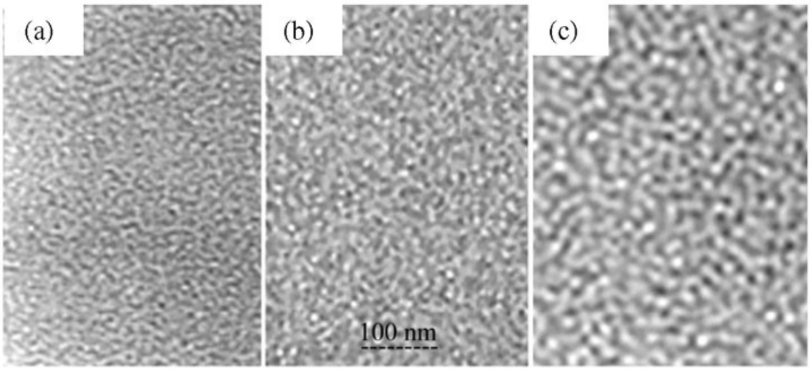
Annealing : Classical and Quantum

Note Title

2015-11-12



Time taken to cool (fixed ΔT)

The basic idea: cool a material (metal, glass, ...) slowly to let large ordered regions form

Widely used in
- metallurgy
- glassmaking
- algorithms ??

In conventional computation: Simulated Annealing

(not too closely related to quantum annealing, but still pretty cool)

"energy"

Q: Given some function E on some (maybe very large) space of states $\{s\}$, how would you tell a computer to find its global minimum?

SA: iterative procedure

- suppose you're in state s with energy $E(s)$

1. Pick some "neighbouring state" s', compute $E(s')$
2. With probability $P(E(s), E(s'); T)$, move to state s'
3. GOTO 1.

What's this?

$$P(E, E'; T) := \begin{cases} 1 & \text{if } E' \leq E \\ \exp\left\{-\frac{E'-E}{T}\right\} & \text{otherwise} \end{cases}$$

T is the "temperature" — should start very big, and slowly decrease as the algorithm progresses

Q: Why is it important to sometimes move to larger E'?

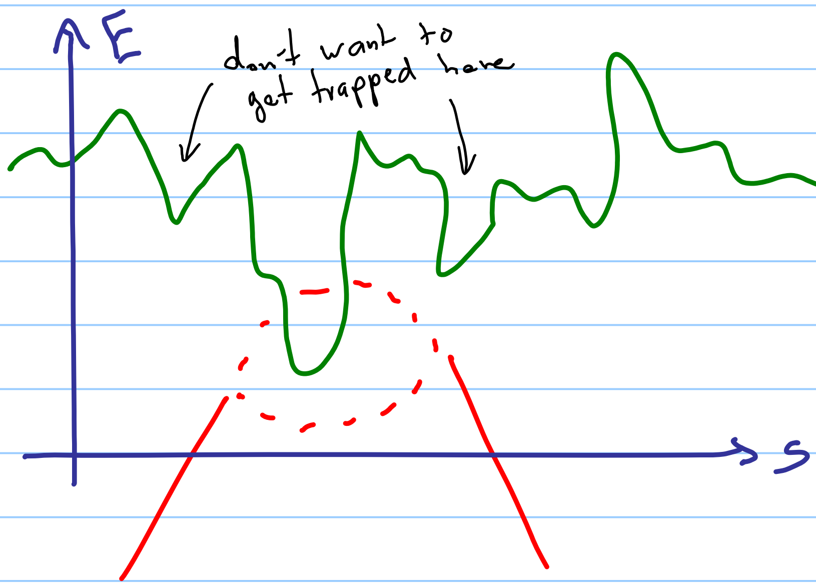
A: avoid getting stuck in local minima

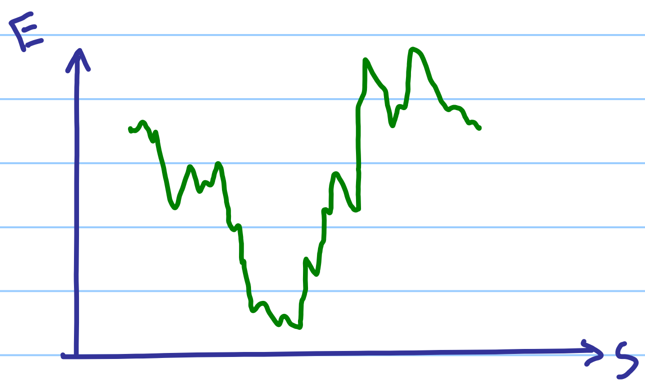
Analogy with annealing:

- at high T, you have a bigger probability to jump to "worse" states
- as T goes down, you start to home in on local minima

i.e. high T: probe large-scale features of the energy function E

low T: probe short-scale features





Quantum Annealing

The problem: obtain the ground state $|\chi_0\rangle$, i.e., state of lowest energy, of some Hamiltonian H_0

ex A collection of spins
- finding the ground state of their Hamiltonian could be very hard!

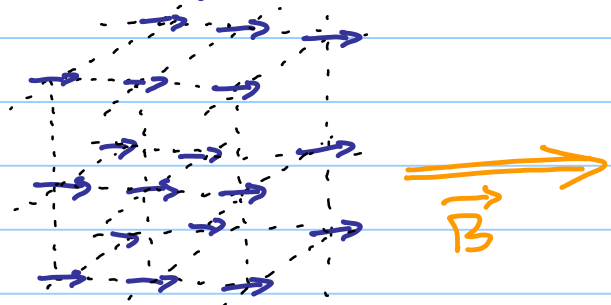
eg, weird layout in space, complicated interactions...

- but if you apply a really strong magnetic field that totally overwhelms H_0, then it's easy to find this configuration's (approx.) ground state

$$\sim \quad H = H_0 - \vec{\mu}\cdot\vec{B}$$

really big

$\Rightarrow$



The idea:
- start in the g.s. with a huge magnetic field
- slowly turn off the B-field
- system should (hopefully) relax to the g.s. of H_0 once $B = 0$

i.e. if $|\psi(t)\rangle \equiv$ state of system at time t, want

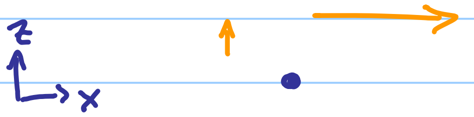
$$|\langle \chi_0 | \psi(t_f)\rangle|^2 \approx 1 \quad \text{at end time } t_f$$

Here, B-field is like the "temperature" in simulated annealing.

ex Annealing a single spin

$$|\psi(t)\rangle = \alpha(t)\,|\uparrow_z\rangle + \beta(t)\,|\downarrow_z\rangle \equiv \begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} \quad ; \; |\alpha|^2+|\beta|^2=1$$

spin up $\equiv \begin{pmatrix}1\\0\end{pmatrix}$ spin down $\equiv \begin{pmatrix}0\\1\end{pmatrix}$



small B-field in z direction

variable B-field in x-direction

Hamiltonian: $\hat{H}(t) = -J\,\hat{\sigma}_z - g(t)\,\hat{\sigma}_x \equiv \begin{pmatrix}-J & -g(t)\\ -g(t) & J\end{pmatrix}$

$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ $\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$

- here, $-J\hat{\sigma}_z$ is playing the role of H_0. Of course, its g.s. is just $|\uparrow_z\rangle$

$$\hat{H}_0|\uparrow_z\rangle = -J\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = -J\begin{pmatrix}1\\0\end{pmatrix} = -J\,|\uparrow_z\rangle$$

- but, lets try annealing the spin, i.e., start with huge $g(0) \gg J$ such that $\hat{H}(0) \approx -g(0)\,\hat{\sigma}_x$ which has g.s. $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \equiv |\psi(0)\rangle$

So the name of the game is

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad \hat{H}(t) = \begin{pmatrix}-J & -g(t)\\ -g(t) & J\end{pmatrix}$$

Evolves according to Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle \;\Rightarrow\; i\hbar\begin{pmatrix}\dot{\alpha}\\ \dot{\beta}\end{pmatrix} = \begin{pmatrix}-J & -g(t)\\ -g(t) & J\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

Q: Want to know $|\langle\uparrow_z|\psi(t)\rangle|^2 = |\alpha(t)|^2$

$\equiv$ probability of being in g.s. of H_0 at time t

$\rightsquigarrow$ need to solve a system of ODE's

$$i\hbar\,\dot{\alpha}(t) = -J\alpha(t) - g(t)\beta(t)$$
$$i\hbar\,\dot{\beta}(t) = -g(t)\alpha(t) + J\beta(t)$$
$$\alpha(0) = \beta(0) = \frac{1}{\sqrt{2}}$$

- can do numerically for generic $g(t)$
- exact sol^{n} for some $g(t)$ (homework)
- or, lets make some approximations...

Suppose: $|g(0)| \equiv |g_0| \gg |J|$

$$|\dot{g}(0)| \ll |g_0| \,, \qquad \dot{g}(0) = -\gamma < 0$$

$\rightsquigarrow$ Taylor: $g(t) \approx g_0 - \gamma t + O(t^2)$

Then $\hat{H}(t) \approx -J\sigma_z - (g_0 - \gamma t)\,\hat{\sigma}_x$

$$= \underbrace{-g_0\,\hat{\sigma}_x}_{H_0} \underbrace{- J\hat{\sigma}_z + \gamma t\,\hat{\sigma}_x}_{H'(t)}$$

$\rightsquigarrow$ perturbation! Should be good as long as $\gamma t \ll g_0$

Time-dependent perturbation primer

eg. $H(t) = H_0 + H'(t)$ ← small time-dependent perturbation

↑ time-indep, ON eigenstates $|\psi_n^0\rangle$, $H_0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle$

- Expand a general state $|\psi(t)\rangle$ as

$$|\psi(t)\rangle = \sum_n c_n(t)\, e^{-iE_n^0 t/\hbar}\, |\psi_n^0\rangle$$

- Reformulate S.E.

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

$$\Rightarrow \quad i\hbar \sum_n \left(\dot{c}_n - \cancel{\frac{iE_n^0}{\hbar} c_n} \right) e^{-iE_n^0 t/\hbar}|\psi_n^0\rangle = (H_0 + H')\sum_n c_n e^{-iE_n^0 t/\hbar}|\psi_n^0\rangle$$

$$= \sum_n c_n \left(\cancel{E_n^0} + H' \right) e^{-iE_n^0 t/\hbar}|\psi_n^0\rangle$$

$$i\hbar \sum_n \dot{c}_n e^{-iE_n^0 t/\hbar}|\psi_n^0\rangle = \sum_n c_n e^{-iE_n^0 t/\hbar} H'|\psi_n^0\rangle$$

$$\langle\psi_m^0| \to \quad i\hbar\, \dot{c}_m(t)\, e^{-iE_m^0 t/\hbar} = \sum_n c_n(t)\, e^{-iE_n^0 t/\hbar} \langle\psi_m^0|H'(t)|\psi_n^0\rangle$$

or $$i\hbar\, \dot{c}_m(t) = \sum_n c_n(t)\, e^{i\omega_{mn} t} H'_{mn}(t)$$

$$\omega_{mn} \equiv \frac{E_m^0 - E_n^0}{\hbar} \qquad H'_{mn} \equiv \langle\psi_m^0|H'(t)|\psi_n^0\rangle$$

- so far no approximations; now expand $c_m(t)$ order by order

$$c_m(t) = c_m^0(t) + c_m^1(t) + \cdots$$

setting $c_m^0(0) = c_m(0)$, $c_m^j(0) = 0 \quad j \geq 1$

$$\Rightarrow \quad i\hbar\,(\dot{c}_m^0 + \dot{c}_m^1 + \dots) = \sum_n (c_n^0 + c_n^1 + \dots)\, e^{i\omega_{mn}t} H'_{mn}(t)$$

Zeroth order: $\quad i\hbar\, \dot{c}_m^0(t) = 0 \quad \Rightarrow \quad c_m^0(t) = c_m(0)$ const

First order: $\quad i\hbar\, \dot{c}_m^1(t) = \sum_n c_n^0\, e^{i\omega_{mn}t} H'_{mn}(t)$

Back to annealing:

$$H(t) = H_0 + H'(t) \qquad H_0 = -g_0 \hat{\sigma}_x \qquad H'(t) = -J\hat{\sigma}_z + \gamma t \hat{\sigma}_x$$

Write $|\psi(t)\rangle$ in eigenbasis of H_0

$$|\psi(t)\rangle = c_1(t)\, e^{-i\omega_1 t} \underbrace{|\uparrow_x\rangle}_{= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}} + c_2(t)\, e^{-i\omega_2 t} \underbrace{|\downarrow_x\rangle}_{= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}}$$

Initial condition $\quad c_1(0) = 1 \quad c_2(0) = 0$

Perturbation:
$$i\hbar\, \dot{c}_1^1(t) = H'_{11}(t)$$
$$i\hbar\, \dot{c}_2^1(t) = e^{i\omega_{21}t} H'_{21}(t)$$

$$H'_{11}(t) = \langle \uparrow_x | -J\hat{\sigma}_z + \gamma t\, \hat{\sigma}_x | \uparrow_x \rangle$$
$$= \frac{1}{2}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}-J & \gamma t\\ \gamma t & J\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}-J+\gamma t\\ \gamma t + J\end{pmatrix}$$
$$= \gamma t$$

$$H'_{21}(t) = \langle \downarrow_x | -J\hat{\sigma}_z + \gamma t\, \hat{\sigma}_x | \uparrow_x \rangle$$
$$= \frac{1}{2}\begin{pmatrix}1 & -1\end{pmatrix}\begin{pmatrix}-J & \gamma t\\ \gamma t & J\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = -J$$

and $\quad \omega_{21} = \dfrac{E_2 - E_1}{\hbar} = \dfrac{g_0 - (-g_0)}{\hbar} = \dfrac{2g_0}{\hbar}$

$\Rightarrow \quad i\hbar\, \dot{c}_1^1(t) = \gamma t$

$\quad\quad i\hbar\, \dot{c}_2^1(t) = -J e^{2ig_0 t/\hbar}$

So $\quad c_1^1(t) = \dfrac{\gamma t^2}{2i\hbar}$ ← not first order!

$$c_2^1(t) = -\frac{J}{i\hbar} \cdot \frac{\hbar}{2ig_0} \left(e^{2ig_0 t/\hbar} - 1 \right)$$

$$= \frac{J}{2g_0} \left(e^{2ig_0 t/\hbar} - 1 \right) \qquad \frac{g_0 t}{\hbar} \ll 1$$

$$= \frac{J}{2g_0} \left(1 + \frac{2ig_0 t}{\hbar} + \dots - 1 \right)$$

$$\approx \frac{iJt}{\hbar} \quad \text{to first order in } t$$

$\therefore \quad c_1(t) \approx 1$

$\quad\quad c_2(t) \approx \dfrac{iJt}{\hbar} \quad$ to first order in t

$$\langle \uparrow_z | \psi(t) \rangle = c_1(t) e^{-i\omega_1 t} \underbrace{\langle \uparrow_z | \uparrow_x \rangle}_{= 1/\sqrt{2}} + c_2(t) e^{-i\omega_2 t} \underbrace{\langle \uparrow_z | \downarrow_x \rangle}_{= 1/\sqrt{2}}$$

$$\approx 1 \cdot (1 - i\omega_1 t) \cdot \frac{1}{\sqrt{2}} + \frac{iJt}{\hbar} \cdot 1 \cdot \frac{1}{\sqrt{2}}$$

$$= \frac{1}{\sqrt{2}} \left(1 - i\left(\frac{-g_0}{\hbar}\right) t + \frac{iJt}{\hbar} \right)$$

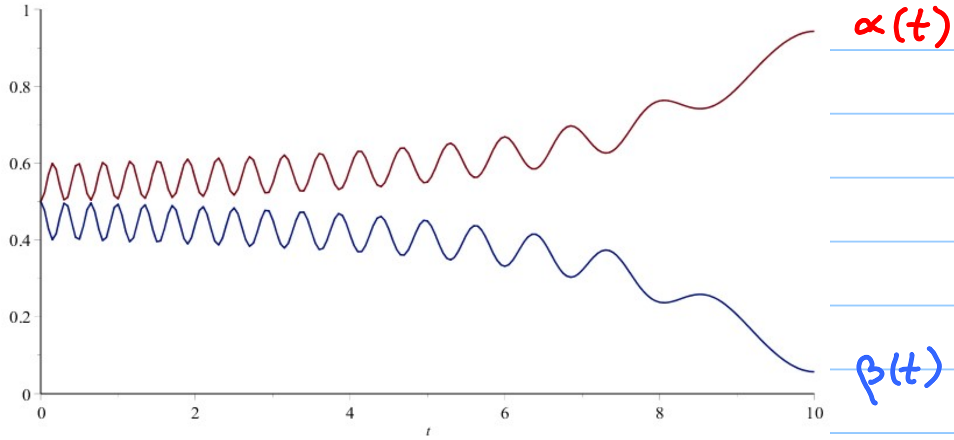
$$= \frac{1}{\sqrt{2}} \left(1 + \frac{i(g_0 + J)t}{\hbar} \right)$$

$$|\langle \uparrow_z | \psi(t) \rangle|^2 = \frac{1}{2} \left(1 + \left(\frac{g_0 + J}{\hbar}\right)^2 t^2 \right) + O(t^4)$$

Increasing! at least for $t \ll \dfrac{\hbar}{g_0}$

We could go to higher orders, or we could just solve the Schrödinger equation numerically

ex $J=1, \quad g_0=10, \quad \gamma=1 \qquad \left(|\psi(t)\rangle = \alpha(t)|\uparrow_z\rangle + \beta(t)|\downarrow_z\rangle \right)$



ex "Cooling" too quickly : $\quad J=1, \quad g_0=10, \quad \gamma=10$