First Steps in the Statistical Analysis of Quantum Adiabatic Computations

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Quantum Computing

- time dependent Schrödinger equation evolves states

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

- lets consider two level systems which maps the bits $b_i = 0, 1$ of a classical computer to quantum "Ising" spins $\sigma_i^z = -1, +1$

$$\sigma_i^z = 1 - 2b_i$$

  with a spin wave function that has 2^N complex components for N spins
- can one benefit from the simultaneous i.e., parallel in time evolution of all these components ?
- answer in "canonical" quantum computing: if one is able find a physical device, that is able to implement logical gates on Q-bits: yes,
  for very specific mathematical problems

Quantum Computing

- very specific mathematical problem: Shor's algorithm: Peter W. Shor (ATT Research), "Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer", quant-ph/9508027 (1995).
- it is however very hard to build a quantum computer from

  - trapped ions, NMR spins, Quantum Dots, Josephson Junctions in a superconductor, ...

  because a large number of logical gates has to be implemented with high precision in a coherent state for long time
- Quantum Adiabatic Algorithm: forget about logical gates: let a quantized spin system evolve into its ground-state with a Quantum Hamiltonian, whose classical counterpart parametrizes a optimization problem of the NP-hard category

$$\mathrm{NP-hard} \;:\; \mathrm{computational\ effort} \propto e^{+\mathrm{const}\,N}$$

Quantum Adiabatic Algorithm

- it has been conjecture by famous people, that the QA algorithm could solve general optimization problems in polynomial time: E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren and D. Preda, Science 292 (2001) 472; T. Kodawaki and H. Nishimori, Phys. Rev. E 58 (1998) 5355.

  -methods : exact diagonalization, real time Schrödinger equation solution for few spins, complexity $\propto N^2$ for $N = 24$ spins

  -recently : A.P. Young, S. Knysh, V.N. Smelyanskiy, Phys. Rev. Lett. 101, 170503(2008) : support for polynomial scaling up to $N = 128$

  -just in October 2009: Young et al., "First order phase transition in the Quantum Adiabatic Algorithm", arXiv:0910.1378v1 at $N = 256$.

Quantum Adiabatic Alg. Basics

- a system remains in instantaneous energy eigenstate if a given perturbation is acting on it slowly enough, M. Born and V. A. Fock (1928), "Beweis des Adiabatensatzes"; C. Zener (1932), "Non-adiabatic Crossing of Energy Levels".

- the Quantum Adiabatic Hamiltonian is a sum

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

- of the driver Hamiltonian $\mathrm{H}_D = -\sum_i \sigma_x$ (transverse field)

- and the problem Hamiltonian H_P, with difficult groundstate calculation

- λ: QA control parameter with time-schedule e.g.,

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

how large the scale $\mathcal{T}_0$ has to be, that an instantaneous eigenstate at groundstate energy for $\lambda = 0$ stays in the ground state up to $\lambda = 1$ **?**

Quantum Adiabatic Alg. Basics

- Answer: the QA Hamiltonian has a spectrum and the mass-gap

  $$\Delta m(\lambda) = m_1(\lambda) - m_0(\lambda)$$

  sets the scale

- in particular there exists a minimum gap on λ-space

  $$\Delta m_{\min} = \{\min_\lambda \Delta m(\lambda)\}$$

  and with avoided level crossings

  $$\mathcal{T}_0 >> \frac{\mathrm{const}}{\Delta m_{\min}^2}$$

  the QA algorithm is expected to converge **!**

- the invariant main difficulty possibly remains: a zero temperature quantum phase transition with small values of the gap at some value λ^* **!**, in particular first order phase transitions will kill polynomial scaling

The Working Program

- define a classical optimization problem, that

  - has a Ising Hamiltonian

  - has a unique ground state solution

  - is NP hard, $\rightarrow 3 - \mathrm{SAT}$, a satisfiability problem

- choose an driver Hamiltonian $\rightarrow$ transverse field

- and quantize that Ising model in the imaginary time formulation and determine its minimum mass-gap within λ space $\rightarrow$ Monte Carlo sampling at few hundred spins (at least in principle)

- compare the complexities classical vs. quantum, with increasing N_{spin}

3 SAT

- 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 $h_{\mathrm{Clause}} = 1$ if $s_1 = s_2 = s_3 = -1$, otherwise it is $h^3_{\mathrm{Clause}} = 0$
- it is a Ising spin version of the Boolean expression $\mathrm{b}_1.\mathrm{OR}.\mathrm{b}_2.\mathrm{OR}.\mathrm{b}_3$
- in Boolean algebra one forms M of such 3 clauses on a set N bits and in addition allows for logical negation, the α clause possibly has the form

  $$\mathrm{b}_{\alpha_1}.\mathrm{OR}.\overline{\mathrm{b}_{\alpha_2}}.\mathrm{OR}.\mathrm{b}_{\alpha_3}$$

  and one asks, whether M of such clauses can be satisfied simultaneously (logical .AND.)

3 SAT

- 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 $i = 1, 2, 3$.

  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 -or- incidence

  <u>**we choose**</u> (non-universal)

- realizations at $M = 5 \times N$ (percolation threshold at $M/N \approx 4.2$ in random 3-SAT)

- we construct forced incidences and filter for unique satisfying assignments : number of ground states exactly one

- random but uniform distribution of ϵ spin to clause assignment $h(n) =< \sum_{\alpha,i} \delta^1(\epsilon_{\alpha_i} \alpha_i - n) >_{\text{Realizations}} = \text{constant}$

Findings Classical

- we do a multicanonical simulation of the classical theory for many realizations and measure an ensemble of ergodicity time scales $\tau_{erg,i} = 1, ..., N_{\text{meas}}$ for "tunneling" in-between $H_{P,\text{min}} = 0$ and $H_{P,\text{max}}$, forth and back, in units of MONTE CARLO STEPS

  the histogram

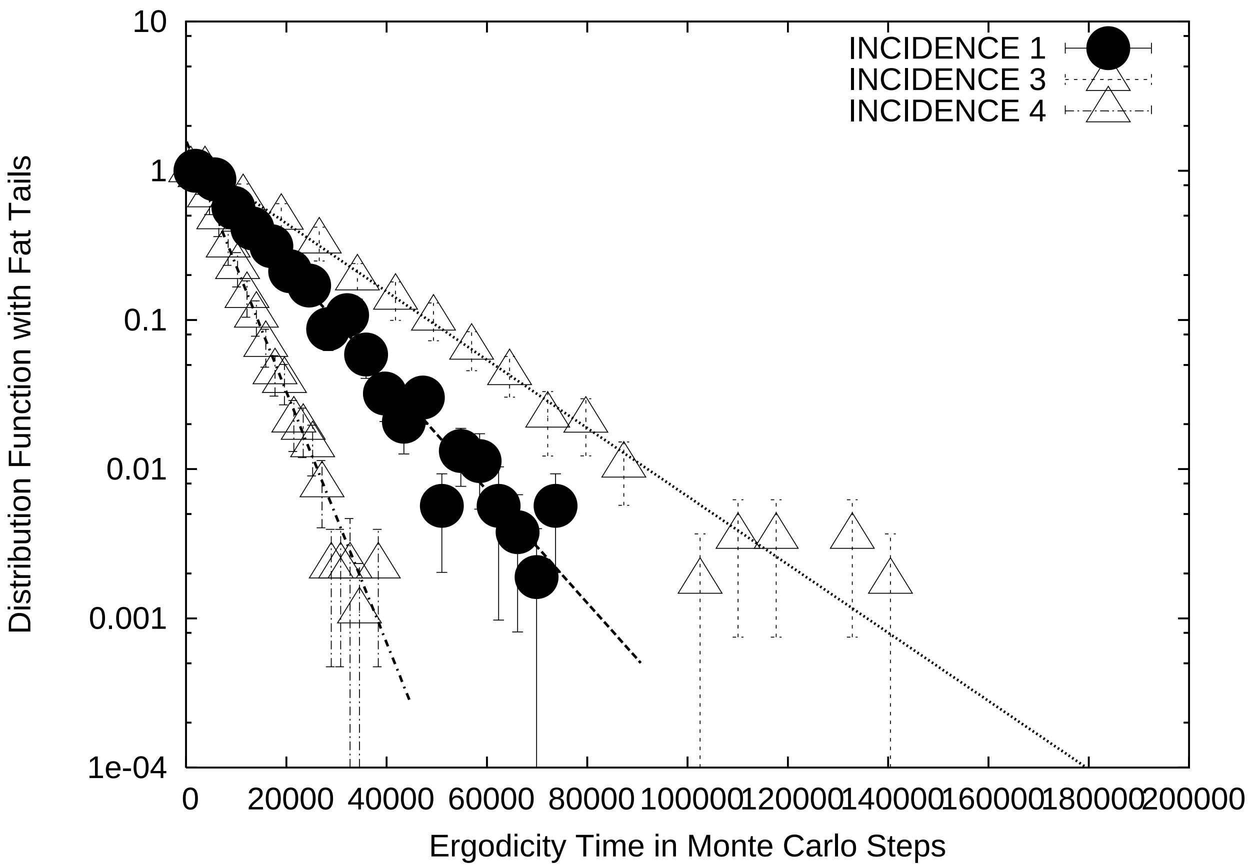
$$h(\tau_{erg}) = \mathcal{N}^{-1} \sum_i \delta^1(\tau_{erg,i} - \tau_{erg})$$

  exhibits <u>"fat tails"</u> $h(\tau_{erg}) \propto e^{-\tau_{erg}/\tau_{erg,exp}}$ with an exponential decay ergodicity time scale $\tau_{erg,exp}$, characterizing each incidence

- similar "fat tails" are observed in the distribution of ergodicity time values $\tau_{erg,exp}$ within the ensemble of incidences !

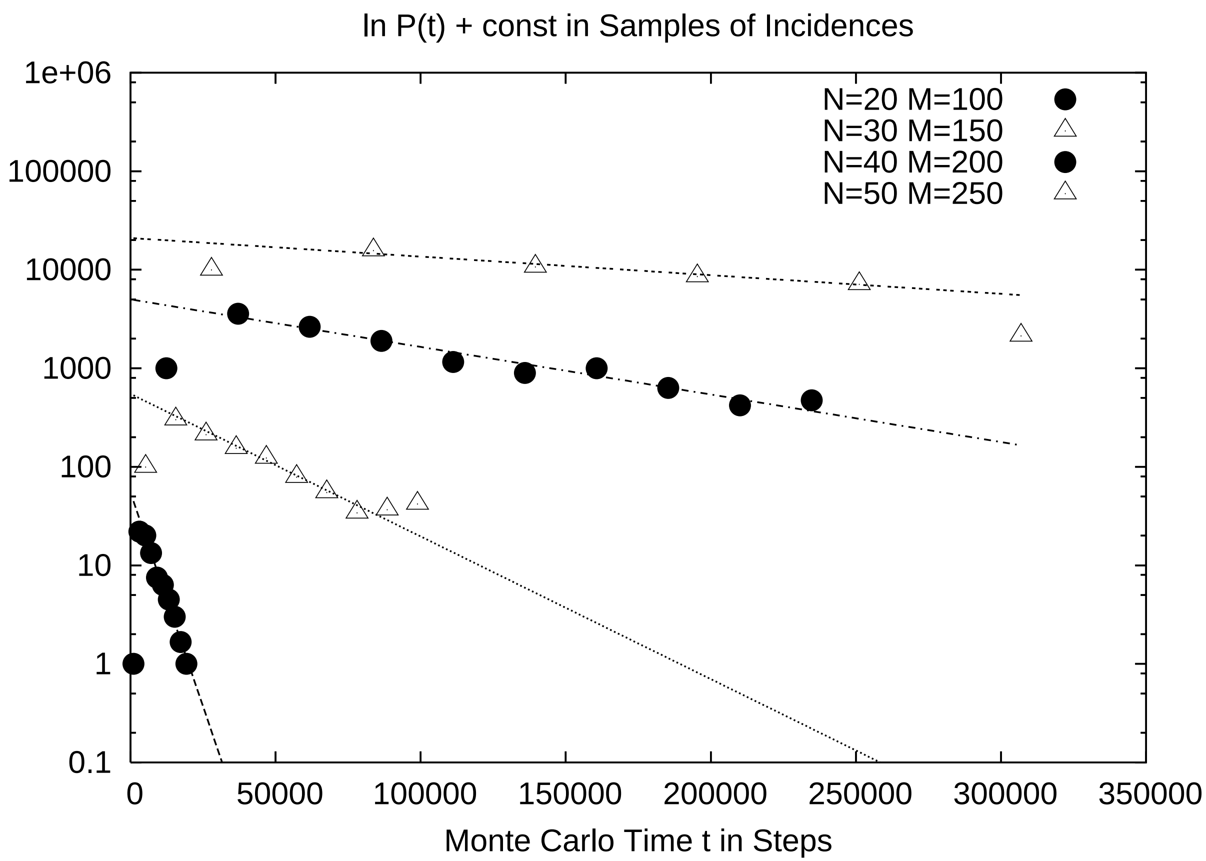
classical complexity

logarithmic distribution $\mathrm{P}(\tau_{\mathrm{erg}})$ with fat tails of ergodicity time scales τ_{erg} in multicanonical simulations as a function of the incidence for $N = 20$ and $M = 100$



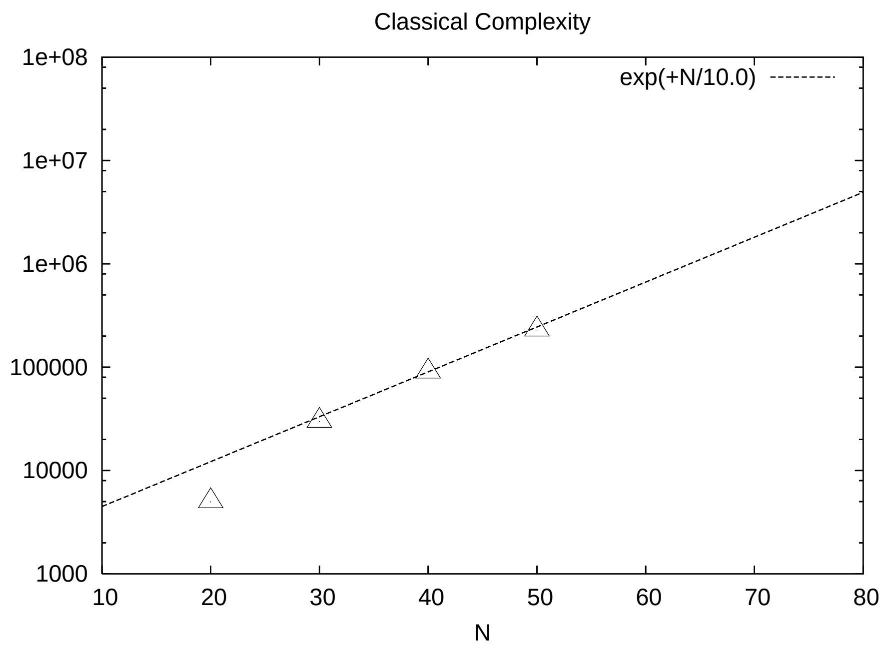
classical complexity

logarithmic distribution $\mathrm{P}(\tau_{\mathrm{erg},\underline{\mathrm{exp}}})$ in ensembles of incidences for "exponential decay" ergodicity time scales $\tau_{\mathrm{erg},\underline{\mathrm{exp}}}$ in multicanonical simulations as a function of the number of spins n for $r = M/N = 5$



classical complexity

- the complexity of the classical problem roughly doubles if $\Delta N \approx \ln 2 \times 10 = 6 - 7$ spins are added to the theory ! (Very, very preliminary !)



Quantization

- Trotter time $m = 0, \ldots, L_\tau - 1$, step $\Delta\tau$, $\beta = L_\tau \Delta\tau = T^{-1}$, p.b.c.

- Boltzmann factor: $e^{-\beta H}$

$$-\beta\lambda H_P \longrightarrow -\lambda \sum_{m=0}^{L_\tau - 1} H_P(\{\sigma_i^z(\tau_m)\})\Delta\tau$$

with driver Hamiltonian $H_D = -\sum_i \sigma_i^x$

$$-\beta(1-\lambda)H_D \longrightarrow \kappa_\tau \sum_{m=0}^{L_\tau - 1} \sum_{i=1}^{N} \sigma_i^z(\tau_m)\sigma_i^z(\tau_m + 1)$$

$$e^{-2\kappa_\tau} = \tanh(\Delta\tau[1-\lambda])$$

overlap order parameter

to the groundstate on the time-slice

$$\mathcal{O}(\tau_m) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i^z(\tau_m) \sigma_i^z |_{\text{Groundstate}}$$

correlation function

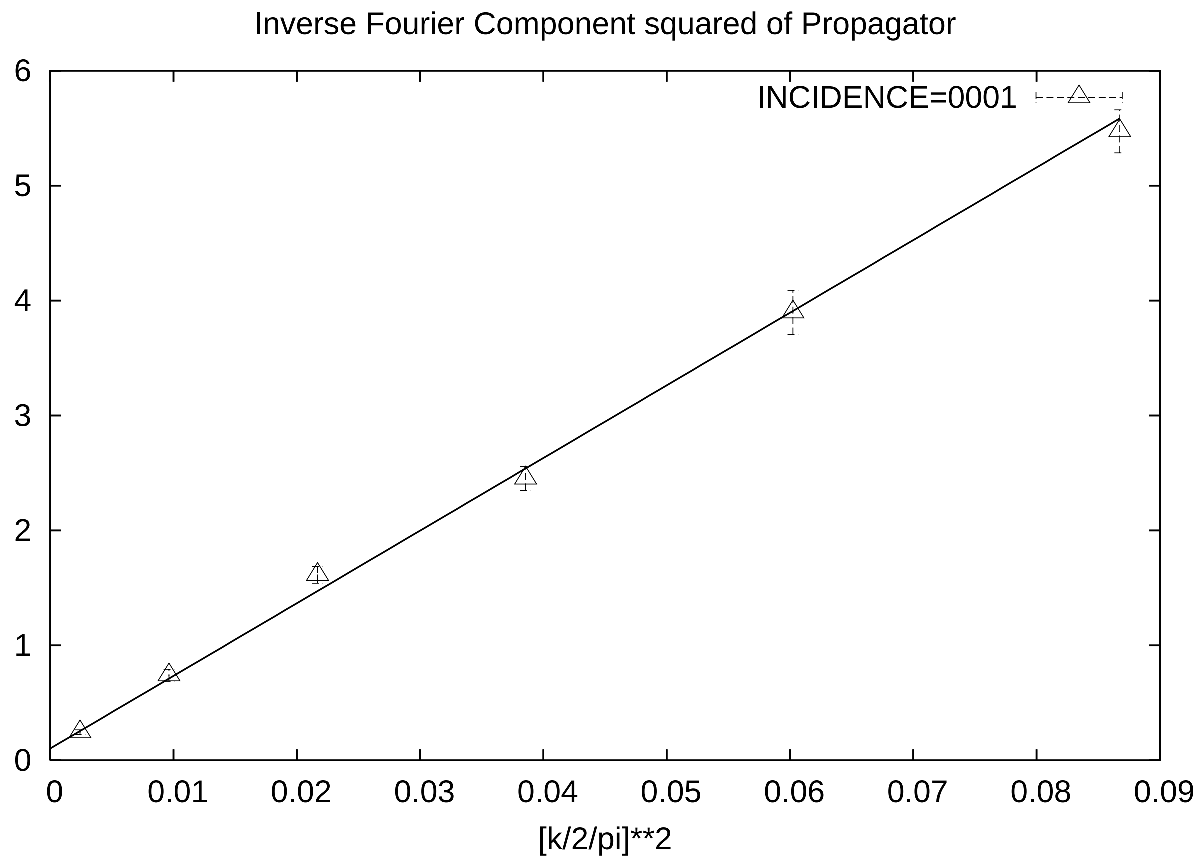
$$\Gamma(\tau) = \frac{1}{L_\tau} \sum_{m=0}^{L_\tau - 1} \mathcal{O}(\tau_m) \mathcal{O}(\tau_m + \tau)$$

gap and order parameter for large τ

$$\Gamma(\tau) \propto e^{-\Delta m(\lambda)\tau} + ||\mathcal{O}_{\text{OrderParameter}}||^2$$

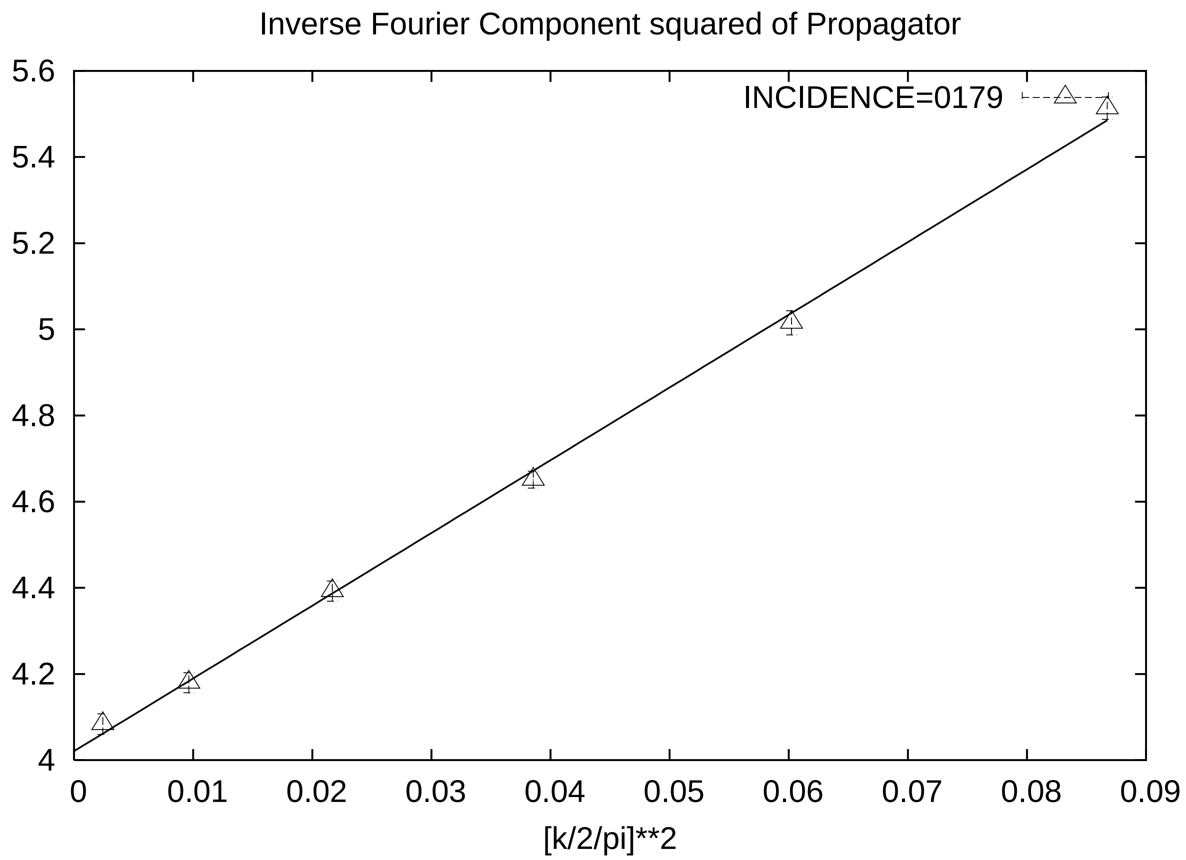
propagator in k-space

INCIDENCE=0001, $L_\tau = 128$, $\lambda = 0.6742$: almost massless !



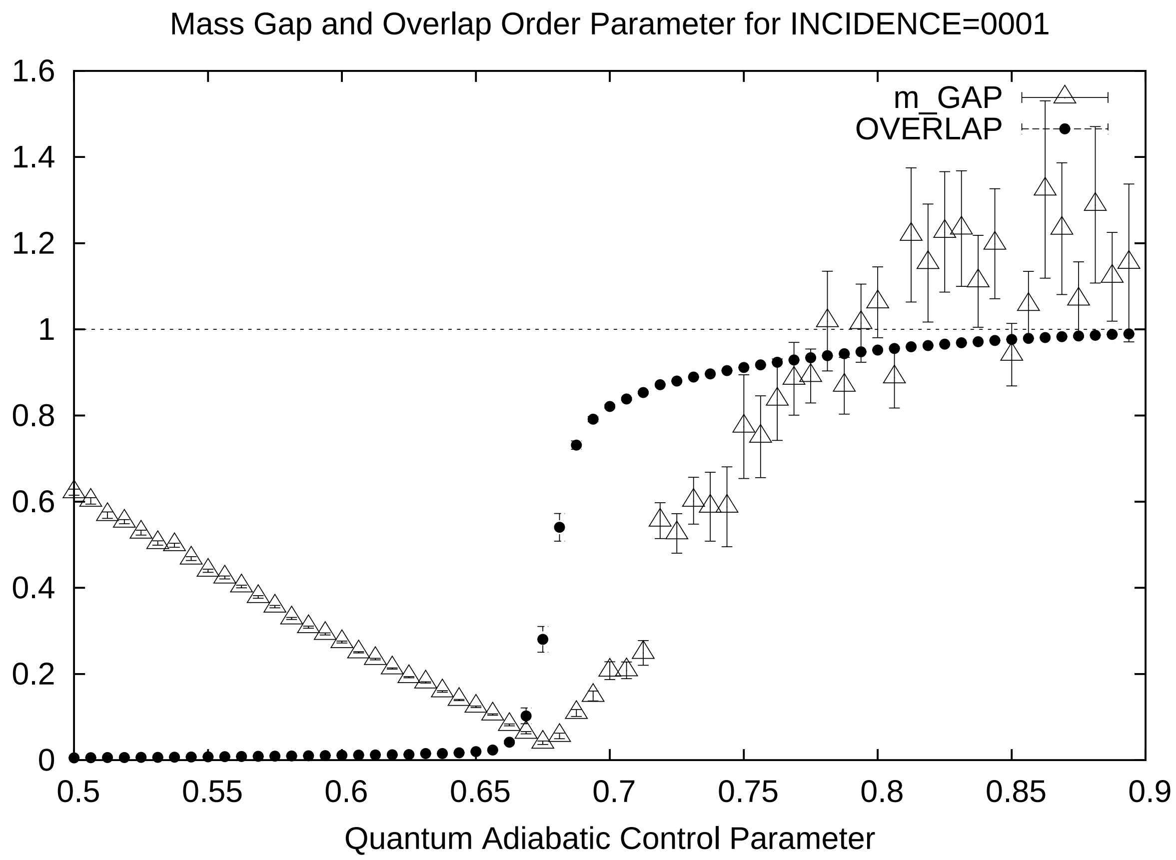
propagator in k-space

INCIDENCE=0179, $L_\tau = 128$, $\lambda = 0.5539$: massive !



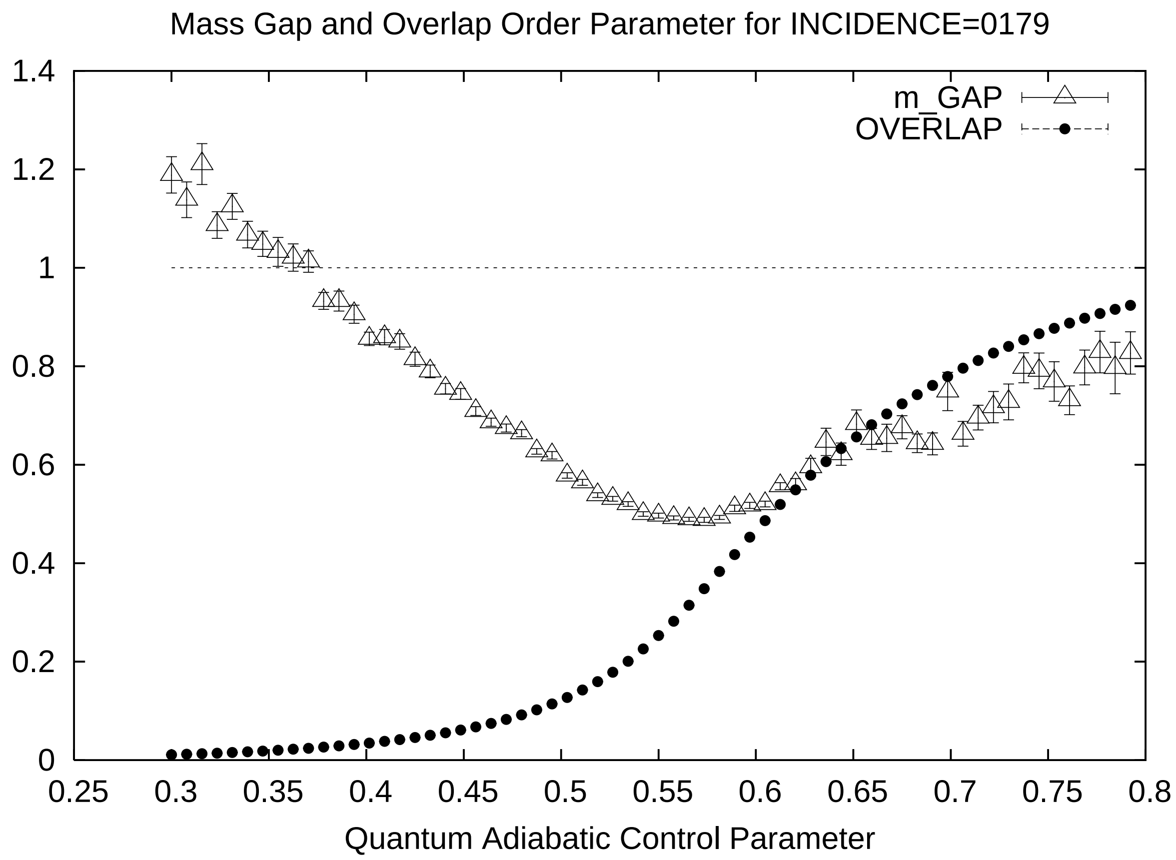
mass gap and order parameter

INCIDENCE=0001, $L_\tau = 128$, $\lambda = 0.6742$: <u>large quantum complexity !</u>



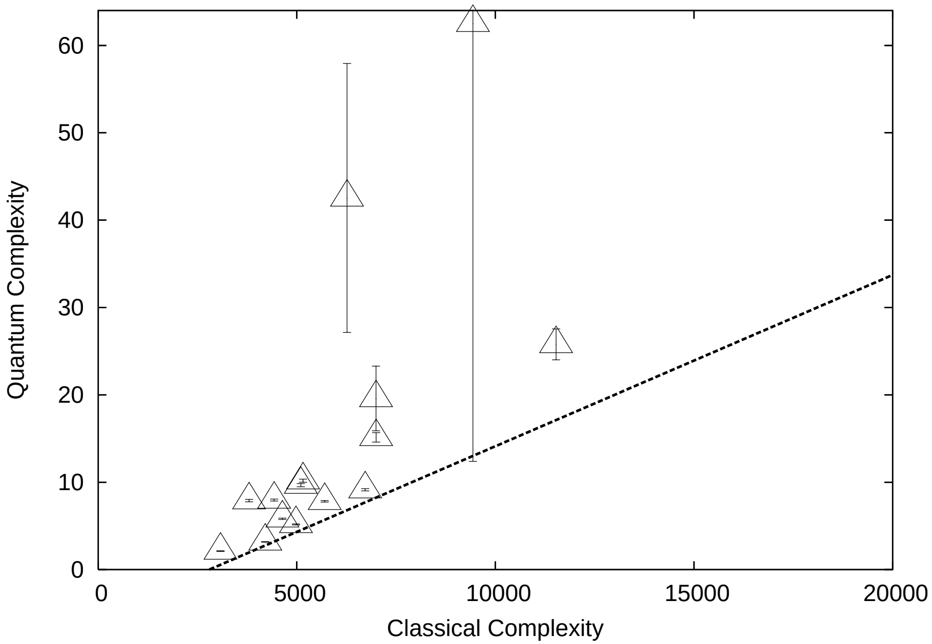
mass gap and order parameter

INCIDENCE=0179, $L_\tau = 128$, $\lambda = 0.5539$: small quantum complexity !



quantum versus classical

Quantization does not apparently boost the efficiency of the optimization problem solver **!**



Conclusion

- in statistical physics there exists a research area, which is cornered by

  1) NP-hard optimization problems given by H_P in terms of Ising spins

  2) the future possibility to built devices that run quantum H_P

  3) a large theory space as parametrized by the form of the driver Hamiltonian H_D

  one would then like to know : is there a minimum mass-gap, that only is polynomial small in the number of degrees of freedom ?

- 3 SAT is a problem leaned to mathematics/informatics: its computational demanding (we have realizations for hundred spins, where we cannot find the known groundstate with stochastic searches)

  -first preliminary results indicate, that Quantum Adiabatic Calculations with transverse field do not improve the situation in 3 SAT

  -P. Young et. al. study Exact Cover, which is a weaker problem