More on Quantum Adiabatic Computations (QAC)

Blatant Failure of QAC in Transverse Field 3SAT with USA

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Abstract

We determine the classical and quantum complexities of a specific ensemble of three-satisfiability problems with a unique satisfying assignment for up to $N = 100$ and $N = 80$ variables, respectively. In the classical case we employ generalized ensemble techniques and measure the time that a Markovian Monte Carlo process spends in searching classical ground states. In the quantum case we determine the maximum finite correlation length along a quantum adiabatic trajectory that uses constant tranverse field. In the median of our ensemble both complexities diverge exponentially with the number of variables. Hence, adiabatic quantum computation fails to reduce intractable classical complexity to a polynomial one. Moreover, the growth-rate constant of the quantum case is 3.8 times as large as the one of the classical case, making classical fluctuations more beneficial than quantum fluctuations in ground-sate searches.

Outline of the Talk.

1. what is QAC ?
   - Landau Zener Theory
2. what is 3SAT ?
3. results for 3SAT
   - Markov Chain Monte Carlo (MCMC)
   - Quantum Mass Gap
4. conclude

Outline of the Talk.

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4. conclude

work in slow progress !

Landau Zener Theory.

- a 1932 Proc. Royal Society paper

Non-Adiabatic Crossing of Energy Levels.

By Clarence Zener, National Research Fellow of U.S.A.

(Communicated by R. H. Fowler, F.R.S.—Received July 19, 1932.)

1. *Introduction.*

The crossing of energy levels has been a matter of considerable discussion.* The essential features may be illustrated in the crossing of a polar and homopolar state of a molecule.

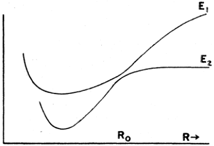


Fig. 1.—Crossing of polar and homopolar states.

Summary.

When a single parameter is varied adiabatically, two eigenwerte of a system may approach each other, and then recede, the corresponding eigenfunctions having exchanged their characters. If the parameter is varied with a finite velocity, the system may jump from one state to the other, thus not suffering a change of character. This transition probability has been rigorously calculated provided the system satisfies certain reasonable restrictions.

Landau Zener Theory..

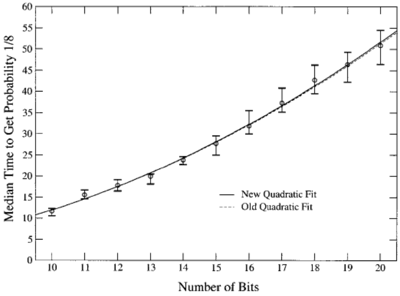
Quantum Adiabatic Evolution

- a 2001 Science article:

A Quantum Adiabatic Evolution Algorithm Applied to Random Instances of an NP-Complete Problem

Edward Farhi,[1]* Jeffrey Goldstone,[1] Sam Gutmann,[2]
Joshua Lapan,[3] Andrew Lundgren,[3] Daniel Preda[3]

A quantum system will stay near its instantaneous ground state if the Hamiltonian that governs its evolution varies slowly enough. This quantum adiabatic behavior is the basis of a new class of algorithms for quantum computing. We tested one such algorithm by applying it to randomly generated hard instances of an NP-complete problem. For the small examples that we could simulate, the quantum adiabatic algorithm worked well, providing evidence that quantum computers (if large ones can be built) may be able to outperform ordinary computers on hard sets of instances of NP-complete problems.



Landau Zener Theory...

- adiabatic passage : a system remains in its instantaneous energy eigenstate if a given perturbation is acting on it slowly enough, M. Born and V. A. Fock (1928), "Beweis des Adiabatensatzes"
- model: single spin in time dependent magnetic field $B = B(t)$ with Hamiltonian matrix $H_{i,j}$:

$$H_{1,1} = +\mu B - \hbar\omega_0/2$$

$$H_{2,2} = -\mu B + \hbar\omega_0/2$$

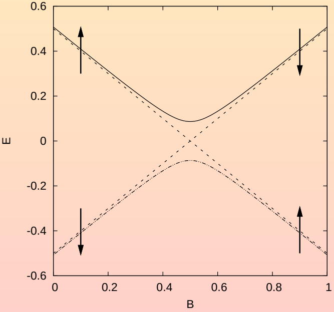
$$H_{1,2} = g \qquad H_{2,1} = g^*$$

Landau Zener Theory....

- instantaneous energy spectrum

$$E_1 = -\frac{1}{2}\sqrt{4gg^* + (\hbar\omega_0 - 2\mu B)^2}$$

$$E_2 = +\frac{1}{2}\sqrt{4gg^* + (\hbar\omega_0 - 2\mu B)^2}$$



the probability of an non-adiabatic i.e., diabatic passage vanishes in the static limit

$$P_{\mathrm{diabatic}} = \exp[-\frac{2\pi gg^*}{\hbar \mid\mid \partial_t(E_2 - E_1) \mid\mid}]$$

$$(E_2 - E_1)\mid_{\mathrm{min}} = \sqrt{4gg^*}$$

Landau Zener Theory.....

how slow the perturbation must vary such that $P_{\text{adiabatic}}$ is small ?

- the scale is set by the minimum energy-gap i.e., mass-gap

$$\Delta m(B) = E_1(B) - E_0(B)$$

$$\Delta m_{\text{min}} = \min_B \{\Delta m(B)\}$$

  and adiabatic passage is guaranteed when

$$\mathcal{T}_0 >> \frac{\text{const}}{\Delta m^2_{\text{min}}}$$

- remark: <u>level crossing</u> kills the adiabatic passage: an <u>avoided level crossing</u> is needed
- for many degrees of freedom : N it is generic that an zero temperature quantum phase transition (PT) appears with small gap values
  $\rightarrow$ 1'st order PT yields exponential small $\Delta m_{\text{min}}(N) \propto \exp[-cN]$
  $\rightarrow$ 2'nd order PT yields polynomial small $\Delta m_{\text{min}}(N) \propto N^{-\alpha}$

Landau Zener Theory......

Quantum Adiabatic Algorithm

- time dependent Schrödinger equation evolves states

$$|\Psi(t)> e^{\frac{i}{\hbar}\mathrm{H}_{\mathrm{QA}}(\mathrm{t})(t-t_0)}|\Psi(t_0)>$$

- map bits $b_i = 0, 1$ of a classical computer to quantum Pauli spins $b_i = (1+\sigma_i^z)/2$ with a $|\Psi(t)>$ that has 2^N complex components for N spins
- Quantum Adiabatic Hamiltonian

$$H_{QA} = [1-\lambda]\mathrm{H}_D + \lambda \mathrm{H}_P \quad 0 \le \lambda \le 1$$

- λ : quantum adiabatic control parameter with schedule

$$\lambda(t) = \frac{t}{\mathcal{T}_0} \quad 0 \le t \le \mathcal{T}_0$$

- driver Hamiltonian $\mathrm{H}_D = -\sum_i \sigma_i^x$ i.e., transverse field
- problem Hamiltonian $\mathrm{H}_P := \mathrm{H}_P(\sigma_i^z)$

Landau Zener Theory.......

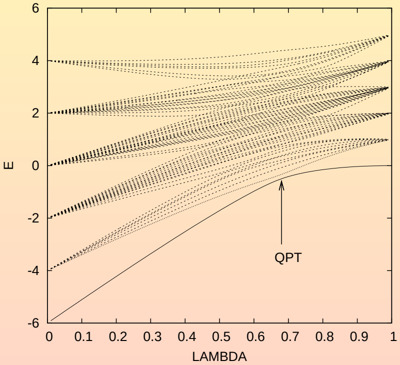
Quantum Adiabatic Algorithm

- quantum adiabatic algorithm solves for the classical ground state of the problem Hamiltonian $\mathrm{H}_P := \mathrm{H}_P(\sigma_i^z)$
- by, first building a configurable nano fabricated device in nature that has a H_{QA} (science fiction now)
- by second, putting there a ground-state of H_D
  - note the spectrum and all wave-functions are known
- by third, performing an adiabatic transition from the ground-state of H_D to the ground-state of H_P in time $\mathcal{T}_0$
- it looks more like an experiment, rather than an actual computation
- in fact it is a model of quantum computation without Q-bits

Landau Zener Theory........

Quantum Adiabatic Algorithm

- the spectrum of H_{QA} for 6 spins and a 3 SAT Hamiltonian



- note the avoided level crossing at the finite N QPT

Landau Zener Theory.........

Quantum Adiabatic Algorithm

- there is the freedom to change the driver Hamiltonian (it should not commute with the problem Hamiltonian)
- there is the freedom to change the problem Hamiltonian if the ground-state stays the same
- there is the freedom to change the path in $Z_{\mathrm{QA}}(\beta, \lambda)$
- there is the freedom to reformulate the problem via polynomial reduction by a ”change of basis”
- there is the freedom to relax the adiabatic condition and correct for it i.e., Jarzynski equality
- but : there is no way to change the Schrödinger wave function dynamics for general Hamiltonian’s of Pauli spins

Landau Zener Theory..........

Quantum Adiabatic Algorithm

- statistical field theory corollary : two parametric QAC partition function at finite temperature $T = \beta^{-1}$

$$Z_{\mathrm{QA}}(\beta, \lambda) = \mathrm{Tr} < \Psi \mid e^{-\beta\{(1-\lambda)H_D + \lambda H_P]\}} \mid \Psi >$$

  - mathematica script for the eigenvalues
  - Lanczos for the eigenvalues
  - Trotter Suzuki Monte Carlo at imaginary time
  - brute force Schrödinger wave function dynamics

- at the point $P^* = (T, \lambda) = (0, 1)$ quantum and thermal fluctuations are frozen ; and the most probable state is the ground-state to H_P
- determine Instanton free energy at the presumed quantum/thermal phase transition line, that separates P^* from high temperature and/or small λ

What is 3 Sat ?.

Intractable !

problems and ground-states ?

- in physics: the ground state mostly is boring, up to
  - random disorder, spin glasses
  - ice , ice models
  - dense packing e.g., liquid crystals, fully packed loop models
  - there can be phase transitions over an ensemble of ground states
- in mathematics:
  - satisfiability problems: exact cover, KSAT, etc
- NP-hard or NP-complete typical run-time

$$\tau \propto e^{\omega N}$$

- ω := rate constant $\omega \leq \ln 2$ (classical) $\omega \leq (\ln 2)/2$ (quantum Grover)

What is 3 Sat ?..

Intractable !

- and even the problem a identifying string theory vacua from a space of 10^{500} different vacua is NP-complete

  F. Denef, M. R. Douglas, ”Computational complexity of the landscape: Part I ”, Ann. of Phys. **322**, Issue 5, (2007) 1096.

  ”We study the computational complexity of the physical problem of finding vacua of string theory which agree with data, such as the cosmological constant, and show that such problems are typically NP hard. In particular, we prove that in the Bousso Polchinski model, the problem is NP complete. We discuss the issues this raises and the possibility that, even if we were to find compelling evidence that some vacuum of string theory describes our universe, we might never be able to find that vacuum explicitly. In a companion paper, we apply this point of view to the question of how early cosmology might select a vacuum.”

What is 3 Sat ?...

Intractable !

- 3SAT is the mother of all Complexity Theories, like the Ising model is for magnets
- given three Ising spins, the three point function

$$h^3_{\mathrm{Clause}}(s_1, s_2, s_3) = \frac{1}{8}(2 - s_1 - s_2 - s_3 + s_1 s_2 + s_1 s_3 + s_2 s_3 - s_1 s_2 s_3)$$

  only is one $h^3_{\mathrm{Clause}} = 1$ <u>if</u> $s_1 = s_2 = s_3 = -1$, otherwise it is zero
- Ising spin version of clause: $\mathrm{b}_1 \vee \mathrm{b}_2 \vee \mathrm{b}_3$
- *M* clauses + logical negation on a set *N* spins/bits in conjunctive normal form

$$\mathrm{CNF} = (\mathrm{b}_{\alpha_1} \vee \overline{\mathrm{b}_{\alpha_2}} \vee \mathrm{b}_{\alpha_3}) \wedge (\overline{\mathrm{b}_{\beta_1}} \vee \mathrm{b}_{\beta_2} \vee \mathrm{b}_{\beta_3}) \wedge (\mathrm{b}_{\gamma_1} \vee \overline{\mathrm{b}_{\gamma_2}} \vee \overline{\mathrm{b}_{\gamma_3}}) \wedge \ldots (M \text{ clauses})$$

  can the CNF be satisfied ?

What is 3 Sat ?....

Intractable !

- Ising Hamiltonian on $s_1, ..., s_N$

$$H_P = \sum_{\alpha=1}^{M} h^3_{\text{Clause}}(\epsilon_{\alpha_1} s_{\alpha_1}, \epsilon_{\alpha_2} s_{\alpha_2}, \epsilon_{\alpha_3} s_{\alpha_3})$$

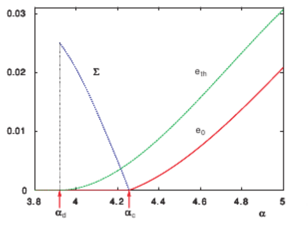
  with $\epsilon_{\alpha_i} = \pm 1$ for $i = 1, 2, 3$ chosen at random
  a choice of the index array α_i, $i = 1, 2, 3$ for $\alpha = 1, ..., M$ and of ϵ_{α_i} is called a realization, we use 1000 realizations
- realizations at $M/N = 5, 8$
- forced unique satisfying assignments (USA): number of ground states at $H_P = 0$ exactly one

What is 3 Sat ?.....

- a single $N = 8$ $M = 64$ realization
  (1,4,-8,7) (2,3,2,4) (3,6,5,-7) (4,6,-1,5) (5,-3,-5,7) (6,7,8,3)
  (7,-1,-2,-6) (8,5,6,2) (9,4,1,8) (10,-3,1,4) (11,-1,-4,5) (12,8,4,1)
  (13,-8,3,7) (14,-5,-8,-1) (15,-3,2,4) (16,-1,-3,7) (17,-1,2,-8)
  (18,5,-7,-3) (19,8,-7,5) (20,-8,7,5) (21,7,6,-4) (22,-7,-1,6)
  (23,-6,-1,-7) (24,-6,1,-3) (25,4,2,3) (26,6,1,7) (27,3,-6,-5)
  (28,6,5,-4) (29,6,8,-2) (30,-5,-8,-3) (31,-8,2,1) (32,6,3,8)
  (33,2,3,5) (34,8,-2,5) (35,6,5,-3) (36,-4,-5,-8) (37,-7,1,8)
  (38,-7,-3,4) (39,-2,-7,8) (40,-2,-5,4) (41,-6,-2,8) (42,7,-5,-2)
  (43,3,7,6) (44,-1,-5,3) (45,4,-6,3) (46,-3,1,4) (47,4,3,-5)
  (48,-3,7,5) (49,2,-8,-5) (50,1,2,3) (51,2,8,6) (52,3,2,-5) (53,8,2,-6)
  (54,-7,-2,-3) (55,-6,-1,-2) (56,-1,4,-8) (57,-7,8,1) (58,-4,-2,7)
  (59,3,6,7) (60,4,-7,-1) (61,1,-7,2) (62,1,-3,-5) (63,-8,-4,-3)
  (64,-2,8,4)
- has the unique satisfying ground-state: $|\ 01010111 >$

Random 3 SAT interludium.

- $\alpha_s(K=3) = 4.26675(15)$:
- Parisi; Science 2002, 1RSB solution
- Borgs 1999, $\Delta\alpha \propto N^{-\tilde{\nu}}$
- D. Wilson, 2002, $\tilde{\nu} \geq 2$
- data for N=50,100,200



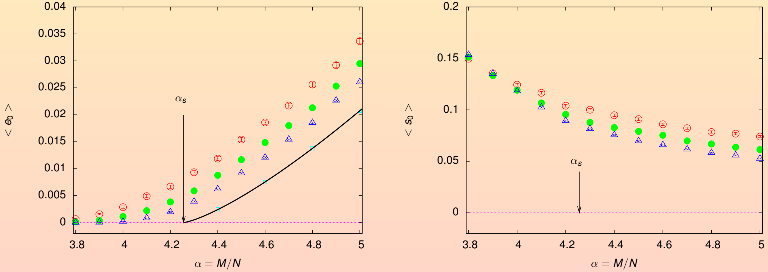


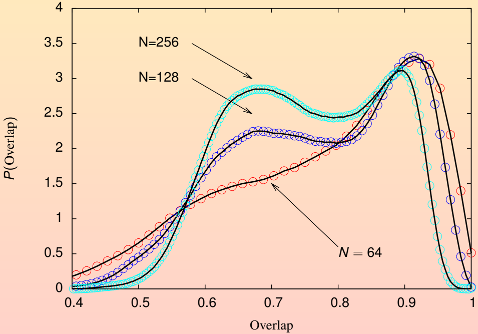
Figure: Left: Ground-state energy $< e_0 >$. Right: Ground-state entropy $< s_0 >$

Random 3 SAT interludium..

$\alpha = 4.0$ large scale

$$\text{Overlap} = [2/N/g_0/(g_0-1)] < \sum_{i,\alpha,\beta>\alpha} \delta^1[s^{\alpha}_{i,gsc}, s^{\beta}_{i,gsc}] >$$

parallel tempering



Hartmann 2010

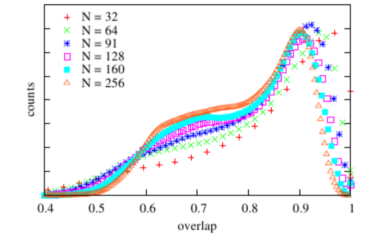
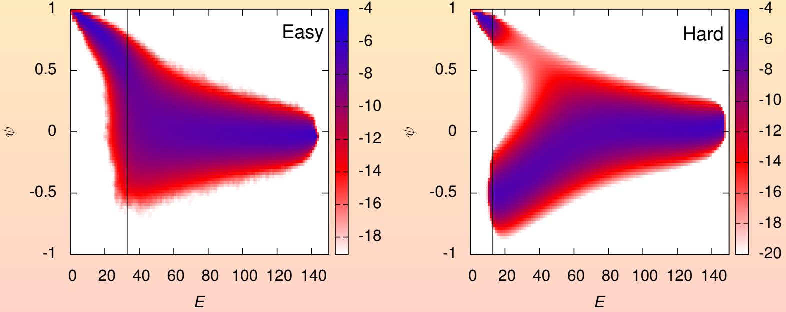


FIG. 13: Overlap $\langle r \rangle$ of solutions in clusters found by Ballistic Networking, for $\alpha = 4.0$. For $\langle r \rangle < 0.4$ the curves are essentially zero.

USA search landscape via density of states.

$$\rho(\psi, E) = \mathcal{N}^{-1}(E) \sum_{\text{conf}} \delta^1(H - E)\delta^1(\psi - \frac{1}{N}\sum_i s_i s_{i,gsc})$$

contour plot of $\rho(\psi, E)$ on two easy/hard realizations



the vertical line denotes E at $C_{V,max}$

Spin Glass landscape via density of states.

Iba, Takahashi 2004

$$P_\beta(\boldsymbol{x}) \propto \exp\left(\beta \sum_{(ijk)\in G} J_{ijk} x_i x_j x_k\right).$$

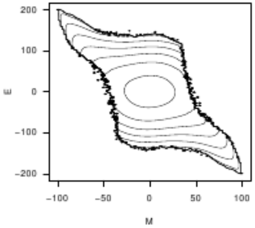


Fig. 1. Density of States: $\log D(E,M)$

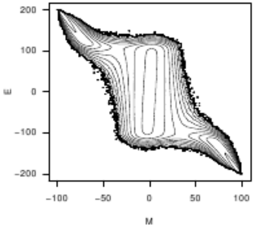


Fig. 2. Multicanonical Density: $\log D(M|E)$

MCMC search complexity in 3 SAT with USA.

random walk in energy, i.e. Multicanonical Ensemble sim.

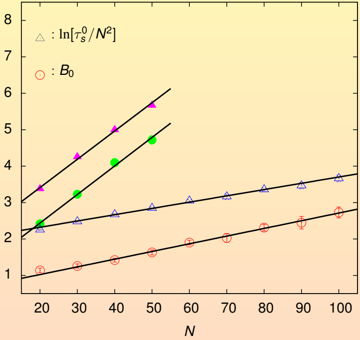


Figure: Logarithmized search time $<\tau_s^0/N^2>$ (triangles) and the nucleation barrier $<B_0>$ (circles). Two data-sets at $M/N = 8$ (open symbols) and at $M/N = 5$ (full symbols). All data are consistent with an exponential singularity $(<\tau_s>, <B_0>) \propto \exp[+\omega N]$. Numerical values: $\omega(M/N = 5) = 0.078(1) \approx \ln 2/9$ and $\omega(M/N = 8) = 0.016(1) \approx \ln 2/43$.

Signature of the Quantum Phase Transition.

using Trotter Susuki time regularization of the quantum system and extensive parallel tempering simulations in λ

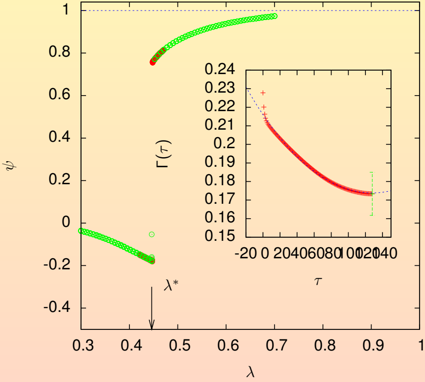


Figure: First order phase transition jump in ground state overlap ψ as a function of λ. Inset: Correlator $\Gamma(\tau)$ at λ^*, that determines the inverse gap, i.e. tunneling correlation length on a $N_\tau = 256$ box.

Quantum search complexity in 3 SAT with USA.

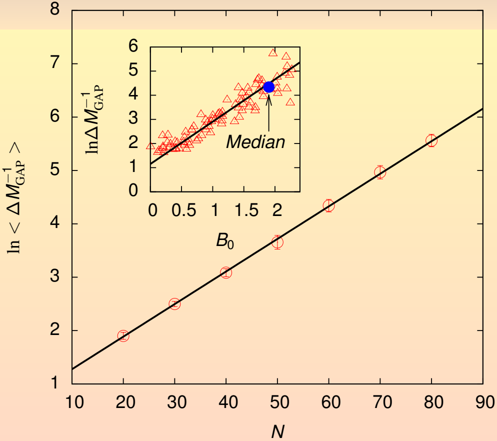


Figure: maximal $\Delta M_{\mathrm{GAP}}^{-1}(< B_0 >)$ as a function of N in logarithmic ordinate scale for N as large as $N = 80$ (with a correlation length as large as $\xi = 259.9$). In 3 SAT there is an indisputable exponential singularity with a rate constant $\omega = 0.061(1) \approx \ln 2/12$ at $M/N = 8$.

Conclusion.

- first order Quantum phase transition in 3SAT with USA with transverse field yielding exponential large quantum search complexity in the Median, which actually behaves worst $12/44$, than a classical/thermal random search in energy !
- calculation in 3 SAT at $N = 80$, related work has been done by P. Young et. al. in exact cover at $N = 256$, PRL 2010

First-Order Phase Transition in the Quantum Adiabatic Algorithm

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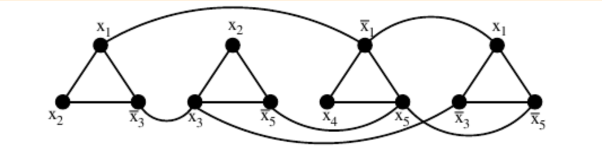
(Received 8 October 2009; published 14 January 2010)

We simulate the quantum adiabatic algorithm (QAA) for the exact cover problem for sizes up to $N = 256$ using quantum Monte Carlo simulations incorporating parallel tempering. At large N, we find that some instances have a discontinuous (first-order) quantum phase transition during the evolution of the QAA. This fraction increases with increasing N and may tend to 1 for $N \to \infty$.

Conclusion..

- it is too early to draw final conclusions for all of the NP problems and for all versions of the QAC algorithm
- paper: T. Neuhaus, M. Peschina, K. Michielsen and H. de Raedt, ”Classical and Quantum Annealing in the Median of Three Satisfiability” submitted to PRA.
- current study: polynomial reduction of 3 SAT to maximum independent set (MIS)



$\rightarrow$ dense packing of hard spheres/atoms on a graph at radius $1 < r < 2$