

# Statistical Analysis for Quantum Adiabatic Computations: Quantum Monte Carlo Annealing

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## Abstract

Quantum adiabatic computations are designed to determine the ground state configurations of a classical problem Hamiltonian  $H_{3SAT}$  within quantum theory and at imaginary time allow statistical mechanics studies for the computational efficiency of the ground state search. We mention a recent determination of the quantum complexity, i.e. the mass-gap  $\Delta m_{GAP}$  for a specific ensemble of three-satisfiability (3SAT) problems with a unique satisfiability assignment, which shows an exponential increase of the gap correlation length  $\xi_{GAP}$  with  $\xi_{GAP} = 1/\Delta m_{GAP}$ . In 3SAT we present numerical data for the behavior of quantum Monte Carlo annealing cycles in search for the ground state. The findings show, that for the specific set of realizations quantum Monte Carlo searches in 3SAT fail above a sharp cut-off  $K_{cut}$  in the complexity  $K$ , which exemplifies the intractable nature of 3SAT.

*Keywords:*

## 1. Introduction

In mathematics one defines optimization problems, that are cast into solving a minimization problem on a discrete set of variables: Given a cost function or problem Hamiltonian  $H_{3SAT}(s)$  that is bounded from below by zero, and given a set of integer variables (Ising spins)  $s_i = \pm 1$  with  $i = 1, \dots, N$ , one may ask: Which assignment or - satisfiability assignment - solves  $H_{3SAT} = 0$ ? Many satisfiability assignment problems with Boolean variables  $b_i = (1 + s_i)/2$  in the class of NP-complete problems have precisely this form. In this work we study the 3-satisfiability (3-SAT) problem, a NP-hard problem at the heart of complexity theory [1] by means of methods used in statistical physics. Under the assumption  $P \neq NP$ , the computational effort for any classical algorithm to solve NP-hard problems is believed to be  $O(e^{gN})$ , where  $g$  denotes the growth-rate constant. For an unstructured search, that is the evaluation of  $H_{3SAT}$  over all configurations,  $g = \ln 2$ . A polynomial solution to a NP-hard problem is expected to have  $g = 0$ . A quantum algorithm with  $g = 0$  for a NP-complete problem would certainly be of interest.

Conventional, standard adiabatic quantum computation (AQC) [2, 3] assumes a linear interpolation between

$$H_{AQC} = (1 - \lambda) H_D + \lambda H_{3SAT} \quad (1)$$

the NP-hard problem Hamiltonian  $H_{3SAT}$  and a non-commuting driver Hamiltonian  $H_D = \sum_i \sigma_i^x$  (the “transverse field”), where  $\sigma_i^x$  is the  $x$ -component of the Pauli matrix. A statistical analysis of AQCs determines the thermodynamic

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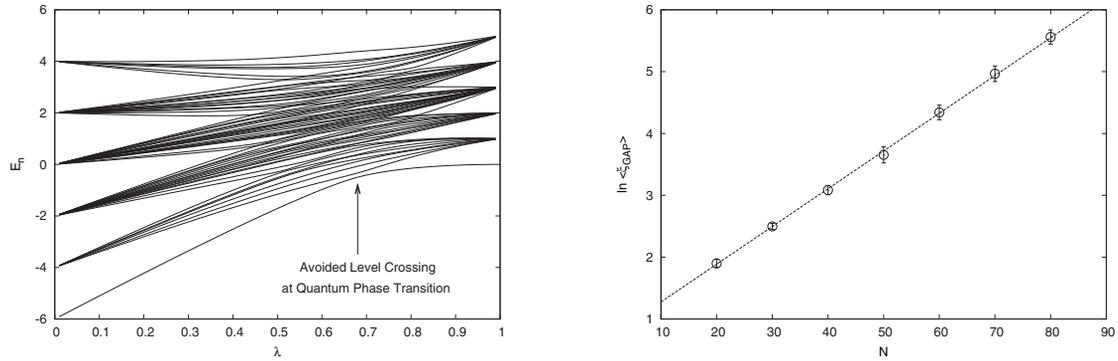


Figure 1: Eigenvalue spectrum as a function of  $\lambda$  of a  $H_{\text{AQC}}$  in 3SAT Figure 2: Exponential divergence in Median gap correlation length for  $N = 6$  spins. There are 64 levels and a unique ground-state (USA).  $\xi_{\text{GAP}}$  of 3SAT from [10] for  $N$  up to  $N = 80$ . Plotted is  $\ln \langle \xi_{\text{GAP}} \rangle (N)$ .

and quantum singularities of the partition function

$$Z_{\text{AQC}}(\beta, \lambda) = \text{Tr} e^{-\beta((1-\lambda)H_D + \lambda H_{\text{3SAT}})}, \quad (2)$$

where  $\beta = 1/k_B T$  denotes the inverse temperature,  $k_B$  is Boltzmann's constant and  $0 \leq \lambda \leq 1$  is the quantum adiabatic control parameter. In the vicinity of the point  $P_0^* = (\beta, \lambda) = (\infty, 1)$  the optimization problem is solved as vanishing thermal and quantum fluctuations lead to the exact ground-state. In particular we study the approach to  $P_0^*$  from regions of large quantum fluctuations on lines of the parameter  $\lambda$  at  $T = 0$ .

In the pure quantum limit one determines the maximal spin-spin correlation length  $\xi_{\text{GAP}}$  i.e., the inverse of the mass gap  $\xi_{\text{GAP}} = 1/\Delta m_{\text{GAP}}$  at the presumed quantum phase transition (QPT), which is positioned at  $\lambda^*$ . The mass gap of the theory simply is defined through the spectral properties of  $H_{\text{AQC}}$

$$\Delta m(\lambda) = E_1 - E_0 \quad (3)$$

with  $E_0$  denoting the ground-state energy and  $E_1$  the first excited one and, at the QPT  $\Delta m(\lambda)$  takes its minimal value  $\Delta m_{\text{GAP}} = \Delta m(\lambda^*)$ . One may either determine the exponential decay of a two point function in imaginary time in Quantum Monte Carlo simulations for large number of spins, or directly diagonalize the Hamiltonian  $H_{\text{AQC}}$  via the Lanczos algorithm for small number of spins. In either case, if there exists an avoided level crossing, see Fig.(1), even the maximum spin-spin correlation length is finite for a finite number of spins. Then and accordance with Landau Zener theory [4], in AQCs the running time of ground-state searches is fundamentally limited to a time scale  $\mathcal{T}$  of order  $\mathcal{O}(\xi_{\text{GAP}}^2)$  from below. Hence, for a NP-hard problem, a spin-spin correlation length growing exponentially with  $N$  - the number of spins - would yield a computational complexity for quantum ground-state searches that is similar to the one expected for a classical search. Also, a correlation length  $\xi_{\text{GAP}}$  only rising polynomially  $\xi_{\text{GAP}} \propto N^p$  would give AQCs a clear advantage over all classical algorithms. It is argued that exponentially small energy gaps are induced by the presence of first-order phase transitions within  $Z_{\text{AQC}}$ , hampering a possible performance gain of AQC in optimization problems related to the 3-SAT problem [5, 6, 7, 8]. A second order phase transition on the other hand signals a polynomial running time.

Adiabatic quantum computations have received attention because of a 2001 research paper of Farhi et. al., which indicated the possibility of a polynomial running time in 3SAT [3]. The work relied on systems with up to twenty  $N = 20$  spins, which from a statistical mechanics point of view presumably is way to small to substantiate asymptotic claims. Recently the issue was studied in another NP-complete theory, namely Exact Cover by P. Young et. al. [9] using up to  $N = 256$  spins and Quantum Monte Carlo (QMC). They encounter a particular nasty situation where the QPT appears to be weak - of second order - for small number of spins, and then slowly turns into first order for the largest number of spins. The author in collaboration with K. Michielson and H. De Raedt at Jülich Supercomputing Center (JSC) has studied 3SAT up to  $N = 80$  spins with QMC methods also. In the Median of a particular designed

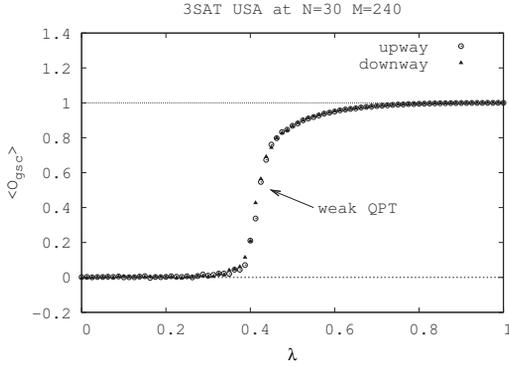


Figure 3: QMC adiabatic cycle on a weak problem realization.

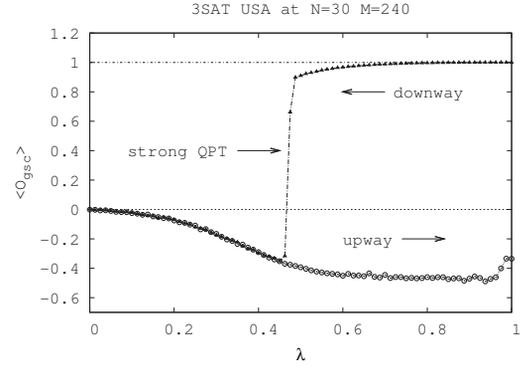


Figure 4: Adiabatic cycle hysteresis on a hard problem realization.

ensemble of 3SAT Hamiltonian's - USA with unique ground-state - and at the principal 3SAT parameter  $\alpha = M/N = 8$ , where  $M$  denotes the number of clauses, the gap correlation length  $\xi_{\text{GAP}}$  diverges exponentially [10] indeed, see Fig.(2) thus reiterating the NP-hard nature of 3SAT for the quantum case also. However, here we present additional material on the efficiency of a related but somewhat different algorithmic approach: We study Quantum Monte Carlo annealing cycles in search for the ground state. These simulations implement an artificial Monte Carlo time dynamics within the quantum partition function for purposes of the ground-state search.

## 2. 3SAT Theory, Quantum Monte Carlo Simulation and QMC adiabatic cycles

3SAT is defined on a set of  $N$  Ising spins  $s_i = \pm 1$  with  $i = 1, \dots, N$ . The Hamiltonian is a sum of  $M$  three point interactions  $\Gamma_\gamma^3(s_1, s_2, s_3)$ , called clauses with  $\gamma = 1, \dots, M$ . The principal parameter of the 3 SAT Hamiltonian is the ratio  $\alpha$  with  $\alpha = M/N$ . The Hamiltonian then is

$$H_{\text{3SAT}} = \sum_{\gamma=1}^M \Gamma^3(\epsilon_{\gamma,1} s_{i[\gamma,1]}, \epsilon_{\gamma,2} s_{i[\gamma,2]}, \epsilon_{\gamma,3} s_{i[\gamma,3]}) \quad (4)$$

and where  $\Gamma^3$  is a direct transcription of the logical .or. in-between three bits to Ising degrees of freedom:

$$\Gamma^3(s_1, s_2, s_3) = \frac{1}{8} \{(s_1 s_2 s_3) + (s_1 s_2 + s_1 s_3 + s_2 s_3) + (s_1 + s_2 + s_3) - 1\}. \quad (5)$$

The theory possesses random disorder as well as frustration. Each Ising spin at each clause  $\gamma$  and clause-position  $p = 1, 2, 3$  carries a sign  $\epsilon_{\alpha,p} = \pm 1$ , that is chosen at random. Finally there exists a map  $[\gamma, p] \rightarrow i$  from the clauses to the set of spins, which also is randomized. We mention that additional constraints are imposed. In particular we only consider realizations i.e., Hamiltonian's  $H_{\text{3SAT}}$  whose ground-state is unique at energy zero. These ground-states are called unique satisfiability assignment's (USA). The theory then is quantized by introducing a standard Trotter-Suzuki time discretization [11]. We choose a regular temporal lattice with  $N_\tau$  time-slices, a finite step-size  $\Delta\tau = 1$  in  $\tau$  direction and periodic boundary conditions in Trotter time. The inverse temperature is  $\beta = 1/k_B T = N_\tau \Delta\tau$  and the Boltzmann factor of the quantized problem at imaginary time is

$$\ln[P_{\text{B,q}}] = -\kappa_0 \sum_{\tau=1}^{N_\tau} H_0(\{s_1(\tau), \dots, s_N(\tau)\}) + \kappa_\tau \sum_i^N \sum_{\tau=1}^{N_\tau} s_i(\tau) s_i(\tau + 1), \quad (6)$$

with positive ferromagnetic hopping parameters  $\kappa_0 = \lambda \Delta\tau$  and  $\kappa_\tau = -\ln[\tanh((1 - \lambda)\Delta\tau)]/2$ . These equations implement the AQC partition function Eq.(2) as a function of  $\lambda$  and  $\beta$ , up to discretization errors caused by the finiteness

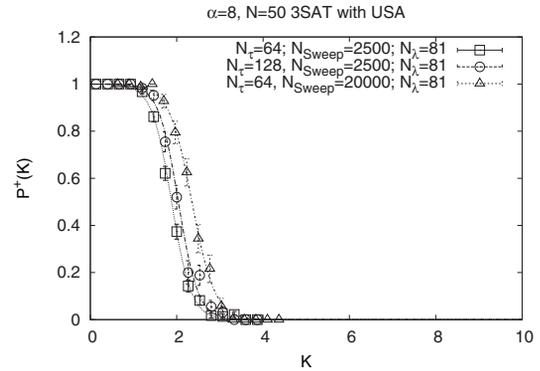
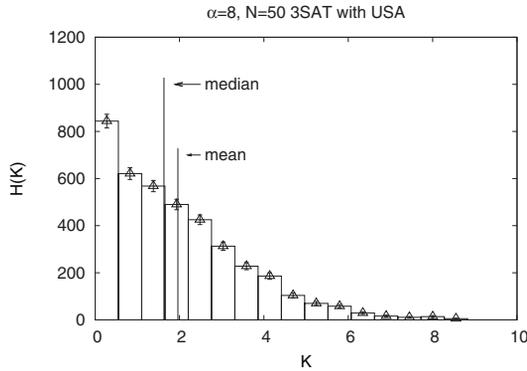


Figure 5: Histogram  $H(K)$  of complexity  $K$  as explained in the text on a set of 4000 3SAT realizations at  $N = 50$  and  $\alpha = 8$ . Figure 6: Success probability  $P^+(K)$  in up-way ground-state searches for three different sets of annealing parameters.

of the regularization. The partition function Eq.(2) is updated with standard Metropolis steps and at each set of the parameters  $\lambda$ ,  $\Delta\tau$  and  $N_\tau$  one sweep touches each of the  $N \times N_\tau$  spins once. The parameters  $\Delta\tau = 1$  and  $\alpha = M/N = 8$  are kept fixed throughout our study. We typically generated several hundred to several thousand different realizations of  $H_{3SAT}$  and present average values over realizations.

The most direct and simple approach to explore properties of the QPT in AQC for 3SAT consists in QMC adiabatic cycles, which as the function of the adiabatic control parameter  $\lambda$  in a up-way simulation on the cycle prepare a ground-state to  $H_{AQC}$  at  $\lambda = 0$ , that is slowly iterated with quantum Monte Carlo updates on a equal spaced grid of  $\lambda$ -values towards the point  $\lambda = 1$ , where the ground state is known to be the ground-state to  $H_{3SAT}$ . Clearly this is simulated annealing in the quantum fluctuations of a Monte Carlo dynamics as controlled by  $\lambda$ . We choose an equal-spaced  $\lambda$ -grid of  $N_\lambda$  grid-points and at each  $\lambda$ -value perform  $N_{sweep}$  sweeps. The cycle is completed by preparing the known ground-state at  $\lambda = 1$ , which then is iterated back to  $\lambda = 0$  in the down-way simulation. We monitor the mean overlap  $\langle O_{gsc} \rangle = N^{-1} \langle \sum s_i s_{i,gsc} \rangle$  on each  $\lambda$ -grid point, where  $s_{i,gsc}$  denotes the ground-state to  $H_{3SAT}$ .

The signature of the QPT is nicely exhibited in Figures (3) and (4), which display simulation data for a  $\lambda$ -grid of  $N_\lambda = 81$  points with  $N_\tau = 64$  and  $N_{sweep} = 2500$  in the QMC simulation. The 3SAT problem has  $N = 50$  spins and at  $\alpha = 8$  there are  $M = 400$  clauses in the Hamiltonian. Both data sets correspond to two different realizations of the 3SAT Hamiltonian  $H_{3SAT}$  at grossly different computational complexity, and while the up-way simulation in Fig.(3) on a weak problem realization converges to the correct ground-state at  $\langle O_{gsc} \rangle = 1$ , the simulation in Fig.(4) on a hard problem realization is trapped at  $\lambda = 1$  in a wrong configuration and does not converge. The observed hysteresis structure of Fig.(4) is reminiscent of a discontinuous i.e., first order behavior at the QPT, if the problem realizations are hard.

During the course of our studies we have classified 4000 3SAT problem realizations at  $N = 50$  spins and at  $\alpha = 8$  with respect to their search-hardness by a complexity measure  $K$ , that is easier to calculate than the gap correlation length itself. However, and for the given set of realizations  $K$  is linearly correlated to the gap correlation length logarithm  $\ln \xi_{GAP}$  within reasonable statistical errors:  $\ln \langle \xi_{GAP} \rangle = \langle K \rangle + \text{const}$ . The numerical value of const is  $\text{const} = 1.44$  here and thus a typical complexity  $K = 2$  implies a gap correlation length of about  $\xi_{GAP} = 30$  Trotter time spacings at  $\Delta\tau = 1$ . We display in Fig.(5) the histogram  $H(K)$  of complexities  $K$  within our set of  $H_{3SAT}$  realizations at  $N = 50$ . The histogram exhibits a fat tail corresponding to large variability of the search complexity. We note that rare i.e., extreme realizations can have complexities  $K = 8$ , which are far above the mean  $K_{\text{mean}} = 1.96$  or Median  $K_{\text{Median}} = 1.63$ , see the vertical lines in Fig.(5).

Our main result concerns the restricted probability  $P^+(K)$  with  $0 \leq P^+ \leq 1$  for a successful ground-state search in the up-way simulation of the cycle at complexity value  $K$ . Repeating cycles with different random number sequences we accumulate additional statistics and Fig.(6) displays the results for three different sets of the annealing parameters.

In all cases we observe a sharp cut-off  $K_{\text{cut}}$  beyond which the search fails and using the form

$$P^+(K) = 1 - \tanh\left(\frac{K - K_{\text{cut}}}{\Delta K}\right) \quad (7)$$

the cut-off values are determined, see the curves in Fig.(6). Firstly the squares within Fig.(6) correspond to annealing parameters  $N_\lambda = 81$ ,  $N_\tau = 64$  and  $N_{\text{sweep}} = 2500$  and have  $K_{\text{cut}} = 1.88$ . This implies that realizations up to mean complexity can be solved with certainty while large value  $K$  realizations are not solved with certainty. Secondly, the circles within Fig.(6) correspond to an annealing schedule, where the small but finite temperature  $T = 1/64$  of the finite Trotter time quantum box, is further lowered to half of its previous value:  $T = 1/128$ . We find a cut-value  $K_{\text{cut}} = 2.03$ , which however only is marginal larger than the previous value at twice the temperature value. The search failure at large complexity  $K$  values consequently is likely not going to be healed in a easy way upon lowering the small albeit finite temperature of the finite Trotter boxes. For this purpose the temperature dependence appears to be too weak. Thirdly, the triangles within Fig.(6) correspond to an annealing schedule, where at temperature  $T = 1/64$  the statistics  $N_{\text{sweep}} = 20000$  was eight-fold larger than as for the firstly mentioned data set at  $N_{\text{sweep}} = 2500$ . We determine  $K_{\text{cut}} = 2.35$  and the finding in total is sobering: There is no way to solve for ground-state configurations in 3SAT with USA at  $\alpha = 8$  and  $N = 50$  spins by means of QMC adiabatic cycles, if the corresponding 3SAT realizations lie in the fat tail of rare and computational hard complexity values  $K = 4, 5, 6, 7$  and  $K = 8$ , compare Fig.(5) and Fig.(6) again. We mention the obvious fact, that the situation worsens for larger spin numbers  $N > 50$ .

### 3. Conclusion

In summary, we have introduced statistical methods that study the quantum running times for ground-state searches in the 3-SAT problem with unique satisfiability assignment. We have mentioned a recent result [10] that excludes a polynomial run-time behavior for quantum searches in 3SAT adiabatic quantum computations, see Fig.(2) for number of spins up to  $N = 80$ . The data in Fig.(2) appear to be asymptotic. We have also illustrated the computational complexity of ground state searches within quantum Monte Carlo adiabatic cycles that fail badly within the extreme value tail of complexity distributions, again demonstrating the intractable nature of the theory. In the future one may determine complexities of systems with modified driver Hamiltonian's, that possibly are optimized with respect to ground state searches. A second line of research can be concerned with polynomial transformations - or polynomial reductions - of 3SAT within the set of NP-complete theories. There exists an elegant transformation of 3SAT to the *Maximum Independent Set* (MIS) problem [12], which transforms the frustrated three-point couplings  $\propto \epsilon^3 s^3$  of the Ising spin Hamiltonian  $H_{3\text{SAT}}$ , eqns.(4,5) into fluctuating but anti-ferromagnetic two-point couplings  $\propto -\kappa s^2$  supplied by magnetic field terms  $\propto +hs$ . It will be interesting to find out how quantum complexities behave under such transformations on an identical set of problem realizations.

### 4. Acknowledgment

The author acknowledges the extended hospitality of the theory department at Bielefeld university. Calculations were performed on the JUMP and JUROPA supercomputers at JSC and on the NICOLE workstation cluster of NIC (VSR grant JJSC02).

- [1] S. A. Cook, Proc. Third Annual ACM Symposium on the Theory of Computing, (ACM, New York, 1971) 151.
- [2] T. Kadowaki and H. Nishimori, Phys. Rev. E **58**, 5355 (1998).
- [3] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, arXiv:quant-ph/0001106, (2001); E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, and D. Preda, Science **292**, 472 (2001).
- [4] L. D. Landau, Phys. Z. Sowjetunion **2**, 46 (1932); C. Zener, Proc. Roy. Soc. London, Series A **137**, 696 (1932).
- [5] R. Schützhold and G. Schaller, Phys. Rev. A **74**, 060304(R) (2006).
- [6] M. H. S. Amin and V. Choi, Phys. Rev. A **80**, 062326 (2009).
- [7] T. Jörg, F. Krzakala, G. Semerjian, and F. Zamponi, Phys. Rev. Lett. **104**, 207206 (2010).
- [8] B. Altshuler, H. Krovi, and J. Roland, PNAS **107**, 12446 (2010)
- [9] A. P. Young, S. Knysh, and V. N. Smelyanskiy, Phys. Rev. Lett. **101**, 170503 (2008) and Phys. Rev. Lett. **104**, 020502 (2010).
- [10] T. Neuhaus, M. Peschina, K. Michielsen and H. De Raedt, Phys. Rev A **83**, 012309 (2011).
- [11] M. Suzuki, S. Miyashita, and A. Kuroda, Prog. Theor. Phys. **58**, 1377 (1977).
- [12] V. Choi in: "Avoid First Order Quantum Phase Transition by Changing Problem Hamiltonians", arXiv:1010.1220v1 [quant-ph], October 2010.