fluctuations
Control parameter	Temperature (from equilibrium at high T to equilibrium at zero T)	Quantum field strength (from ground state at strong field to ground state at no field)

- Cost function given by the Hamiltonian of a a (classical) Ising model:
- Transverse field to control quantum fluctuations:

$$H = -\sum_{i,j} J_{ij}\sigma_z^i\sigma_z^j - \sum h_i\sigma_z^i$$

$$\mathcal{H}(t) = H + \Gamma(t) \sum_{i} \sigma_x^i$$

#### Which dynamics, SA vs QA, comes closer/faster to the ground state ?

(I) Ferromagnetic model

 $\Gamma(t) = T(t) \sim 1/\ln(t+1)$ 





#### (II) Spin glass model

 $\Gamma(t) = T(t) \sim 1/t$ 



#### Results:

- Slow decay: Both SA and QA reproduce stationary states
- Fast decay: QA gets closer to ground state
- QA works particularly well in glassy system

#### **Disordered quantum magnet**

25

20

**15** H<sup>15</sup> H<sup>10</sup>

5

0

0

G

0.1

0.2

Doped material with randomly distributed spins:

 $H_J=-\sum_{i,j}J_{ij}\sigma^i_z\sigma^j_z$ Transverse magnetic field term:  $H_t=-\Gamma\sum_i\sigma^i_x$ Phase diagram:

 $LiHo_{0.44} Y_{0.56}F_4$ 

**Disordered Ferromagnet** 

PM

FM

0.3

В

0.4

T (K)

0.5

0.6

0.7

0.8

# Cooling schedule and ac susceptibility (at 15Hz) as a function of time:



J. Brooke, D. Bitko, T. F. Rosenbaum, G. Aeppli Science 284, 779 (1999)

### Quantum annealing for Exact Cover Problem

#### **Relation to computer science:**

Can quantum annealing solve an NP-hard computational problem?

Example in early proposal: "Exact Cover 3"

- Given N bits {z<sub>1</sub>,...,z<sub>N</sub>} and M clauses
   Each clause selects three bits {z<sub>i</sub>, z<sub>j</sub>, z<sub>k</sub>}, demanding z<sub>i</sub>+z<sub>i</sub>+z<sub>k</sub>=2
- Is there a bit assignment which satisfies all clauses simultaneously?



Can quantum annealing solve an NP-hard computational problem?

Early proposal: Exact cover.

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- Is there a bit assignment which satisfies all clauses simultaneously?

# • Spin language: $H = \sum_{C} h(C)$ with $h(C_{ijk}) = (\sigma_z^i + \sigma_z^j + \sigma_z^k - 1)^2$ Is the ground state energy E=0 or E>0?



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- Is there a bit assignment which satisfies all clauses simultaneously?
- Spin language:  $H_p = \sum_{C} h(C)$  with  $h(C_{ijk}) = (\sigma_z^i + \sigma_z^j + \sigma_z^k 1)^2$ Is the ground state energy E=0 or E>0?

Exponentially many  
satisfying assignments
$$\left(\frac{M}{N}\right)_{c} \sim 0.6$$
  
No satisfying assignment  
EASY $M$   
NEASYHARDEASY

• Generate generically hard instances by constructing clauses with unique satisfying assignment (USA)

Annealing schedule:  $\mathcal{H}(t) = (1 - \frac{t}{T})H_t + \frac{t}{T}H_p$  with  $H_t = B\sum_i \sigma_x^i$ What is the probability of being in the ground state of  $H_p$  at time t=T?





#### Quantum annealing for Exact Cover Problem

#### Numerical results:

• Success probability:

$$p = |\langle \text{GS of } H_{\text{p}}| \text{State at } t = T \rangle|^2$$

For a given system size N, find runtime T such that p is fixed, e.g., p=1/8

• *T* is found to scale polynomially with *N* 



- Averaged over the worst 10%, the probability remains relatively constant with *N*
- Accessible system size too small to make strong claims regarding scalability





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### Adiabatic theorem and Landau-Zener problem

Spin-1/2 particle in a time-dependent magnetic field:

$$H(t) = \frac{1}{2}\gamma t\sigma_z + \frac{1}{2}\Delta\sigma_x$$



- Time-dependent Schroedinger equation:  $i\hbar \begin{pmatrix} \dot{a}(t) \\ \dot{b}(t) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \gamma t & \Delta \\ \Delta & -\gamma t \end{pmatrix} \cdot \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$
- Leads to one second-order differential equation which can be solved exactly
- Probability of excitation during the evolution:  $P_{\rm LZ} = e^{-\pi\Gamma^2/2}, \quad \Gamma \equiv \frac{\Delta}{\sqrt{\hbar\gamma}}$
- Adiabatic condition:  $\Gamma \gg 1 \Rightarrow \Delta^2 \gg \hbar \gamma$
- The annealing time has to scale as  $T \sim rac{1}{\Lambda^2}$

### Scaling of the gap in Exact Cover QA Algorithm

### Anderson localization makes adiabatic quantum optimization fail

Boris Altshuler, Hari Krovi, and Jérémie Roland PNAS July 13, 2010. 107 (28) 12446-12450; https://doi.org/10.1073/pnas.1002116107



#### Perturbative expansion:

$$E(\lambda, \mathbf{s}) = E_{\text{cost}}(\mathbf{s}) + \sum_{m=1}^{\infty} \lambda^{2m} F^{(m)}$$

$$E_1(\lambda) - E_2(\lambda) = \sum_{m=2}^{\infty} \lambda^{2m} [F_1^{(m)} - F_2^{(m)}]$$

$$N \gg 1$$
:  $F_i^{(m)} \cong \sum_{k=1}^N r_k, \quad r_k = \mathcal{O}(1)$ 

First-order correction is the same for all configurations

For large N, the coefficients F<sup>(m)</sup> behave like sum of random numbers

 $\mathcal{O}(N)$ = leading order:  $\Rightarrow |E_1(\lambda) - E_2(\lambda)| \cong \sqrt{N} \sum \lambda^{2m} \sim \sqrt{N} \lambda^4 \stackrel{!}{\sim} 4 \quad \Rightarrow \quad \lambda_{\text{crossing}} \sim N^{-1/8}$ m=2 $m_{\rm f} \sim f({\rm M/N}) {\rm N}$ 

"spin-flip-distance"

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$$V \gg 1: \quad F_i^{(m)} \cong \sum_{k=1} r_k, \quad r_k = \mathcal{O}(1)$$
  
+  $\langle F_1^{(m)} - F_2^{(m)} \rangle = 0, \quad \langle (F_1^{(m)} - F_2^{(m)})^2 \rangle$ 

$$k=1 \\ \Rightarrow \langle F_1^{(m)} - F_2^{(m)} \rangle = 0, \quad \langle (F_1^{(m)} - F_2^{(m)})^2 \rangle = \mathcal{C}$$

 $\Delta \sim \lambda_{\text{crossing}}^{m_{\text{f}}} \sim \exp\{[-f(M/N)N/8]\ln(N/N_0)\}$ 

#### • Modify cost function?

Exponentially small gaps have also been seen for other cost functions of similar complexity [T. Joerg, F. Krzakala, J. Kurchan, A.C. Maggs, PRL 101, 147204 (2008)]

• Modify the initial Hamiltonian?

Standard protocol:  $\mathcal{H}(t) = (1 - \gamma)H_t + \gamma H_p$  with  $H_t = B \sum_i \sigma_x^i$ Modified protocol:  $H_t = B \sum_i \mu_i \sigma_x^i$ [E. Farhi, J. Goldstone, D. Gosset, S. Gutmann, H. Meyer, P. Shor, Quant. Inf. Comp. 11, 181 (2011)]

• Make the Hamiltonian non-stoquastic?

Stoquastic: No sign problem. All off-diagonal elements (in z-basis) are positive (e.g. transverse Ising) Introducing terms which render the Hamiltonian non-stoquastic can turn 1<sup>st</sup> order phase transitions to  $2^{nd}$  order transitions:

Example:

 $\mathcal{H}(\gamma, \lambda) = \gamma H_{\rm p} + (1 - \gamma) \mathbf{H}_{\rm t} + \gamma (1 - \lambda) \mathbf{H}_{\rm XX}$ 

[H. Nishimori and K. Takada Front. ICT 4:2 (2017)]

Thermal assisted quantum annealing?
 [N. Dickson et al., Nat. Commun. 4, 1903 (2013)]



### Experimental realization: D-wave



- Up to 2048 superconducting flux qubits
- Programmable Josephson couplings in blocks of 8 qubits and between blocks (chimera geometry)
- Individual longitudinal fields and global transverse field

$$\mathcal{H}(t) = A(t) \left( \sum_{\langle i,j \rangle} J_{ij} \sigma_z^i \sigma_z^j + \sum h_i \sigma_z^i \right) \\ + B(t) \sum_i \sigma_x^i$$

Does it work? – Maybe!

Output matches expectations [S. Boixo et al., Nature Phys. 10, 218 (2014)]

No clear sign of quantum speedup [T. Ronnow et al., Science Science 345, 420 (2014)]

### Alternative platforms: Trapped ions

- Raman spin-flip transition coupled to different phonon modes m •
- Second-order: effective Ising model  $H = -\sum_{m} \sum_{ij} \frac{\hbar \Omega^{(i)} \eta_m^{(i)} \Omega^{(j)} \eta_m^{(j)}}{\delta_m} \sigma_z^{(i)} \sigma_z^{(j)}$ Close to a resonance we get a Mattis model:  $H = -\text{sign}(\delta) \sum_{ij} \xi^{(i)} \xi^{(j)} \sigma_z^{(i)} \sigma_z^{(j)}$ .
- •

Energy:  $E(s_1, \cdots, s_N) = -\operatorname{sign}(\delta) \Big( \sum_{s_i=\uparrow} \xi^{(i)} - \sum_{s_i=\downarrow} \xi^{(i)} \Big)^2$ 

#### Ferromagnetic coupling ( $\delta > 0$ ):

Two ground states, all spins either aligned or anti-aligned with the parameter  $\xi_i$ 

#### Antiferromagnetic coupling ( $\delta < 0$ ):

Many ground states are possible. Hamiltonian represents the "number partitioning" problem

Can we anneal the ions into the solution of this NP-hard problem? . Exact diagonalization for 6 ions and phonons: Solution obtained on experimentally feasible time scales

Semiclassical simulation for 22 ions and phonons: Annealing time scales as  $~~ au \propto N^4$ 

12 13 17 20 9 2+9+12+20 - 6 - 7 - 13 - 17 = 06+17+20 - 2 - 7 - 9 - 12 - 13 = 0

T. Grass, D. Raventos, B. Julia-Diaz, C. Gogolin, M. Lewenstein Nat. Commun. 7, 11524 (2016)

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Statistical physics analysis applied to the number partitioning problem

Phase transition in the number partitioning problem

# PHYSICAL REVIEW LETTERS

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NUMBER 20

#### Phase Transition in the Number Partitioning Problem

Stephan Mertens\*

Universität Magdeburg, Institut für Physik, Universitätsplatz 2, D-39106 Magdeburg, Germany [T. Joerg, F. Krzakala, J. Kurchan Reviewe Maggs, 1999, 101, 147204 (2008)]



Theoretical Computer Science

Volume 265, Issues 1–2, 28 August 2001, Pages 79-108



# A physicist's approach to number partitioning

Stephan Mertens 😤 🖾

# Classical algorithm for number partitioning



# Complexity of the problem



$$E = \left|\sum_{j=1}^{N} a_j s_j\right|$$

$$E = \left|\sum_{j=1}^{N} a_j s_j\right|$$
$$Z = \sum e^{-\frac{1}{T}\left|\sum_j a_j\right|}$$

Partition function:

$$Z = \sum_{\{s_j\}} a_j s_j$$
$$Z = \sum_{\{s_j\}} e^{-\frac{1}{T} |\sum_j a_j s_j|}$$

$$E = \left|\sum_{j=1}^{N} a_j s_j\right|$$

Partition function:

$$Z = \sum_{\{s_j\}}^{j=1} e^{-\frac{1}{T} |\sum_j a_j s_j|}$$

Without the absolute value, life would be easy:

$$\sum_{\{s_j\}} e^{-\frac{1}{T}\sum_j a_j s_j} = \sum_{\{s_j\}} \prod_{j=1}^N e^{-\frac{1}{T}a_j s_j}$$
$$= \sum_{s_1=\pm 1} e^{-\frac{1}{T}a_1 s_1} \cdot \sum_{s_2=\pm 1} e^{-\frac{1}{T}a_2 s_2} \cdot \ldots \cdot \sum_{s_N=\pm 1} e^{-\frac{1}{T}a_N s_N}$$
$$= 2\cosh\frac{a_1}{T} \cdot 2\cosh\frac{a_2}{T} \cdot \ldots \cdot 2\cosh\frac{a_N}{T}$$
$$= 2^N \prod_{j=1}^N \cosh\frac{a_j}{T}$$

$$E = \left|\sum_{j=1}^{N} a_j s_j\right|$$

Partition function:

$$\overline{j=1}$$

$$Z = \sum_{\{s_j\}} e^{-\frac{1}{T} |\sum_j a_j s_j|}$$

Use Dirac function:

$$Z = \sum_{\{s_j\}} \int_{-\infty}^{\infty} dx \, e^{-|x|} \, \delta\left(x - \frac{1}{T} \sum_{j=1}^{N} a_j s_j\right)$$

$$\stackrel{\bigstar}{=} \int_{-\infty}^{\infty} dx \, e^{-|x|} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\hat{x} e^{ix\hat{x}} \sum_{\{s_j\}} e^{-i\frac{\hat{x}}{T} \sum_j a_j s_j}$$

$$= 2^N \int_{-\infty}^{\infty} \frac{d\hat{x}}{2\pi} \prod_{j=1}^{N} \cos\left(\frac{a_j}{T}\hat{x}\right) \int_{-\infty}^{\infty} dx \, e^{-|x| + i\hat{x}x} \quad \bigstar$$

$$\bigstar \,\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\hat{x} e^{ix\hat{x}}$$

$$\bigstar \quad \int_{-\infty}^{\infty} dx \ e^{-|x| + i\hat{x}x} = \frac{2}{1 + \hat{x}^2}$$

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Rewriting

it: 
$$Z = 2^N \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{dy}{\pi} e^{NG(y)} \quad \text{with} \quad G(y) = \frac{1}{N} \sum_{j=1}^N \ln \cos(\frac{a_j}{T} \tan(y))$$
$$= \left\langle \ln \cos(\frac{a}{T} \tan(y)) \right\rangle$$

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$$y = \arctan \hat{x}$$

$$Z = 2^N \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{dy}{\pi} e^{NG(y)} \quad \text{with} \qquad G(y) = \frac{1}{N} \sum_{j=1}^N \ln \cos(\frac{a_j}{T} \tan(y))$$

$$= \left\langle \ln \cos(\frac{a}{T} \tan(y)) \right\rangle$$

Laplace method / Steepest descent method / Saddle-point method:

Rewriting it:

$$\int e^{NG(y)} dx \approx e^{NG(y_0)} \int e^{-\frac{N}{2}G''(y_0)(y-y_0)^2} dy = e^{NG(y_0)} \sqrt{\frac{2\pi}{NG''(y_0)}}$$

$$y = \arctan \hat{x}$$
$$Z = 2^N \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{dy}{\pi} e^{NG(y)} \quad \text{with} \qquad G(y) = \frac{1}{N} \sum_{j=1}^N \ln \cos(\frac{a_j}{T} \tan(y))$$
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Laplace method / Steepest descent method / Saddle-point method:

$$\int e^{NG(y)} dx \approx e^{NG(y_0)} \int e^{-\frac{N}{2}G''(y_0)(y-y_0)^2} dy = e^{NG(y_0)} \sqrt{\frac{2\pi}{NG''(y_0)}}$$

Saddle points:

Rewriting it:

$$G'(y) = \left\langle \frac{a}{T} \tan\left(\frac{a}{T} \tan y\right) \right\rangle \cdot (1 + \tan^2 y) = 0$$
$$y_k = \arctan\left(\frac{\pi T}{\Delta a}k\right) \qquad k = 0, \pm 1, \pm 2, \dots$$
Numbers are discrete!

$$G''(y_k) = \frac{\langle a^2 \rangle}{T^2} \left[ 1 + \left(\frac{\pi T}{\Delta a}\right)^2 k^2 \right]^2$$

Result:

$$Z \approx 2^{N} \sum_{k} \int_{-\infty}^{\infty} \frac{dy}{\pi} e^{-\frac{N}{2}G''(y_{k})y^{2}} = 2^{N} \frac{\sqrt{2}}{\sqrt{\pi N}} \sum_{k} \frac{1}{\sqrt{G''(y_{k})}}$$

$$\stackrel{\bigstar}{=} 2^{N} \cdot \frac{\Delta a}{\sqrt{\frac{\pi}{2}N} \langle a^{2} \rangle} \cdot \coth \frac{\Delta a}{T}$$

$$\bigstar \sum_{k=0,\pm 1,\dots} \frac{1}{1+(xk)^2} = \frac{\pi}{x} \cdot \coth \frac{\pi}{x}$$

Partition Function: Z

$$= 2^N \cdot \frac{\Delta a}{\sqrt{\frac{\pi}{2}N \langle a^2 \rangle}} \cdot \coth \frac{\Delta a}{T}$$

Free energy:

$$F(T) = -TN\ln 2 + \frac{T}{2}\ln \frac{\pi N \langle a^2 \rangle}{2\Delta a^2} - T\ln \coth \frac{\Delta a}{T}$$

Thermal energy:

$$\langle E \rangle_T = \frac{\Delta a}{\sinh \frac{\Delta a}{T} \cosh \frac{\Delta a}{T}}$$

$$\lim_{T \to 0} \langle E \rangle_T = 0$$

 $\begin{array}{ll} \mbox{Partition} & Z &= 2^N \cdot \frac{\Delta a}{\sqrt{\frac{\pi}{2}N \left\langle a^2 \right\rangle}} \cdot \coth \frac{\Delta a}{T} \\ \mbox{Function:} & F(T) = -TN \ln 2 + \frac{T}{2} \ln \frac{\pi N \left\langle a^2 \right\rangle}{2\Delta a^2} - T \ln \coth \frac{\Delta a}{T} \end{array}$ 

Entropy:

$$S = N(\kappa_c - \kappa) \ln 2 + \tilde{S}(\frac{\Delta a}{2T}),$$

with

$$\kappa_c = 1 - \frac{\ln\left(\frac{\pi}{6}N\right)}{N 2 \ln 2}$$
$$\kappa = \frac{\ln\frac{3}{\Delta a^2} \langle a^2 \rangle}{N 2 \ln 2}$$
$$\tilde{S}(\frac{\Delta a}{T}) = \ln \coth\frac{\Delta a}{T} + \frac{\Delta a}{T} \frac{\coth^2\frac{\Delta a}{T} - 1}{\coth\frac{\Delta a}{T}}$$

Free energy:  $F(T) = -TN\ln 2 + \frac{T}{2}\ln \frac{\pi N \langle a^2 \rangle}{2\Delta a^2} - T\ln \coth \frac{\Delta a}{T}$ 

Entropy:

$$S = N(\kappa_c - \kappa) \ln 2 + \tilde{S}(\frac{\Delta a}{2T}),$$

with

$$\kappa_c = 1 - \frac{\ln\left(\frac{\pi}{6}N\right)}{N\,2\ln2}$$

$$\kappa = \frac{\ln \frac{3}{\Delta a^2} \left\langle a^2 \right\rangle}{N \, 2 \ln 2}.$$

$$\tilde{S}(\frac{\Delta a}{T}) = \ln \coth \frac{\Delta a}{T} + \frac{\Delta a}{T} \frac{\coth^2 \frac{\Delta a}{T} - 1}{\coth \frac{\Delta a}{T}}$$

- $\kappa < \kappa_{\rm c}$  :
- extensive entropy
- exponentially many solutions
- "easy" phase

$$\kappa > \kappa_{\rm c}$$
:

- negative entropy?
- not at finite temperature
- There is no absolute zero → Energy will remain finite!
- "hard" phase

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$$F(T) = -TN\ln 2 + \frac{T}{2}\ln \frac{\pi N \langle a^2 \rangle}{2\Delta a^2} - T\ln \coth \frac{\Delta a}{T}$$

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$$\tilde{S}(\frac{\Delta a}{T}) = \ln \coth \frac{\Delta a}{T} + \frac{\Delta a}{T} \frac{\coth^2 \frac{\Delta a}{T} - 1}{\coth \frac{\Delta a}{T}}$$
$$T_0 = 2\Delta a \, 2^{N(\kappa - \kappa_c)} = \sqrt{2\pi N \langle a^2 \rangle} \, 2^{-N}$$

Minimum temperature and thermal energy when  $\kappa > \kappa_{\rm C}$ :

$$\langle E_1 \rangle = T_0 = \sqrt{2\pi N \langle a^2 \rangle} \ 2^{-N}$$

- $\kappa < \kappa_{\rm c}$  :
- extensive entropy
- exponentially many solutions
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$$\kappa > \kappa_{\rm c}$$
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- negative entropy?
- not at finite temperature
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# **Comparison with numerical results**



# **Comparison with numerical results**



# 1) Simulated annealing:

- Simple sampling algorithm (Metropolis)
- Slow changes in control parameter ("temperature")

# 2) Quantum annealing:

- Adiabatic quantum time evolution
- Control parameter: transverse field
- Fails when small gaps occur along the annealing path

# 3) Analysis of the number partitioning problem:

"Entropy" becomes negative  $\rightarrow$  phase transition to "hard" phase. "Absolute" zero at finite temperature/energy.