Adiabatic quantum optimization and Anderson localization

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NEC

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Outline

1. Introduction: Adiabatic optimization for NP-complete problems
2. Exact Cover 3 problem
3. Anderson Localization on the hypercube
4. Small gaps in the Adiabatic approach to EC3
5. Exponentially large number of solutions (Knysh and Smelyanskiy, 2010)

Computational Complexity Classes

P

Polynomial time
$< N^p$
N is the size of the problem

Solution can be found in a polynomial time, e.g. multiplication

NP

Nondeterministic polynomial time

Solution can be checked in a polynomial time, e.g. factorization

NP complete

Every NP problem can be reduced to this problem in a polynomial time

Cook – Levin theorem (1971):
SAT problem is NP complete

Quantum algorithms for NP complete problems ?

Circuit quantum computer - no good ideas
Adiabatic quantum computer - promising

home

what we are trying to build

Quantum Co

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The Economist

SCIENTIFIC AMERICA

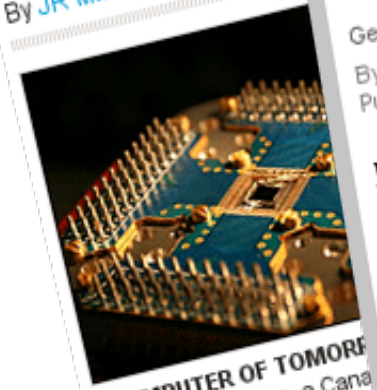
February 13, 2007 | 0 comm

First "Comm

Solves Sudo

Quantum computing co

By JR Minkel



COMPUTER OF TOMORR

D-Wave Systems, a Cana

company, has ap

The New York Times

Geordie Rose, the founder of D-Wave Systems, says he has created a commercial quantum com

By JASON PONTIN
Published: April 8, 2007

DID **D-Wave Systems** achieve the incredible — a startling advance in computing that would radically expand human capacities for industrial activity and scientific discovery, long before experts believed it possible?

It says it did

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Adiabatic quantum optimization

Edward Farhi, Jeffrey Goldstone, Sam Gutmann, and Michael Sipser. "Quantum computation by adiabatic evolution", 2000. arXiv:quant-ph/0001106.

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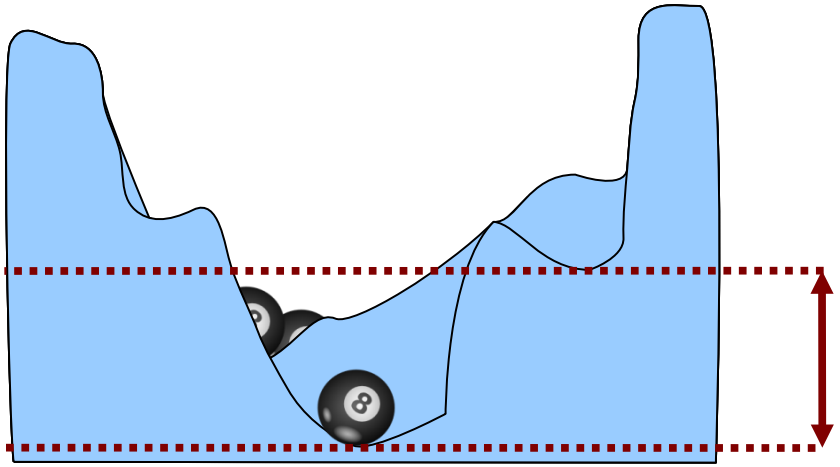

Slowly varying $\hat{H}(t)$

$\longrightarrow$ system stays at the ground state

Probability of excitation depends on:

- Total time T (slower is better)
- Gap $\Delta(t)$ (larger gap is better)

Probability to stay in the ground state $\propto \frac{\Delta_{\min}^2}{T}$

Adiabatic quantum optimization

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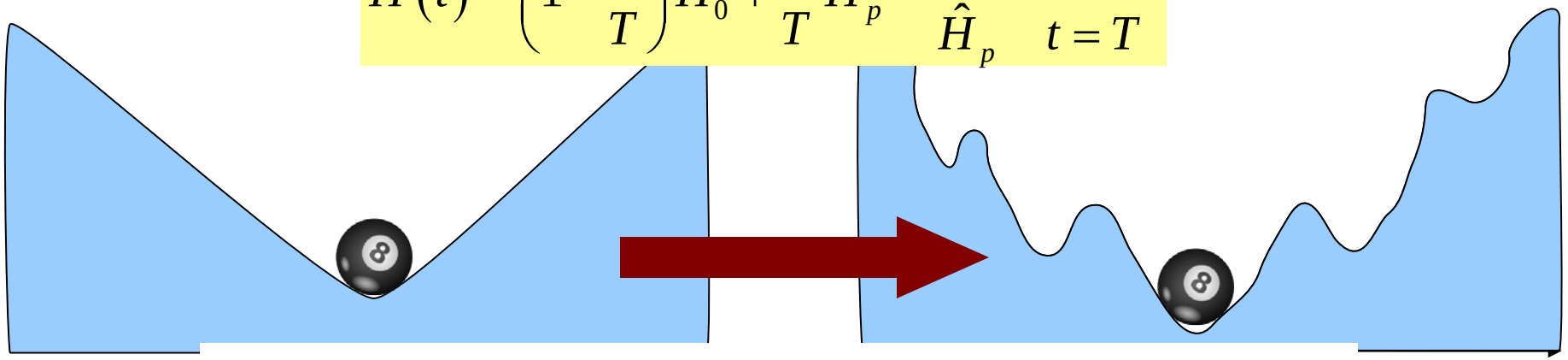
Problem:
Find minimum of a function $f(x)$

1. Choose initial Hamiltonian H_0 with known ground state
2. Change Hamiltonian to H_P "matching" $f(x)$

$$\hat{H}(t) = \left(1 - \frac{t}{T}\right)\hat{H}_0 + \frac{t}{T}\hat{H}_p = \begin{cases} \hat{H}_0 & t = 0 \\ \hat{H}_p & t = T \end{cases}$$



T large enough $\Rightarrow$ measuring reveals the minimum

How powerful is it?

- It is quantum! Unstructured search in time (cf Grover)

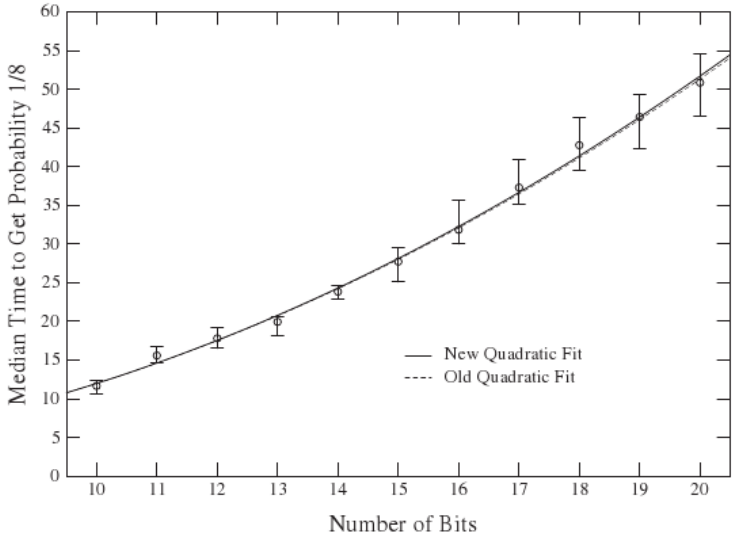
[vanDam-Mosca-Vazirani'01,Roland-Cerf'02]

- It is universal for quantum computation

[Aharonov *et al.*'05]

Good, but what about NP-complete problems?

- Numerical simulations: promising scaling



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Good, but what about NP-complete problems?

- Numerical simulations: promising scaling

[Farhi *et al.*'00,Hogg'03,Banyuls *et al.*'04,Young *et al.'08*]

- But exponentially small gap
  - for bad choice of initial Hamiltonian [Znidaric-Horvat'06,Farhi *et al.*'08]
  - for specifically designed hard instances [vanDam-Vazirani'03,Reichardt'04]

But maybe **typical** gaps are only polynomial?

1 in 3 SAT = exact cover problem

N bits / laterals / Ising spins $\quad \sigma_i = \pm 1 \quad i = 1, 2, \ldots, N$

M clauses $\{i_c, j_c, k_c\}$

$c = 1, 2, \ldots, M$

$1 \le i_c, j_c, k_c \le N$

Definition

Clause c is satisfied if one of the three spins is down and other two are up

$$\sigma_{i_c} = -1, \quad \sigma_{j_c} = 1, \quad \sigma_{k_c} = 1$$

or

$$\sigma_{i_c} = 1, \quad \sigma_{j_c} = -1, \quad \sigma_{k_c} = 1$$

or

$$\sigma_{i_c} = 1, \quad \sigma_{j_c} = 1, \quad \sigma_{k_c} = -1$$

Otherwise the clause is not satisfied

Task: to satisfy all M clauses

1 in 3 SAT = exact cover 3 (EC3) problem

N bits / laterals / Ising spins $\quad \sigma_i = \pm 1 \quad i = 1, 2, \ldots, N$

M clauses $\quad \{i_c, j_c, k_c\} \quad c = 1, 2, \ldots, M$

Clause c is satisfied if one of the three spins is down and other two are up. Otherwise the clause is not satisfied

Task:
to satisfy all M clauses

Important:
We will considering ensemble of randomly selected clauses, not some families of artificially designed instances

1 in 3 SAT = exact cover 3 (EC3) problem

N bits / laterals / Ising spins $\quad \sigma_i = \pm 1, \; i = 1, 2, \ldots, N$

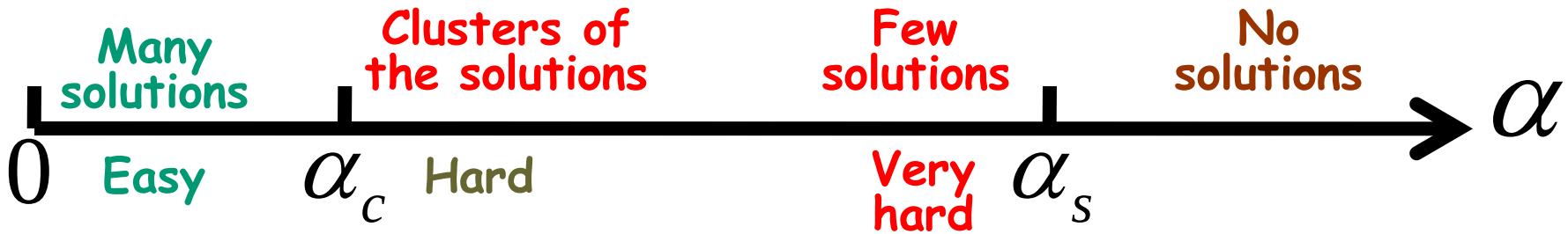
M clauses $\quad \{i_c, j_c, k_c\}, \; c = 1, 2, \ldots, M$

Clause c is satisfied if one of the three spins is down and other two are up. Otherwise the clause is not satisfied

Task:
to satisfy all M clauses

Size of the problem:

$$N \to \infty, M \to \infty, \quad \frac{M}{N} \to \alpha$$



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M clauses $\quad \{i_c, j_c, k_c\}, \; c = 1, 2, \ldots, M$

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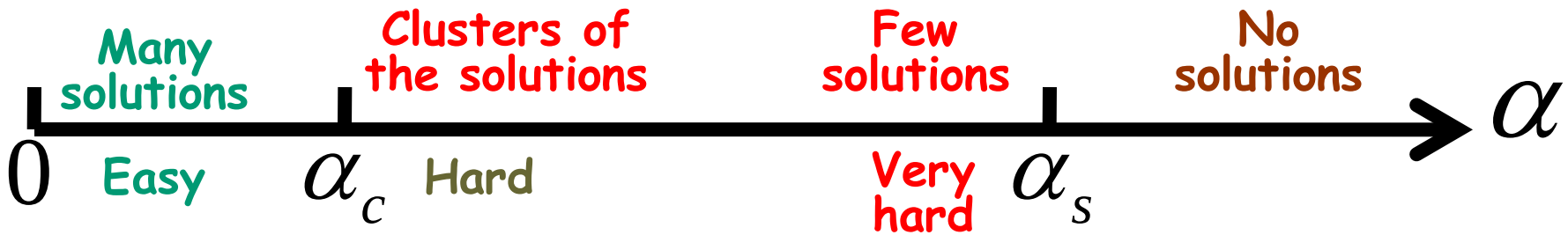

α_c clustering threshold

α_s satisfiability threshold

$$0.546 < \alpha_s < 0.644$$

J. Raymond, A. Sportiello, & L. Zdeborova, Physical Review E 76, 011101 (2007).

$$\left\{\begin{array}{l}\sigma_{i_c}=-1,\sigma_{j_c}=1,\sigma_{k_c}=1\\ \sigma_{i_c}=1,\sigma_{j_c}=-1,\sigma_{k_c}=1\\ \sigma_{i_c}=1,\sigma_{j_c}=1,\sigma_{k_c}=-1\end{array}\right\} \Leftrightarrow \left(\sigma_{i_c}+\sigma_{j_c}+\sigma_{k_c}-1\right)^2=0$$

Otherwise $\left(\sigma_{i_c}+\sigma_{j_c}+\sigma_{k_c}-1\right)^2>0$

Solutions $\{\sigma_i\}$ and only solutions are zero energy ground states of the Hamiltonian

$$H_p=\sum_{c=1}^{M}\frac{\left(\sigma_{i_c}+\sigma_{j_c}+\sigma_{k_c}-1\right)^2}{4}=\frac{M}{4}-\sum_{i=1}^{N}\frac{B_i}{4}\sigma_i+\sum_{i\neq j}\frac{J_{ij}}{2}\sigma_i\sigma_j$$

B_i – number of clauses, which involve spin i

J_{ij} – number of clauses, where both i and j participate

Adiabatic Algorithm for EC3

Recipe: 1. Construct the Hamiltonian

$$\hat{H}_s\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = s\hat{H}_p\left(\left\{\hat{\sigma}_i^z\right\}\right) + (1-s)H_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right)$$

2. Slowly change adiabatic parameter s from 0 to 1

$$H_p = \sum_{c=1}^{M} \frac{\left(\sigma_{i_c} + \sigma_{j_c} + \sigma_{k_c} - 1\right)^2}{4} = \frac{M}{4} - \sum_{i=1}^{N} \frac{B_i}{4}\sigma_i + \sum_{i\neq j} \frac{J_{ij}}{2}\sigma_i\sigma_j$$

$$\hat{H}_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \sum_{i=1}^{N} \hat{\sigma}_i^x$$

$$\hat{H}_\lambda\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \hat{H}_p\left(\left\{\hat{\sigma}_i^z\right\}\right) + \lambda H_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right); \quad \lambda = \frac{1-s}{s} = \frac{T-t}{t}$$

$$0 \longleftarrow \lambda \longrightarrow \infty$$

Adiabatic Algorithm for EC3

$$H_p = \sum_{c=1}^{M} \frac{\left(\hat{\sigma}^z_{i_c} + \hat{\sigma}^z_{j_c} + \hat{\sigma}^z_{k_c} - 1\right)^2}{4} = \frac{M}{4} - \sum_{i=1}^{N} \frac{B_i}{4}\hat{\sigma}^z_i + \sum_{i\neq j} \frac{J_{ij}}{2}\hat{\sigma}^z_i\hat{\sigma}^z_j; \quad \hat{H}_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \sum_{i=1}^{N}\hat{\sigma}^x_i$$

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Ising model (determined on a graph) in a random parallel and a uniform perpendicular field λ

Adiabatic Algorithm for exact cover

$$\hat{H}_p = \sum_{c=1}^{M}\left(\hat{\sigma}_{i_c}^z + \hat{\sigma}_{j_c}^z + \hat{\sigma}_{k_c}^z - 1\right)^2 = \sum_{i=1}^{N} B_i \hat{\sigma}_i^z + \sum_{i\neq j} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z; \qquad \hat{H}_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \sum_{i=1}^{N}\hat{\sigma}_i^x$$

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Another way of thinking:

$\{\sigma_i\}$ determines a site of N-dimensional hypercube

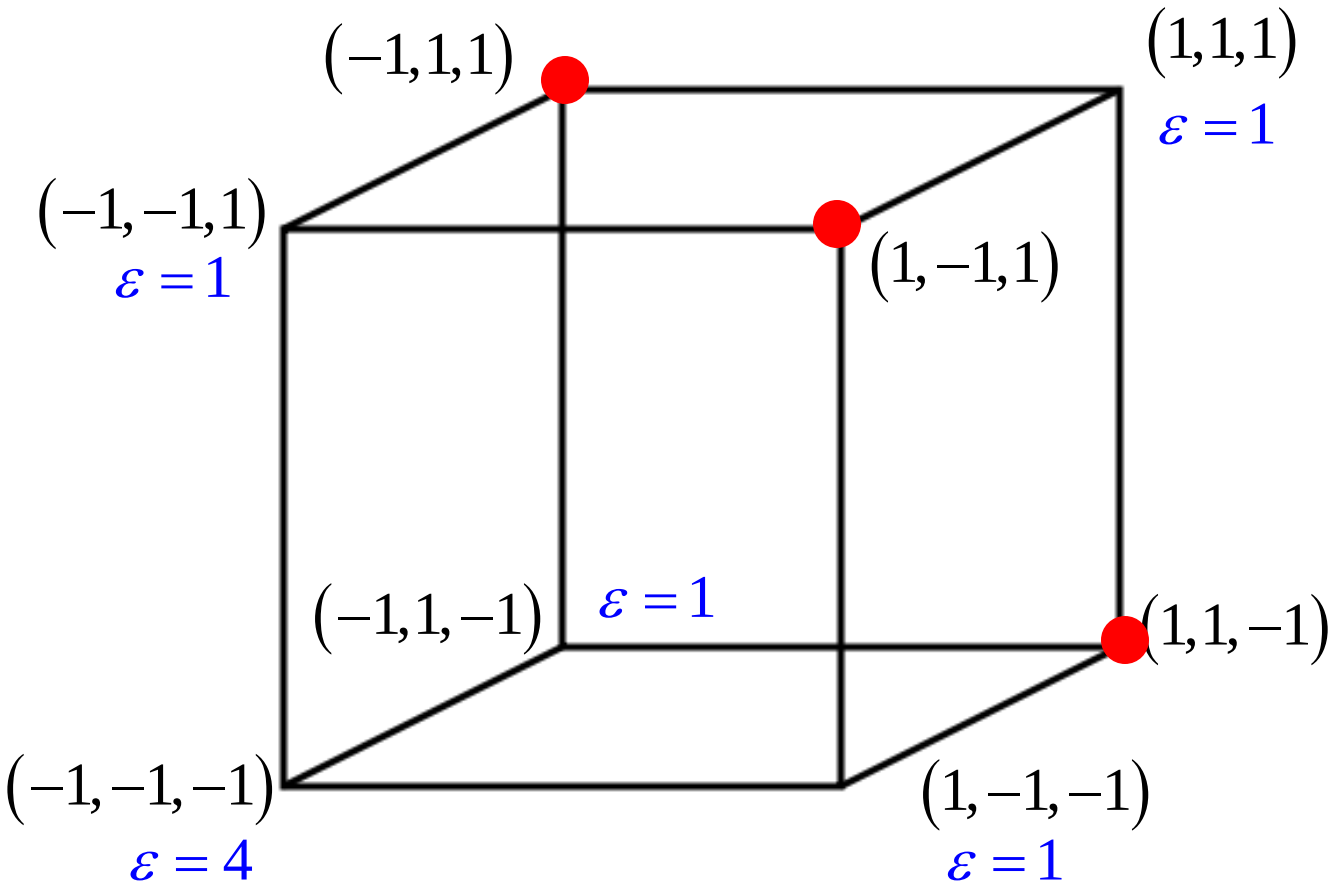
$H_p\left(\{\sigma_i\}\right)$
onsite energy

$\lambda\hat{H}_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \lambda\sum_{i=1}^{N}\hat{\sigma}_i^x \qquad \hat{\sigma}^x = \hat{\sigma}^+ + \hat{\sigma}^-$

hoping between nearest neighbors

The simplest example:

3 qubits
1 clause
} ⇒ 3d cube, 3 solutions



Adiabatic Algorithm for exact cover

$$\hat{H}_p = \sum_{c=1}^{M}\left(\hat{\sigma}_{i_c}^z + \hat{\sigma}_{j_c}^z + \hat{\sigma}_{k_c}^z - 1\right)^2 = \sum_{i=1}^{N} B_i \hat{\sigma}_i^z + \sum_{i\neq j} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z; \qquad \hat{H}_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \sum_{i=1}^{N}\hat{\sigma}_i^x$$

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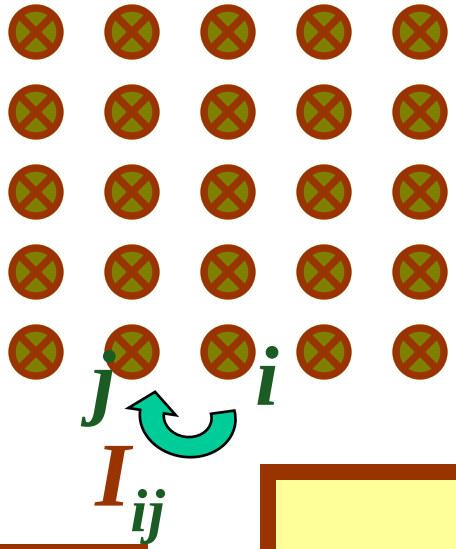
hoping between nearest neighbors

Anderson model for Localization on N-dimensional cube

Anderson Model



- *Lattice - tight binding model*
- *Onsite energies* ε_i *- random*
- *Hopping matrix elements* I_{ij}

$$-W < \varepsilon_i < W$$

uniformly distributed

$$I_{ij} = \begin{cases} I & i \text{ and } j \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Anderson Transition

$I < I_c$

Insulator

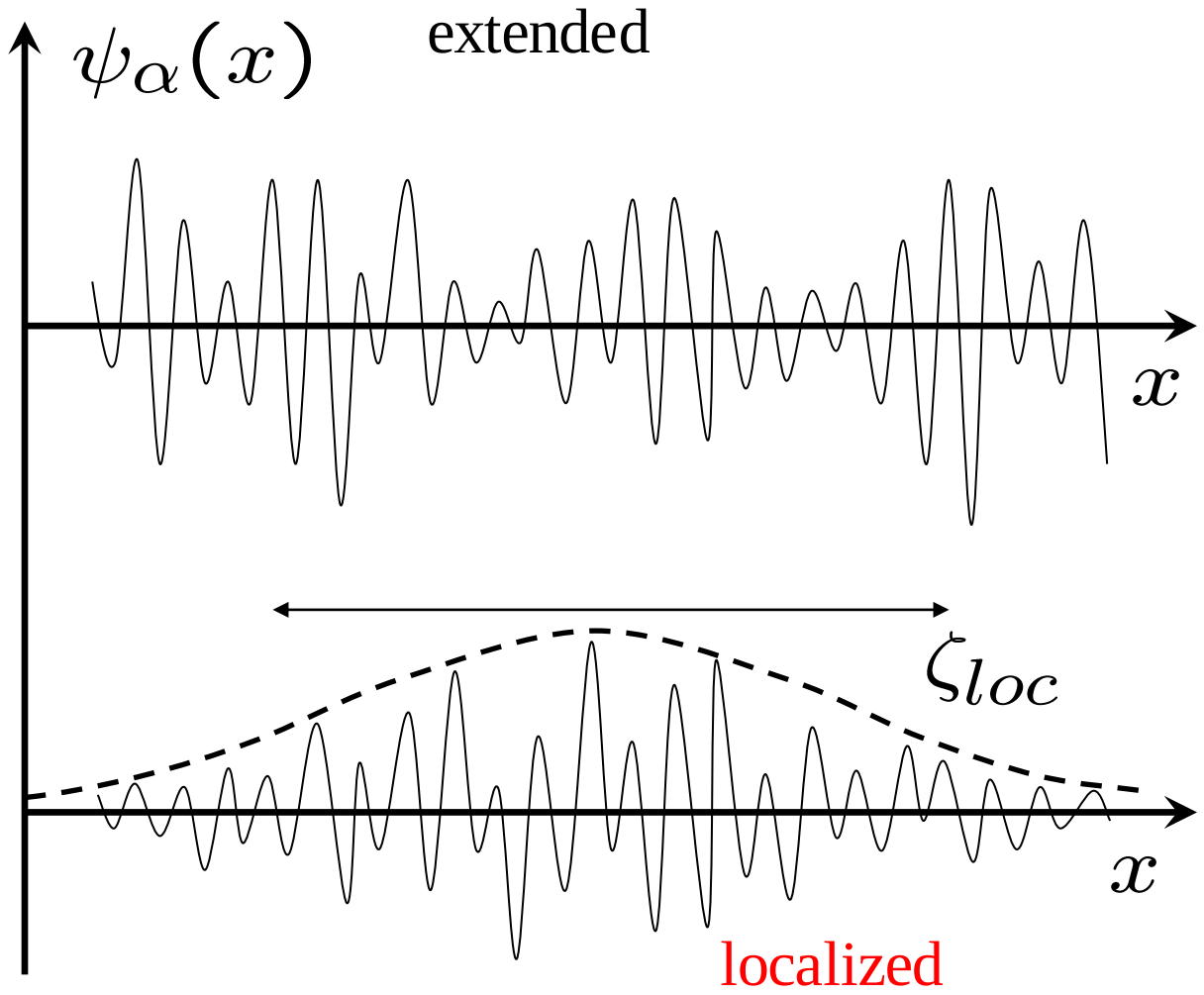
All eigenstates are localized

Localization length ζ_{loc}

$I > I_c$

Metal

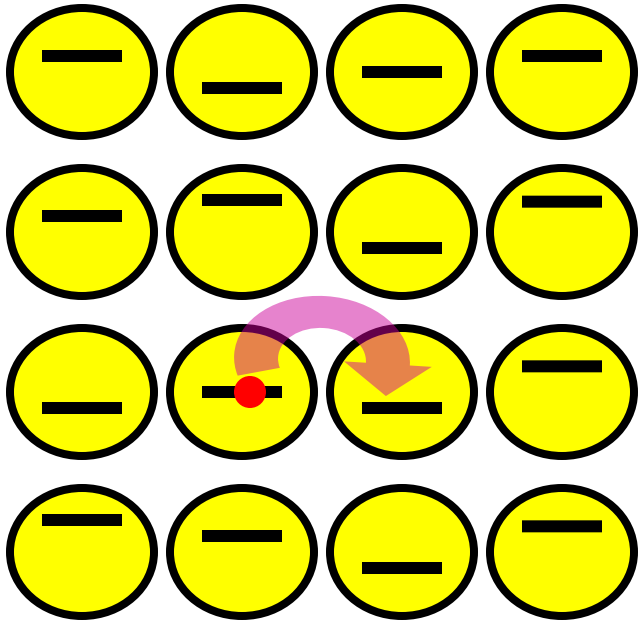
There appear states extended all over the whole system


$\psi_\alpha(x)$
extended
x
ζ_{loc}
x
localized

Conventional Anderson Model

- one "particle",
- one level per site,
- onsite disorder
- nearest neighbor hoping

Basis: $|i\rangle$, i **labels sites**



Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\hat{H}_0 = \sum_i \varepsilon_i |i\rangle\langle i|$$

$$\hat{V} = \sum_{i,j=n.n.} I |i\rangle\langle j|$$

Adiabatic Quantum Algorithm for 1 in 3 SAT

$$\hat{H}_p = \sum_{c=1}^{M} \left(\hat{\sigma}_{i_c}^z + \hat{\sigma}_{j_c}^z + \hat{\sigma}_{k_c}^z - 1 \right)^2 = \sum_{i=1}^{N} B_i \hat{\sigma}_i^z + \sum_{i \neq j} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z ; \qquad \hat{H}_0 \left(\left\{ \hat{\vec{\sigma}}_i \right\} \right) = \sum_{i=1}^{N} \hat{\sigma}_i^x$$

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Anderson Model on N-dimensional cube

Usually:

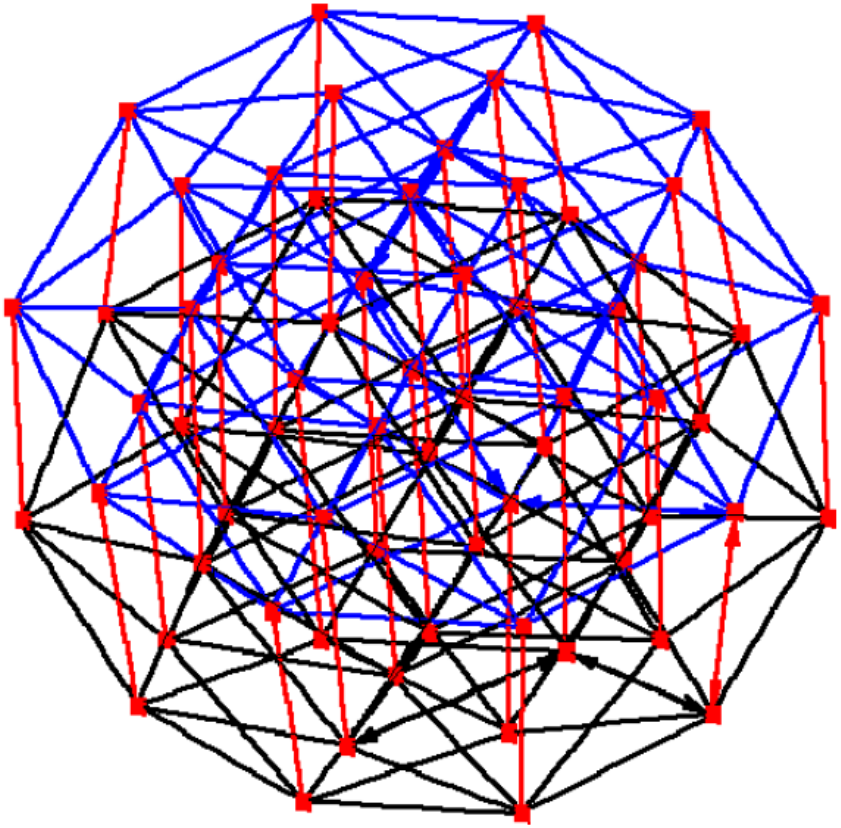
# of dimensions $d \to const$

system linear size $L \to \infty$

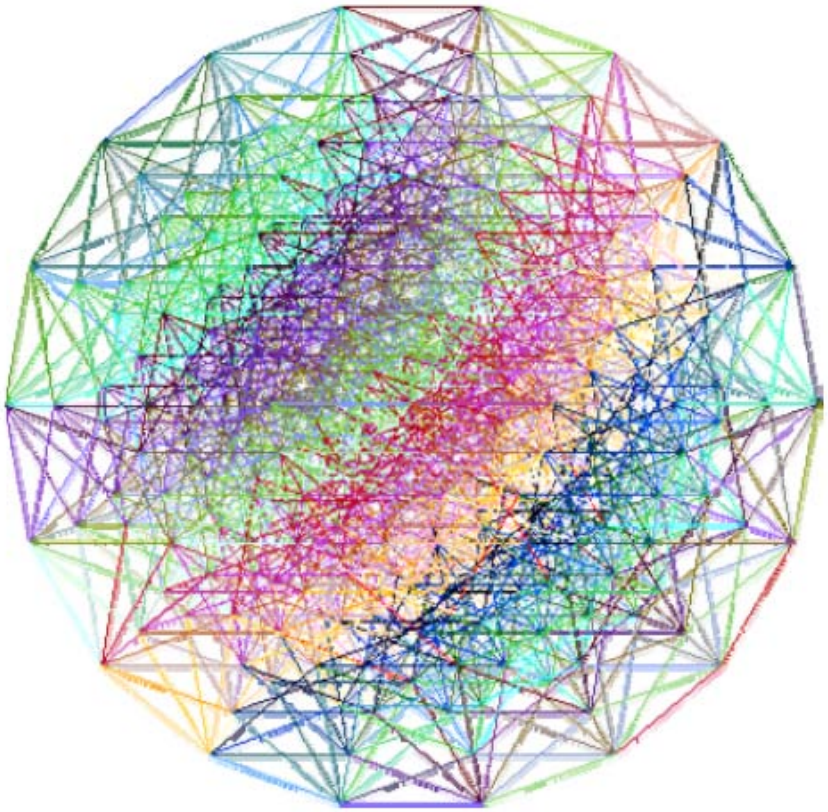
Here:

# of dimensions $d = N \to \infty$

system linear size $L = 1$

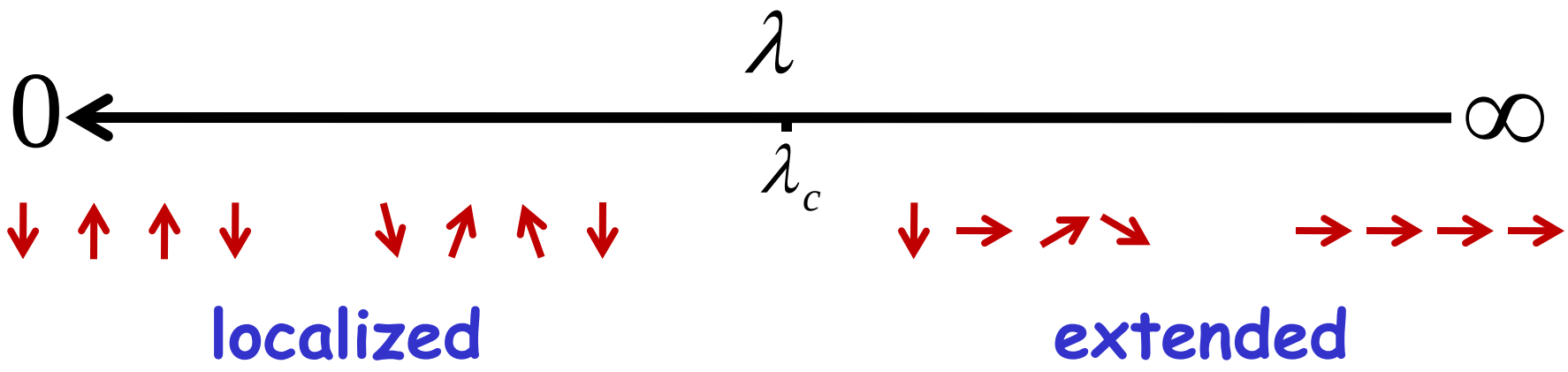


6-dimensional cube



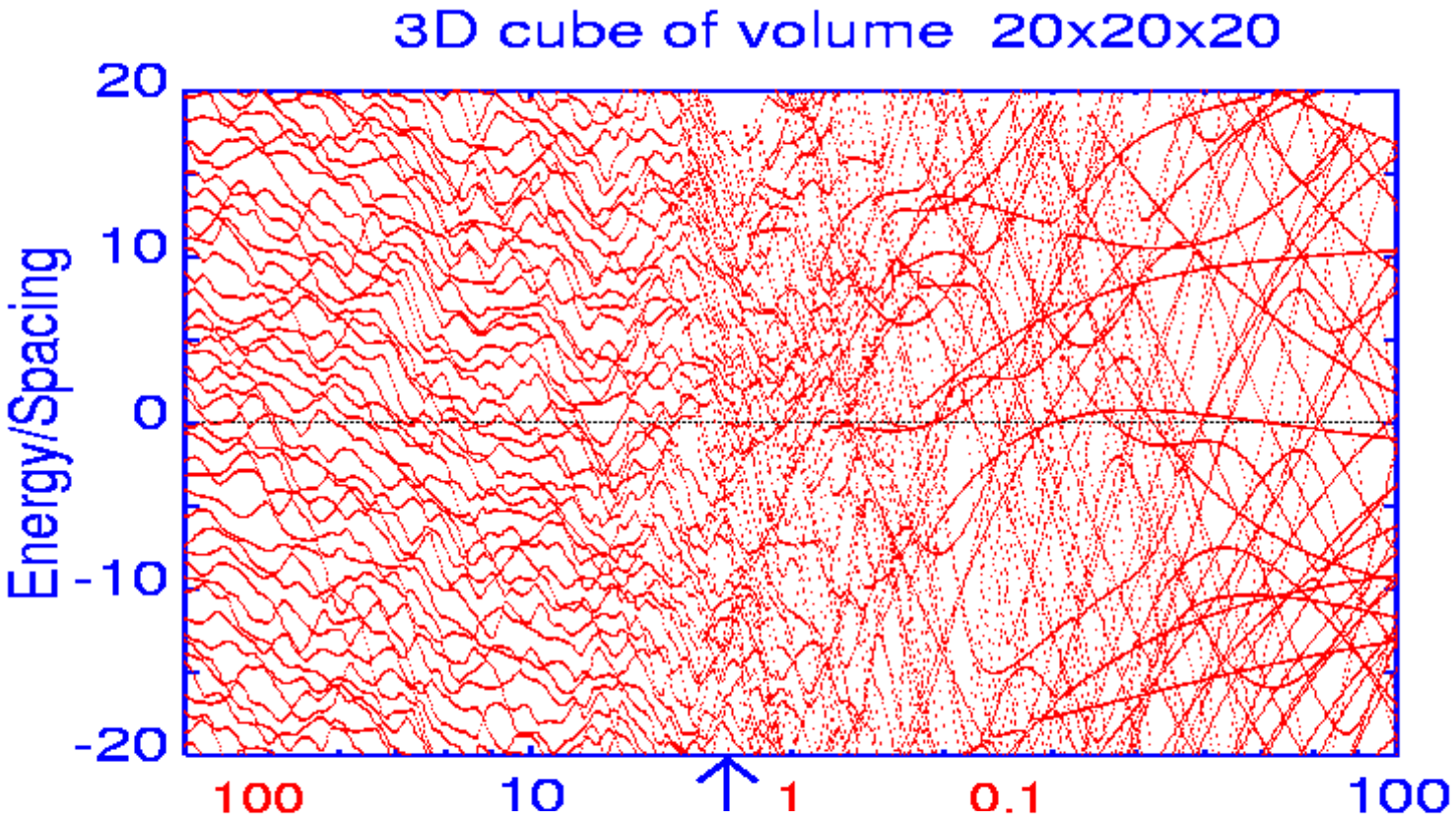
9-dimensional cube

$$\hat{H}_\lambda\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \hat{H}_p\left(\left\{\hat{\sigma}_i^z\right\}\right) + \lambda H_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right)$$



Zharekeschev & Kramer.

Exact diagonalization of the Anderson model



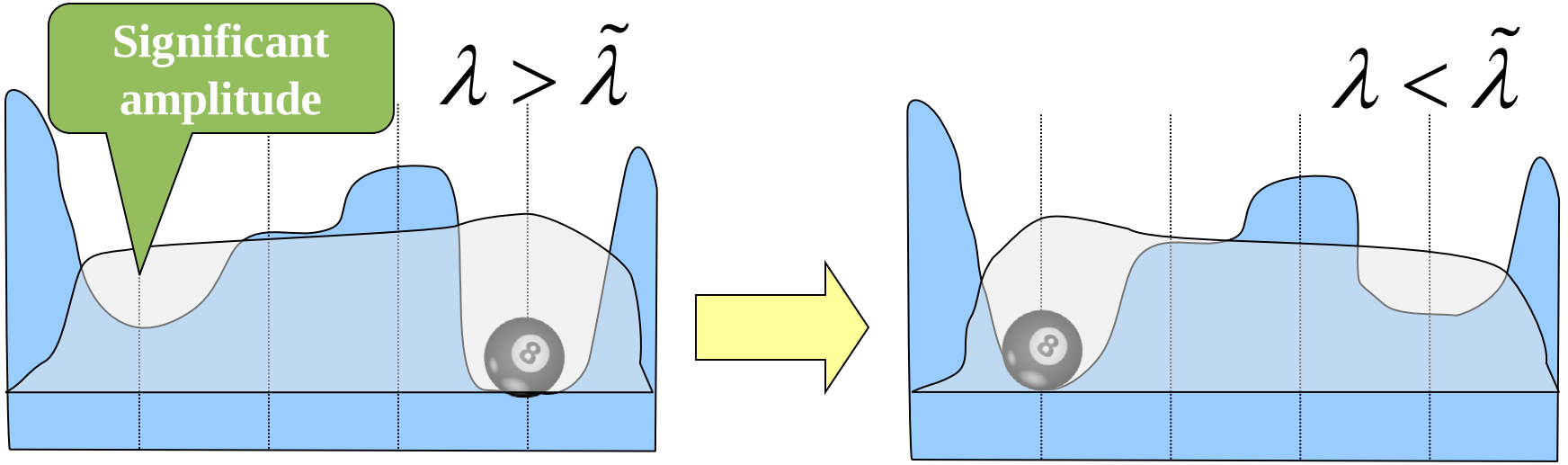
Disorder $W \sim \lambda^{-1}$

Avoided crossing gaps

- extended → large
- localized → small

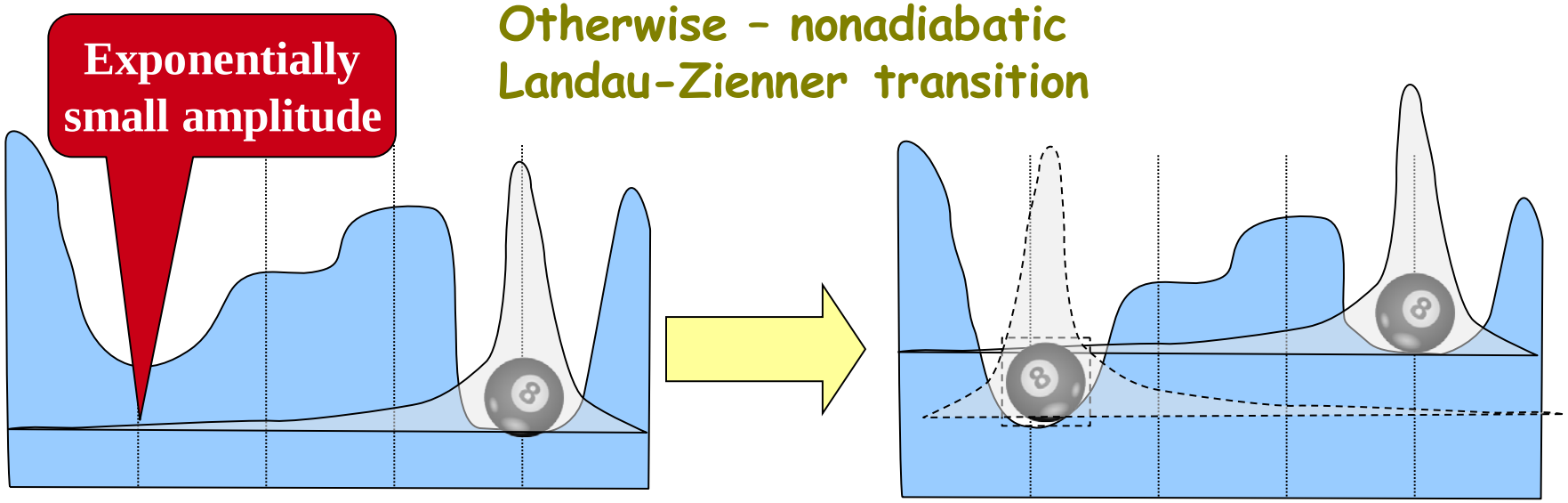
Adiabatic transition:

1. Extended states – can be performed quickly



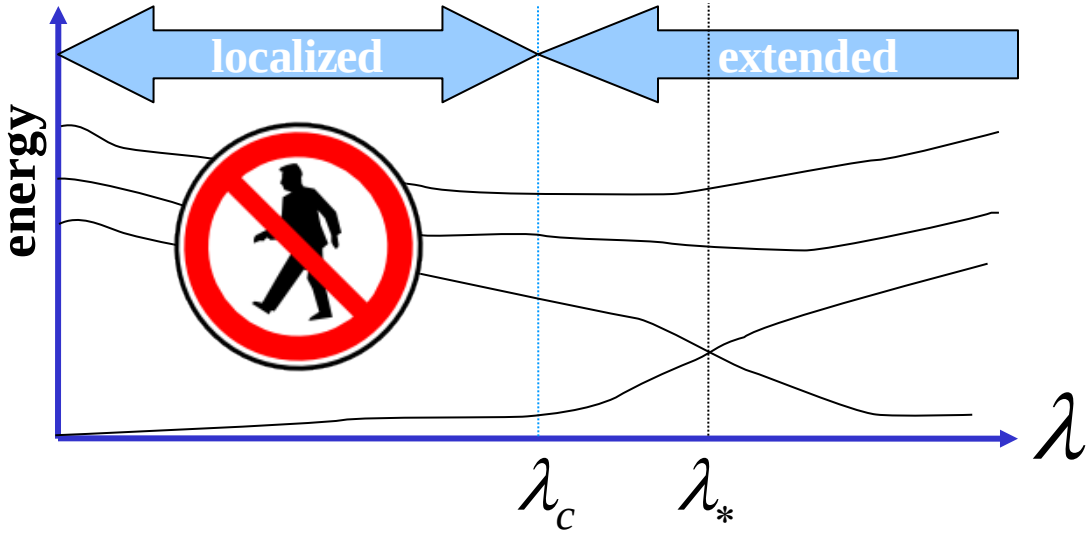
2. Localized states – need exponentially long time

Otherwise – nonadiabatic Landau-Zienner transition



Localized states ⇒ Exponentially long tunneling times ⇒ Exponentially small anticrossing gaps

Our result:



As the size of the problem N increases

1) Anderson localization would imply $\lambda_c = \Omega\left(1/\log N\right)$
2) Anti-crossings between solutions and not-solutions – as long as λ exceeds $\lambda_* \approx \left(CN\right)^{-1/8}$

For $N > \left(C\lambda_c^8\right)^{-1}$ we have $\lambda_* < \lambda_c$

The algorithm fails (stuck in a local minimum)

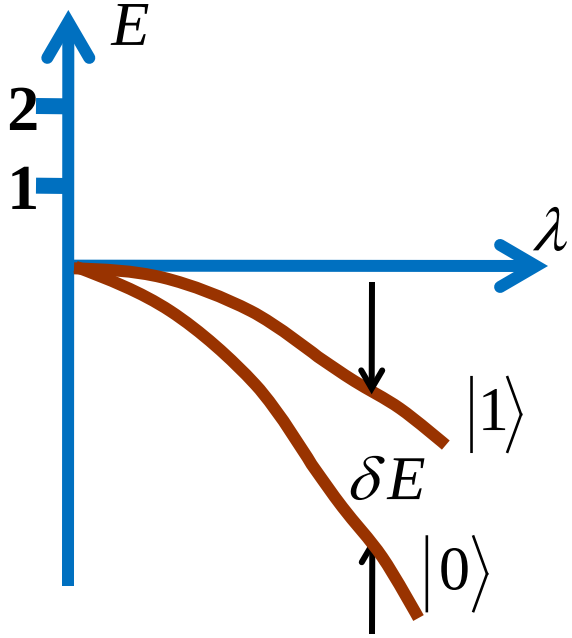
When $N \to \infty$ the gaps decrease even quicker than exponentially

$$\hat{H}_\lambda\left(\left\{\hat{\vec{\sigma}}_i\right\}\right) = \hat{H}_p\left(\left\{\hat{\sigma}_i^z\right\}\right) + \lambda H_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right)$$

1. Hamiltonian $\hat{H}_p\left(\left\{\hat{\sigma}_i^z\right\}\right)$ is **integrable**: it commutes with all $\hat{\sigma}_i^z$. Its states thus can be degenerated. These degeneracies should **split** at finite λ since $\hat{H}_\lambda\left(\left\{\hat{\vec{\sigma}}_i\right\}\right)$ is **non-integrable**

2. For α is close to α_s there typically are several solutions separated by distances $O(N)$. Consider two.

3. Let us add one more clause, which is satisfied by $|1\rangle$ but not by $|0\rangle$



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1. Hamiltonian $\hat{H}_p\left(\left\{\hat{\sigma}_i^z\right\}\right)$ is integrable: it commutes with all $\hat{\sigma}_i^z$. Its states thus can be degenerated. These degeneracies should be split by finite λ in non-integrable $\hat{H}_\lambda\left(\left\{\hat{\vec{\sigma}}_i\right\}\right)$

2. For α is close to α_s there typically are several solutions separated by distances $O(N)$. Consider two.

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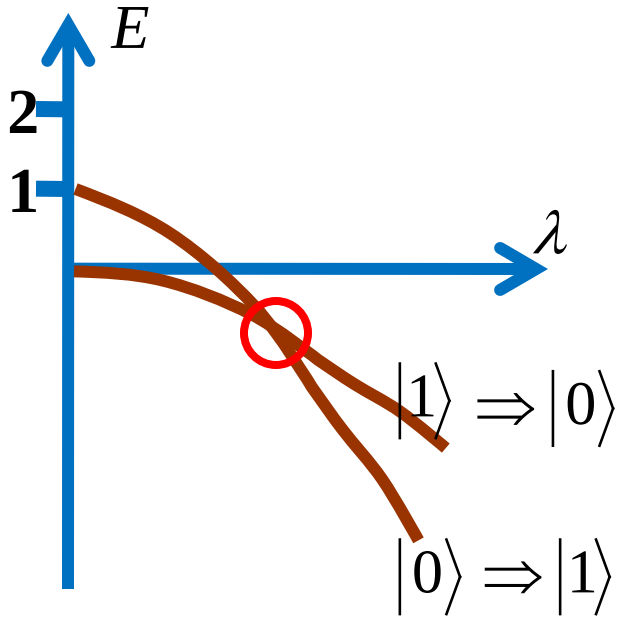
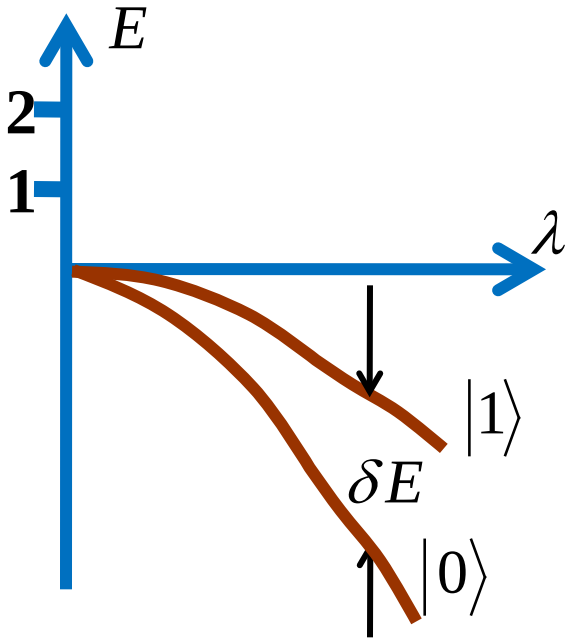
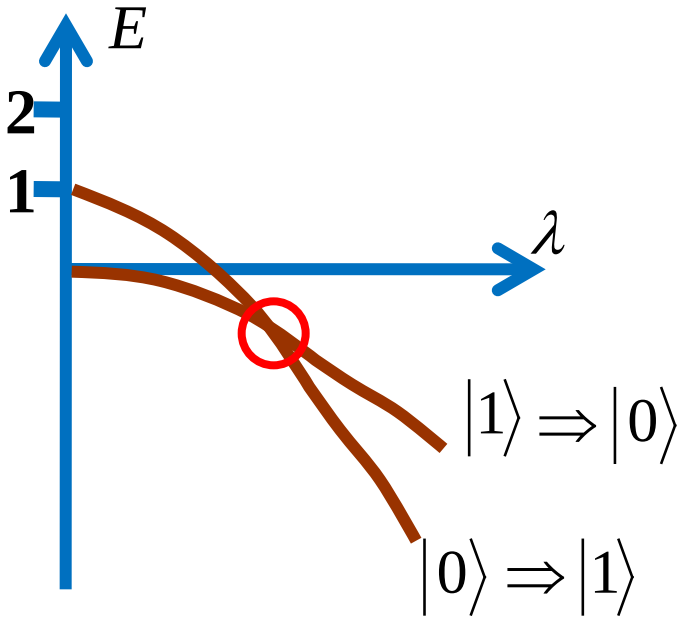






Q1: Is the splitting δE big enough for $|0\rangle$ to remain the ground state at large λ ?

Q2: How big would be the anticrossing gap ?

Q1: Is the splitting δE big enough for $|0\rangle$ to remain the ground state at large λ ?

Perturbation theory in λ

$$E_\alpha(\lambda) = N\sum_k \lambda^{2k} C_k^{(\alpha)}$$

$N \to \infty$

$\frac{M}{N} \to \alpha = const$

$\Longrightarrow E_\alpha(\lambda) \propto N$

Cluster expansion:
~N terms of order 1

1. $C_1^{(\alpha)}$ is exactly the same for all $E_\alpha(\lambda = 0) = 0$ states, i.e. for all solutions. In the leading order $\delta E \propto \lambda^4$

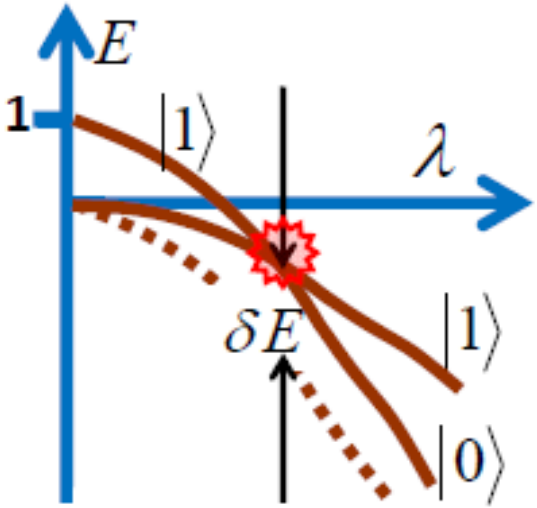
2. In each order of the perturbation theory δE a sum of $O(N)$ terms with random signs.

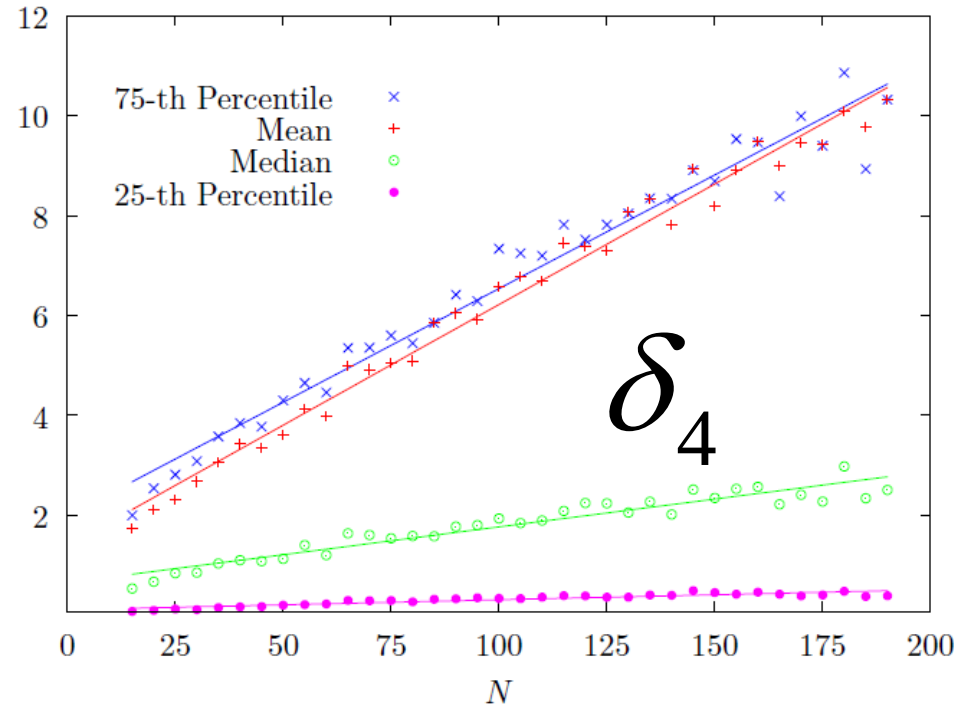
In the leading order in λ

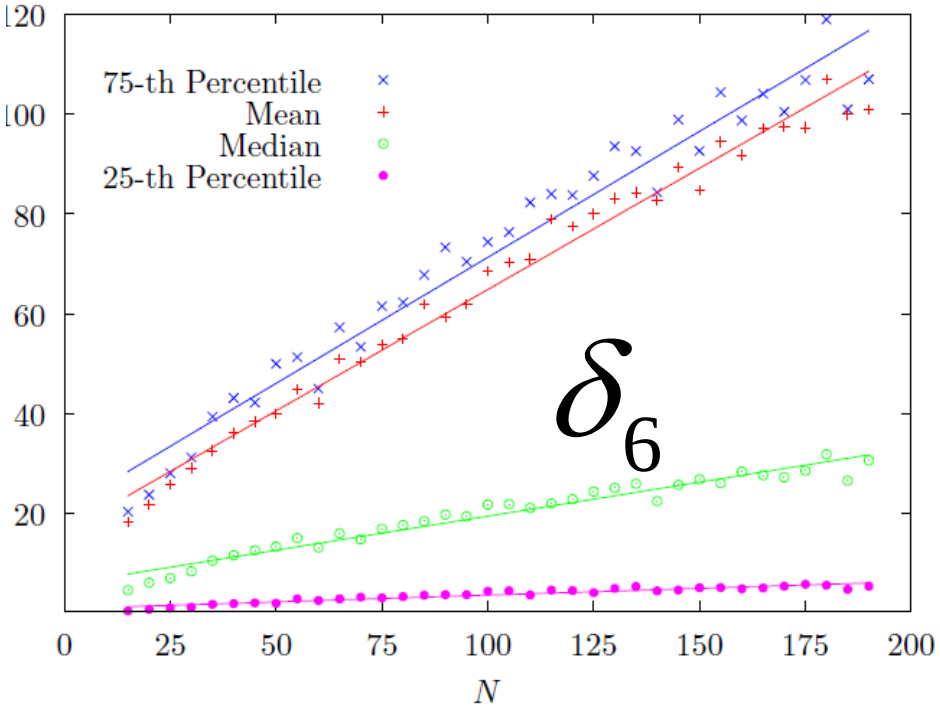
$$\delta E \propto \lambda^4 \sqrt{N}$$

$$\left[\delta E(\lambda, N)\right]^2 = \lambda^4 \delta_4 + \lambda^6 \delta_6 + \ldots$$

$$\delta_4, \delta_6, \ldots \propto N$$

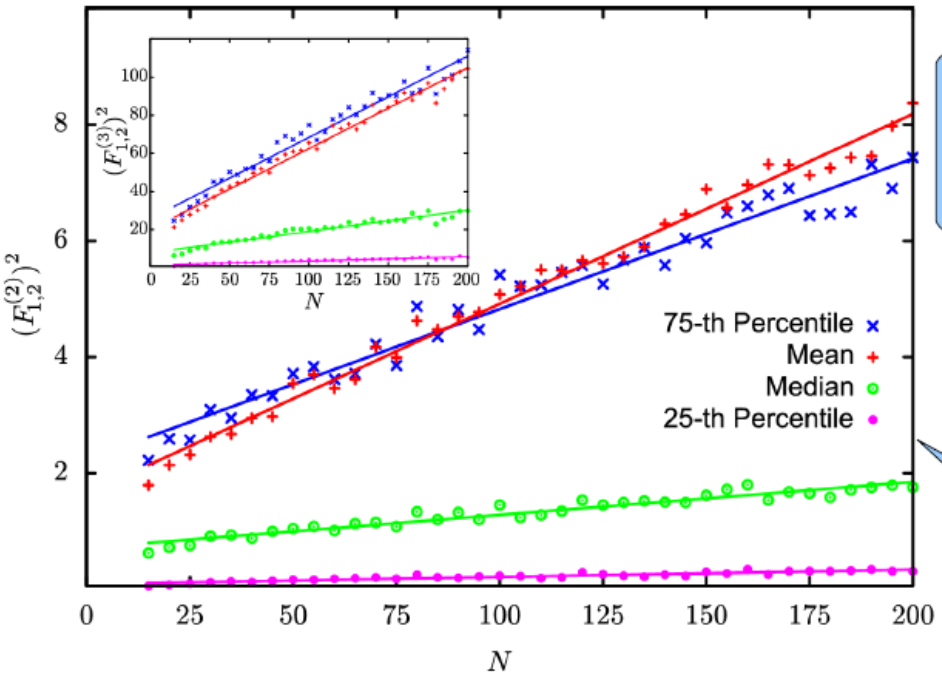






Numerical Simulations

- We generated EC3 random instances with >2 solutions
- then computed $E_1(\lambda) - E_2(\lambda)$ by order 4 perturbation theory



Leading order because:
- Odd orders are zero
- Order 2 is solution-independent for EC3

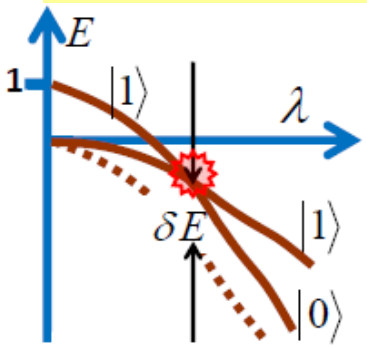
$$(E_1(\lambda) - E_2(\lambda))^2 \approx CN\lambda^8$$

Each data point computed from 2500 instances

We have $E_1(\lambda) - E_2(\lambda) > 4$ for $\lambda > \sqrt{2}(CN)^{-1/8}$

Q1: Is the splitting δE big enough for $|0\rangle$ to remain the ground state at finite λ ?

$$\hat{H}_\lambda\left(\{\hat{\vec{\sigma}}_i\}\right) = \hat{H}_p\left(\{\hat{\sigma}_i^z\}\right) + \lambda \hat{H}_0\left(\{\hat{\vec{\sigma}}_i\}\right)$$



In the leading order in λ

$$\delta E \propto \lambda^4 \sqrt{N}$$

$$\delta E(\lambda) \geq 1 \quad \Rightarrow \quad \lambda \geq (CN)^{-1/8}$$

Q1.1: How big is the interval in λ, where perturbation theory is valid ?

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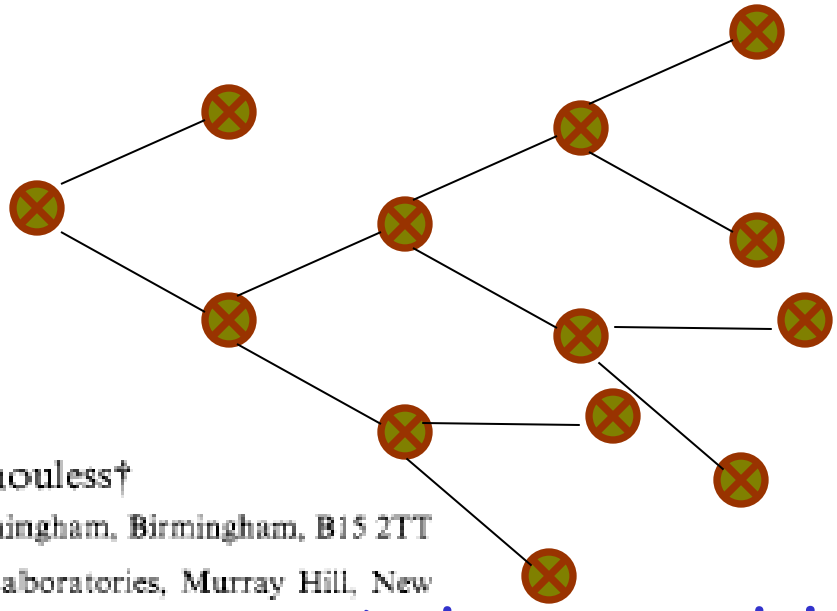
A1.1: 1.Perturbation theory = locator expansion works as long as $\lambda < \lambda_c$ -Anderson localization !

J. Phys. C : Solid State Phys., Vol. 6, 1973. Printed in Great Britain.

Cayley tree



A selfconsistent theory of localization

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Anderson model

W,I

K **– branching #**

Abstract. A new basis has been found for the theory of localization of electrons in disordered systems. The method is based on a selfconsistent solution of the equation for the self energy in second order perturbation theory, whose solution may be purely real almost everywhere (localized states) or complex everywhere (nonlocalized states). The equations used are exact for a Bethe lattice. The selfconsistency condition gives a nonlinear integral equation in two variables for the probability distribution of the real and imaginary parts of the self energy. A simple approximation for the stability limit of localized states gives Anderson's 'upper limit approximation'. Exact solution of the stability problem in a special case gives results very close to Anderson's best estimate. A general and simple formula for the stability limit is derived; this formula should be valid for smooth distribution of site energies away from the band edge. Results of Monte Carlo calculations of the selfconsistency problem are described which confirm and go beyond the analytical results. The relation of this theory to the old Anderson theory is examined, and it is concluded that the present theory is similar but better.

$$I_c = \# \frac{W}{K \ln K}$$

Q1.1: How big is the interval in λ, where perturbation theory is valid ?

A1.1: 1. Perturbation theory = locator expansion works as long as $\lambda < \lambda_c$ - Anderson localization !

2. N-dimensional cube $\approx$ Cayley tree with brunching number $K=N$.

almost no loops

no loops

3. Abou-Chacra, Anderson, Thouless; PRL, 1973

$$I_c = \#\frac{W}{K \ln K} \quad \Rightarrow \quad \lambda_c = O\left(\frac{1}{\ln N}\right)$$

first extended state appears

A1.1: 1.Perturbation theory = locator expansion works as long as $\lambda < \lambda_c$ -Anderson localization !

$$I_c = \# \frac{W}{K \ln K} \quad \Rightarrow \quad \lambda_c = O\left(\frac{1}{\ln N}\right)$$

first extended state appears, i.e. it is a strong underestimation

Important: $\lambda_c = O\left(\frac{1}{\ln N}\right) >> \lambda_* = O\left(N^{-1/8}\right)$

Perturbation theory is valid starting with $\lambda >> \lambda_*$

Q2: How big is the anticrossing gap ?

$$\left\{ \begin{array}{l} \delta E \sim \lambda^{\#N} \\ \lambda \sim \#N^{-1/8} \end{array} \right\} \Rightarrow \delta E \sim \exp\left(-\#N \ln N\right) << e^{-\#N}$$

Adiabatic quantum computer badly fails at large enough N

$$\lambda < \lambda_c \quad \Longrightarrow \quad N > N^* \sim 10^4$$

Existing classical algorithms for solving 1 in 3 SAT problem work for $N < \left(3 \div 4\right) \times 10^3$

The arguments are robust:

N-dimensional hypercube

$H_p\left(\left\{\sigma_i\right\}\right)$ onsite energy

} Correct for any Adiabatic optimization scheme for any problem

$\hat{H}_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right)$ hoping between the neighboring sites of the hypercube

This is not necessary !

For Anderson Localization it is sufficient that $\hat{H}_0\left(\left\{\hat{\vec{\sigma}}_i\right\}\right)$ is local, i.e. contains only products of finite number of spins. Under this condition the arguments are valid for any adiabatic path in the Hamiltonian space

Sergey Knysh and Vadim Smelyanskiy

"On the relevance of avoided crossings away from quantum critical point to the complexity of quantum adiabatic algorithm",
arXiv:1005.3011v1[quant-ph]

- Away from α_s the number of solutions is exponential: $S_0 \sim \exp(\eta N) \quad \eta \xrightarrow[\alpha \to \alpha_s -]{} 0$
- For a typical solution $\left(E - \langle E \rangle\right)^2 \sim \lambda^8 N$
- However the minimum over S_0 solutions

$$\left(E_{\min} - \langle E \rangle\right)^2 \sim \lambda^8 N \log S_0 \sim \eta \lambda^8 N^2$$

- # of states with energy **1** is $S_1 \sim N S_0$
- Energy difference between the true ground state and the E=**1** state at finite λ is $E_{\min} - E^1{}_{\min} \sim -1 + O\left(\lambda^4 \eta^{-1/2} \log N\right)$

$$\lambda_* > (\log N)^{-1/4} \eta^{1/8}$$

$$\lambda_* > (\log N)^{-1/4} \eta^{1/8}$$

Formally small in the $N \to \infty, \eta << 1$ limit, but …

However the exponentially small gap requires only that λ is small

Moreover:

1. Under reasonable restrictions on the allowed sequences a typical sequence in the ensemble can have few solutions or even a unique one and be at the same time hard to solve.

   Zdeborova & Mezard, 2008,
   Krzakala & Zdeborova,2009
   Zdeborova to be published

$$\lambda_* > (\log N)^{-1/4}\,\eta^{1/8}$$

Formally small in the $N \to \infty, \eta << 1$ limit, but …

However the exponentially small gap requires only that λ is small

Moreover:

2. **Upper bound:** given the evolution time T the state of the system would be a linear combination of low energy eigenstates separated by more than $\log T$. Number of "attempts" is thus ~T rather than $\exp(\eta N)$. Provided that $\log T/N \to 0$ we return to more or less previous estimation.

Conclusion

Original idea of adiabatic quantum computation **will not** work

Hopes

- Sampling different trajectories?
  Farhi, Goldstone, Gosset, Gutmann, Meyer, & Shor, arXiv:1004.5127
- Maybe the **delocalized** ground state at finite λ contains information that can speed up the classical algorithm?
- Large number of the solutions?
- Probability to find a solution.
- . . .