Physics Based Approaches to Quantum Computing

Edward Farhi
Center for Theoretical Physics
MIT

Conventional Quantum Computing Paradigm is a sequence of gates that are Unitary Operators

$$\boxed{i \frac{d}{dt} |\psi(t)\rangle = H(t)|\psi(t)\rangle} \qquad \hbar = 1$$

implies

$$\boxed{|\psi(t_2)\rangle = U(t_2, t_1)|\psi(t_1)\rangle}$$

where U is Unitary $\qquad U^\dagger U = 1$

Physics based approach to Quantum Algorithms is Hamiltonian Based

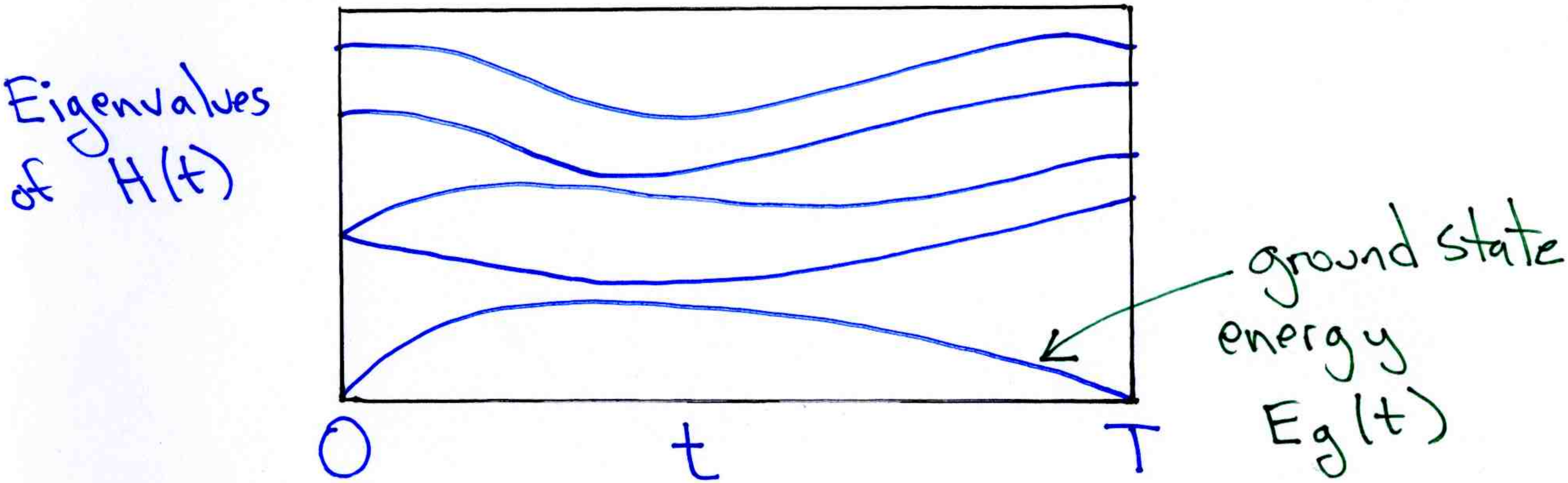
General Quantum Algorithm

* Problem to solve
* Design $H(t)$
* Pick the initial state $|\psi(0)\rangle$
* Pick Run Time T
* Evolve $i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$
* Get $|\psi(T)\rangle$
* Measure some operator $\hat{O}$
* Result of measurement encodes solution to problem

How does T scale with probem size?

How do resources needed to build H scale with problemsize?

Time dependent Hamiltonian $H(t)$



Instantaneous Ground State $H(t)|E_g(t)\rangle = E_g(t)|E_g(t)\rangle$

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle \qquad |\psi(0)\rangle = |E_g(0)\rangle$$

$\boxed{|\psi(t)\rangle \text{ stays near } |E_g(t)\rangle \text{ if } H \text{ changes slowly enough}}$

Adiabatic Theorem

$\boxed{\text{Combinatorial Search}}$

n bits $\quad 2^n$ values $X_1, X_2, \ldots X_n$ each $X_i = 0, 1$

m clauses $\quad$ Each clause is a truth table acting on a subset of the bits.

example of a clause involvings bits 7, 99 and 103

True iff $X_7 + X_{99} + X_{103} = 1$

Mother of all Computational Problems

Find the assignment of the bits that minimizes the number of violated clauses

$\boxed{\text{NP-hard}}$ $\quad$ Considered intractable on a conventional computer

Cost Function

Penalize violated clauses

$$\boxed{E(x_1, x_2, \ldots x_n) = \text{number of clauses violated by string } x_1, x_2, \ldots x_n}$$

If you find the global minimum of E you solve the combinatorial search problem

E is easy to describe but hard to minimize

Find minimum of cost function

$h(z) \qquad z = z_1 z_2 \dots z_n$

$h(w) = 0 \qquad h(z) > 0 \quad z \neq w$

Want to find w.

Quantum Version

$$H_p = \sum_z h(z) |z\rangle$$

Want to find $|w\rangle$, the ground state of H_p

Adiabatic designed for classical combinatorial optimization problems

$$H(s) = (1-s) H_B + s H_P \qquad 0 \leq s \leq 1$$

H_B is beginning Hamiltonian.

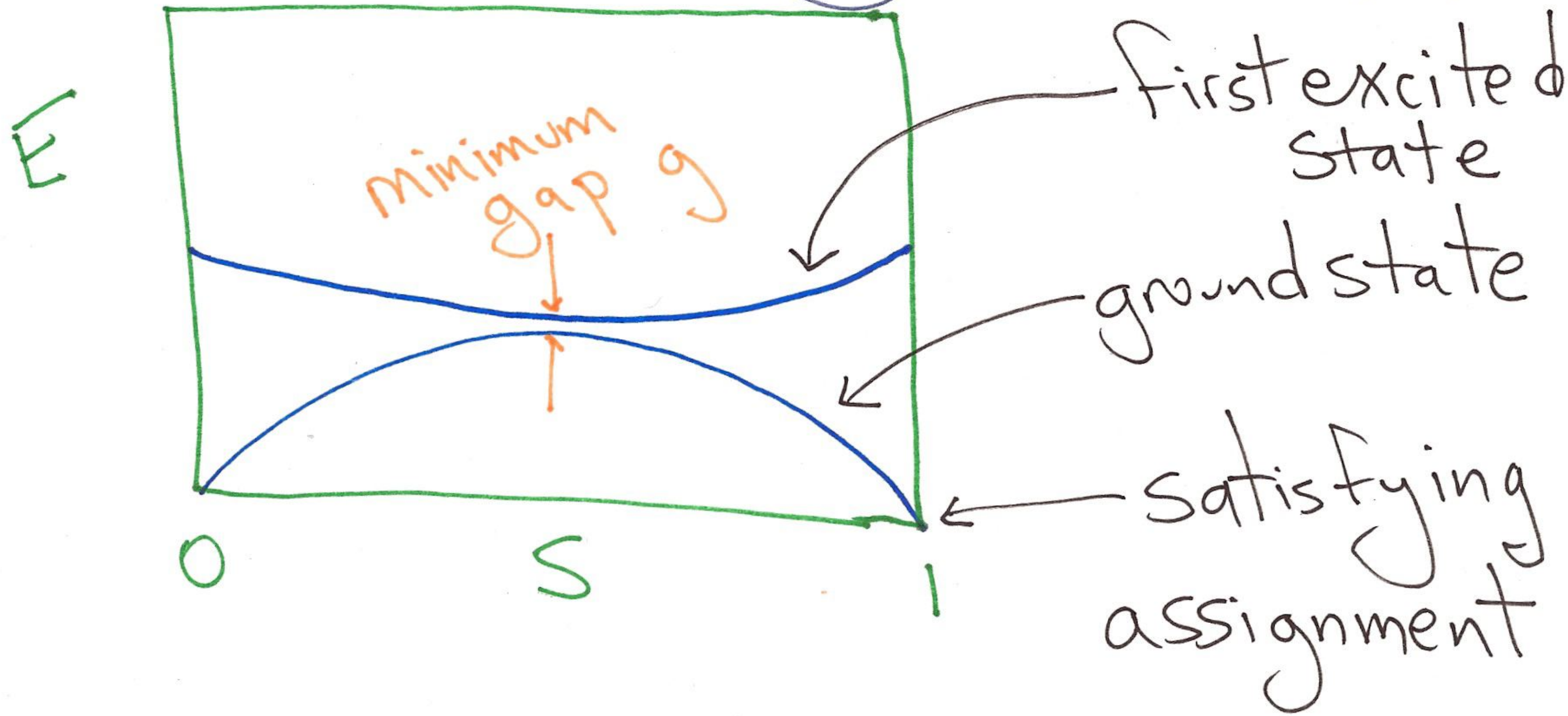
H_P is instance dependent problem Hamiltonian.

Ground state of H_P encodes solution.

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

$$0 \leq t \leq T$$

Run time determined by minimum gap



$$T \gtrsim \frac{1}{g^2}$$

How small is g?

Algorithm designer designs a Hamiltonian

$$\boxed{H(t) = H_D(t) + c(t) H_P}$$

$$|c(t)| \leq 1$$

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

Start in $|\psi(0)\rangle$

Evolve for time T

Success if $|\psi(T)\rangle$ is near $|w\rangle$

Grover Problem: Unstructured Search

$$H_p(z) = \begin{cases} 0 & z = w \\ 1 & z \neq w \end{cases} \qquad 0 \leq z \leq N-1$$

$$N = 2^n$$

Success means $|\psi(T)\rangle = |w\rangle$ for all w

then $\boxed{T > \frac{N^{1/2}}{2}}$

Farhi
Gutmann 1998

Based on BBBV

Information Theory $\Longrightarrow$

Linear Algebra Result

Scrambled Cost Function

Start with $h(z)$ which may be structured

Mininum at $z=0$ $\quad h(0) < h(z) \quad z = 1, 2, \ldots N-1$

[Example $h(z) = z_1 + z_2 + \ldots z_n \quad N = 2^n$
structured. Easy to minimize]

Let π be a permutation of $0, 1, \ldots N-1$

$$h^{[\pi]}(z) = h(\pi^{-1}(z))$$

There are $N!$ permutations of N things

$$w = \pi(0)$$

All structure is gone in $h^{[\pi]}$

Scrambled!

Farhi, Goldstone
Gutmann, Nagaj
2005

Evolve with

$$H(t) = H_D(t) + c(t)\, H_{P,\pi}$$

$$H_{P,\pi} = \sum_z h^{[\pi]}(z)\, |z\rangle\langle z| = \sum_z h(z)\, |\pi(z)\rangle\langle\pi(z)|$$

Evolve for time T from some π independent starting state to $|\psi_\pi(T)\rangle$

Success $\boxed{|\langle\psi_\pi(T)|\pi(0)\rangle|^2 \geq b}$

If this occurs for a set of $\boxed{\varepsilon N!}$ permutations

then $\left\{ T \geq \frac{\varepsilon^2 b}{16 h^*}(N-1)^{1/2} - \frac{(\varepsilon^3/2)^{1/2}}{4h^*} \right\}$

h^* is some average h

This means that if you have a random cost function, a quantum computer can not find the minimum in time less than $N^{1/2}$

Apply to Adiabatic

Information Theory Result

$\Longrightarrow$ Linear Algebra Result about gaps!

Is this a rigorous information theoretic proof of Anderson Localization?

There is no conclusion to be drawn about structured cost functions such as 3-SAT

Attempts to demonstrate failure

Van Dam, Mosca, Vazirani – Non local cost function

van Dam, Vazirani – Local cost function

fixed by Path Change

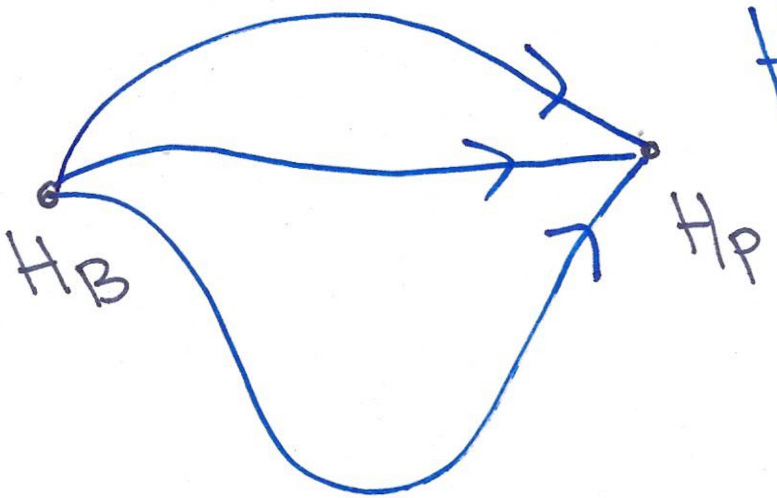
Fisher, Reichardt

Random couplings

$T \sim c\sqrt{n}$ Path Change?

Path Change

$$H = (1-s) H_B + s H_p + s(1-s) H_{EXTRA}$$



Hamiltonian Space

Run each instance many times with different Paths.

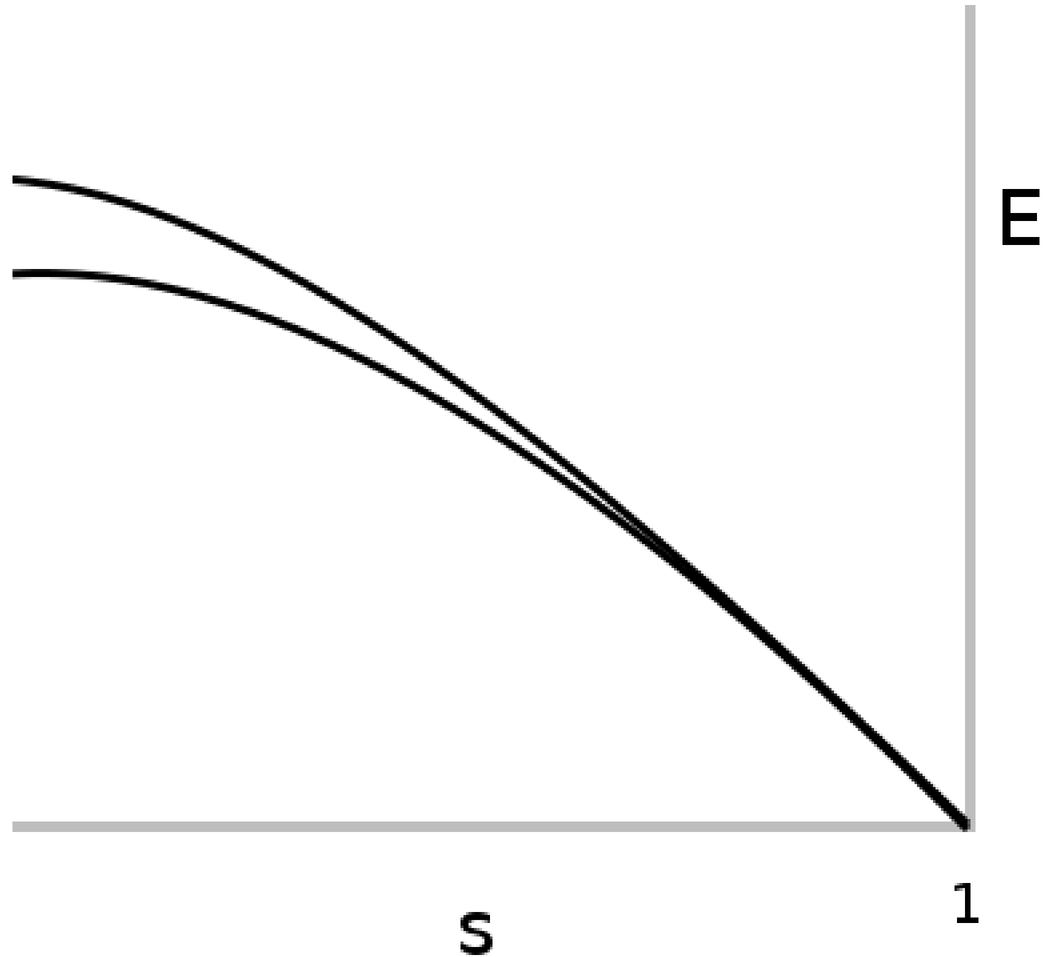
New way to make trouble

Start with a problem Hamiltonian H_p' with two degenerate ground states

$|z_1\rangle$ and $|z_2\rangle$

The strings z_1 and z_2 are far apart in Hamming weight

$$H'(s) = (1-s)H_B + sH_p'$$


E
s
1

Suppose the lower curve approaches $|z_1\rangle$

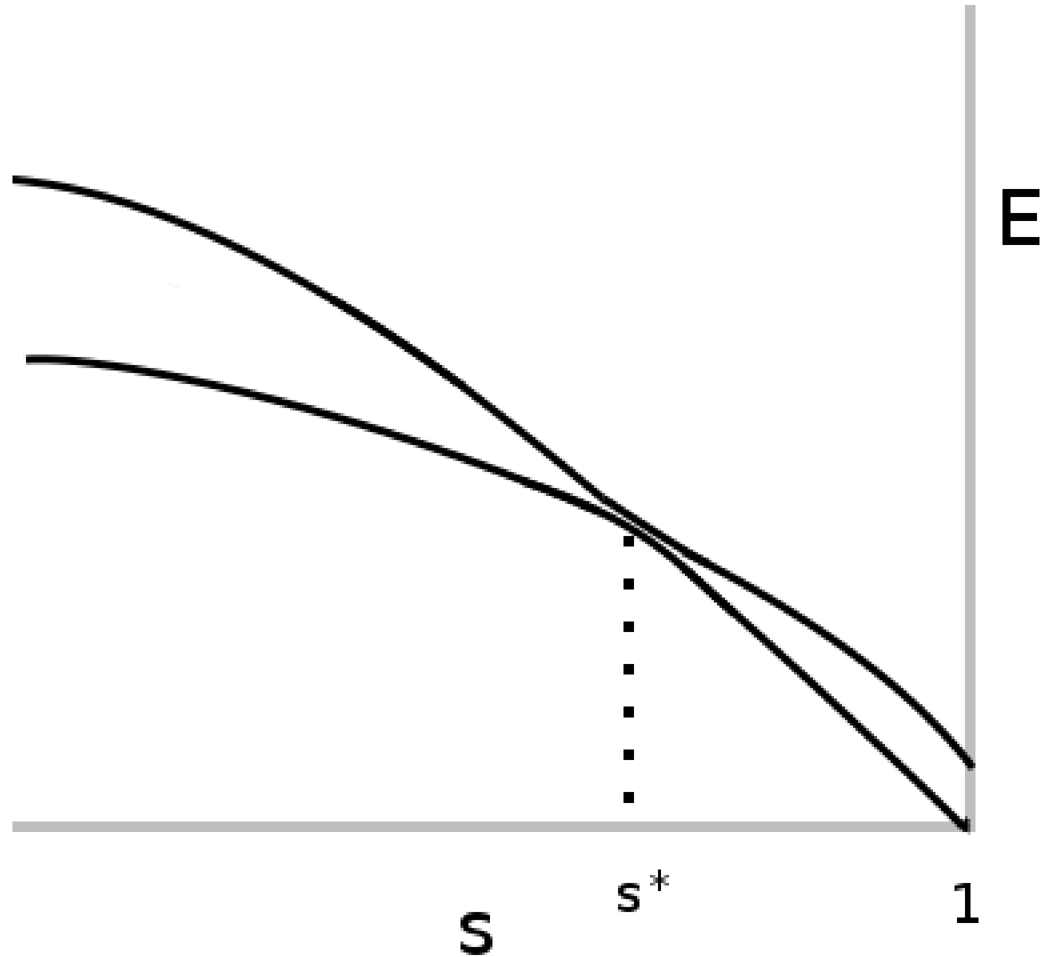
Add a single clause that penalizes z_1

$$H_p = H_p' + h$$

h penalizes z_1 but not z_2

$$H(s) = (1-s)H_B + s H_p$$

Expect to get a tiny gap!


E
s*
1
s

Generate this type of instance

<u>Double</u> <u>Plants</u>

3-SAT Each clause does not like one of the eight possible assignments of the 3 bits

Randomly pick clauses which do not like

001
010
011
100
101
110

The Strings 00000000
and 11111111
will always satisfy

Add enough clauses and these will be the only winners!

The ground state for values of s near 1 will approach either $|000000\rangle$ or $|111111\rangle$. Suppose it is $|000000\rangle$.

Add a clause which penalizes 000 on the first 3 bits.

This creates the situation outlined earlier.

For s near 1 we can write

$$H = H_p + \lambda V \qquad V = -\sum_{j=1}^{n} \sigma_x^{(j)}$$

λ small

We will use low order perturbation Theory to locate the near cross

$$H = H_p + \lambda V$$

$$H_p|z\rangle = E_p(z)|z\rangle \qquad (\lambda = 0)$$

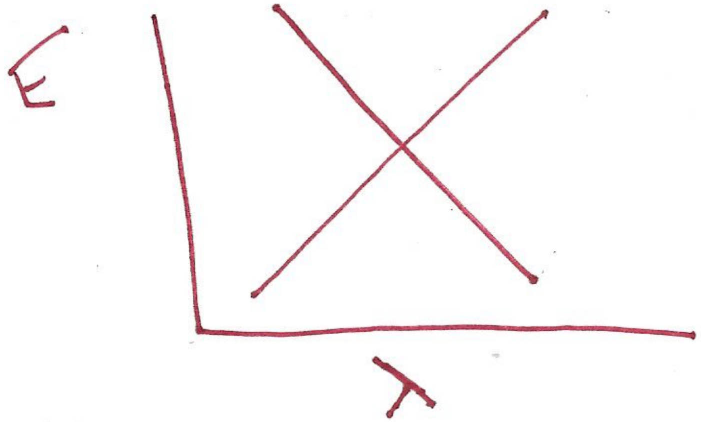
Ground state at $\lambda = 0$ is $|\bar{z}\rangle$ $\qquad E_p(\bar{z}) < E_p(z)$

Ground state for general λ

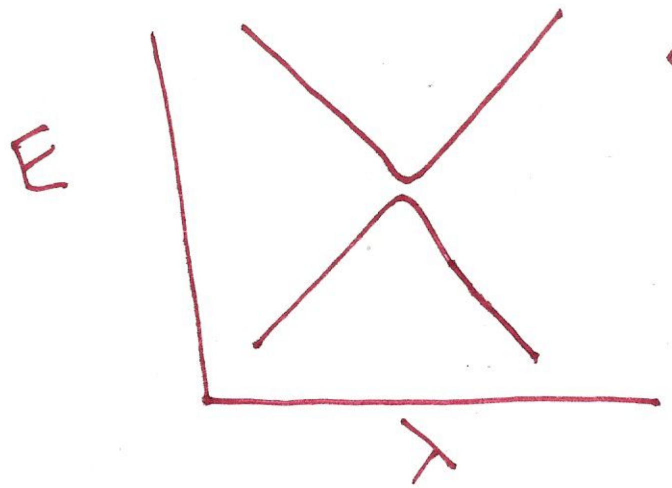
$$H(\lambda)|g\rangle = E_g(\lambda)|g\rangle$$

$$E_g(\lambda) = E_p(\bar{z}) + \lambda\langle\bar{z}|V|\bar{z}\rangle - \lambda^2 \sum_{z \neq \bar{z}} \frac{|\langle z|V|\bar{z}\rangle|^2}{E_p(z) - E_p(\bar{z})} + \dots$$

Usually perturbation theory is not valid at a near cross

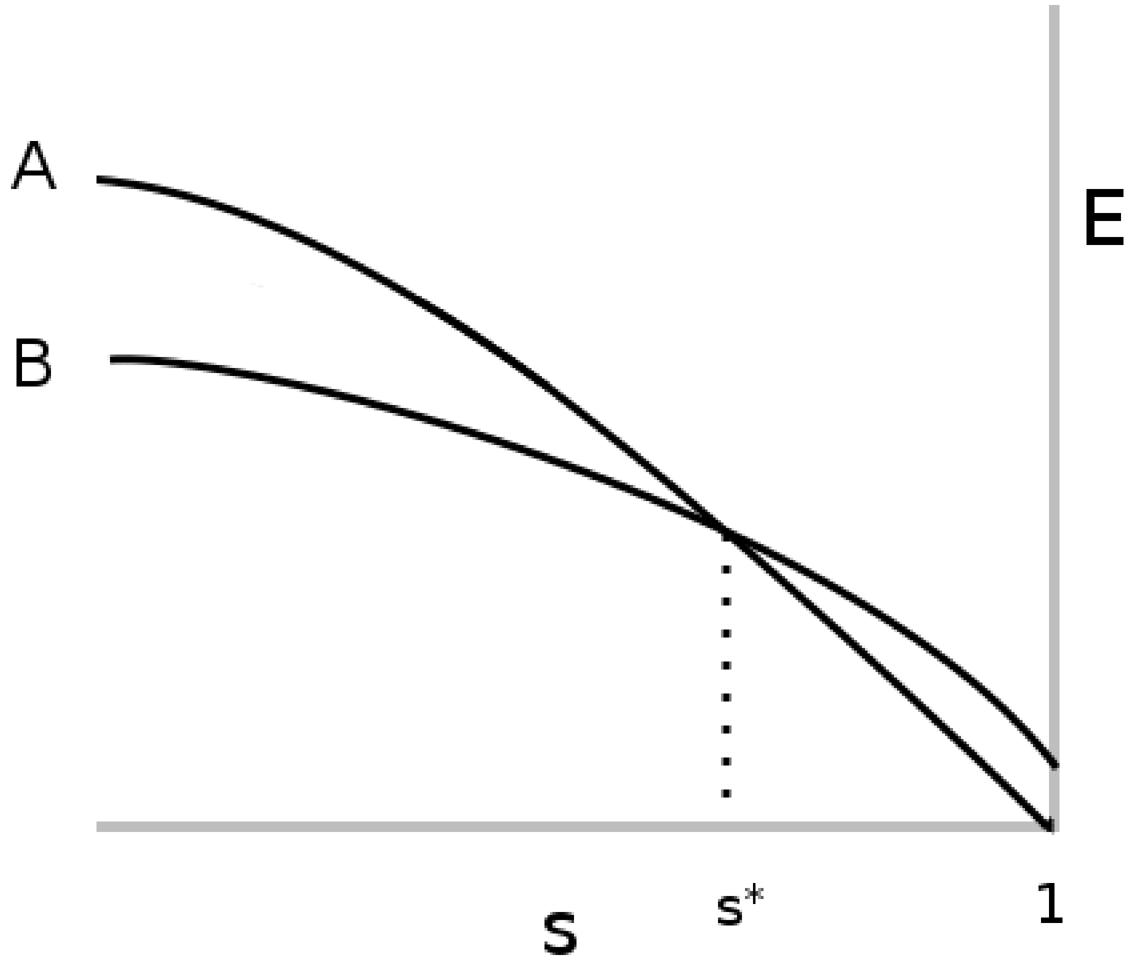


Ground state energy is not an analytic function of λ



Perturbation theory does not work near the cross

Suppose $H = \begin{bmatrix} H_A(s) & 0 \\ 0 & H_B(s) \end{bmatrix}$


A
B
E
s*
1
s

It takes n powers of $V = -\sum_{j=1}^{n} \sigma_x^{(j)}$

to connect $|00000\rangle$ to $|11111\rangle$

Low orders can be used to get cross.

$$E_L(\lambda) = \lambda^2 \mathcal{E}_L^{(2)} + \cdots$$

$$E_U(\lambda) = 1 + \lambda^2 \mathcal{E}_U^{(2)} + \cdots$$

Cross occurs at $\lambda^2 \left(\mathcal{E}_L^{(2)} - \mathcal{E}_U^{(2)} \right) = 1$

$\mathcal{E}_L^{(2)}$ and $\mathcal{E}_U^{(2)}$ are of order n but

the difference is $\Theta(n^{1/2})$

$\lambda = \Theta\left(\frac{1}{n^{1/4}}\right)$ $\boxed{s^* = 1 - \Theta\left(\frac{1}{n^{1/4}}\right)}$

The cross occurs because

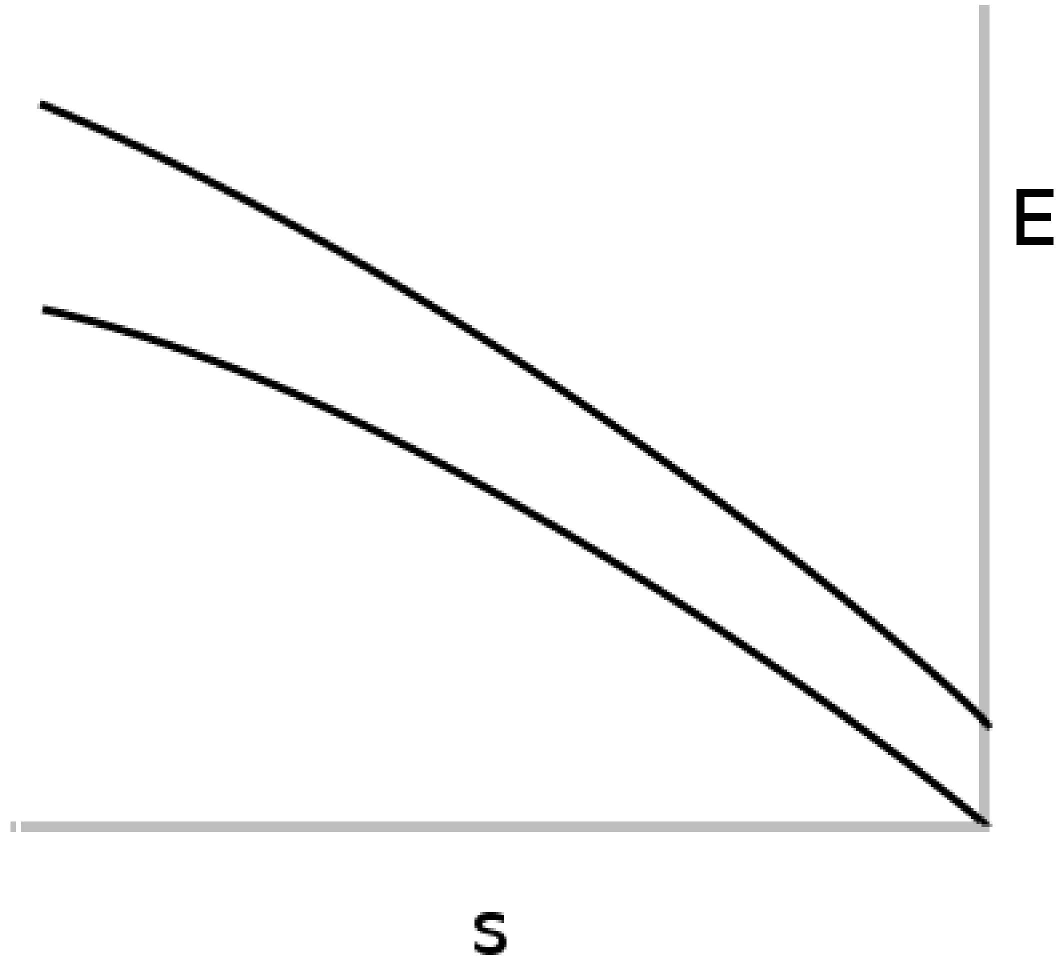
$$\mathcal{E}_U^{(2)} < \mathcal{E}_L^{(2)}$$

$$\mathcal{E}_L^{(2)} = -\sum_{z \neq \bar{z}} \frac{|\langle z | V | \bar{z} \rangle|^2}{E_p(z) - E_p(\bar{z})}$$

n terms, only fires if z differs from $\bar{z}$ by a single bit flip

Randomize the path and get

$$\mathcal{E}_U^{(2)} > \mathcal{E}_L^{(2)}$$


E
S

We used $V = -\sum_{j=1}^{n} \sigma_x^{(j)}$

Try $V = -\sum_{j=1}^{n} c_j \sigma_x^{(j)}$

each $c_j = .5$ or 1.5 with equal probability

This gives a substantial probability that $\mathcal{E}_U^{(2)} > \mathcal{E}_L^{(2)}$

To test these ideas we did a numerical simulation

Continuous Time Quantum* Monte Carlo

~ 600 processors

~ few months

* Not a quantum computer! Classical algorithm for studying quantum systems

a

$$H = H_0 + \lambda V$$

H_0 is diagonal in the z basis

V is purely off diagonal $\quad \langle z|V|z'\rangle \leq 0$

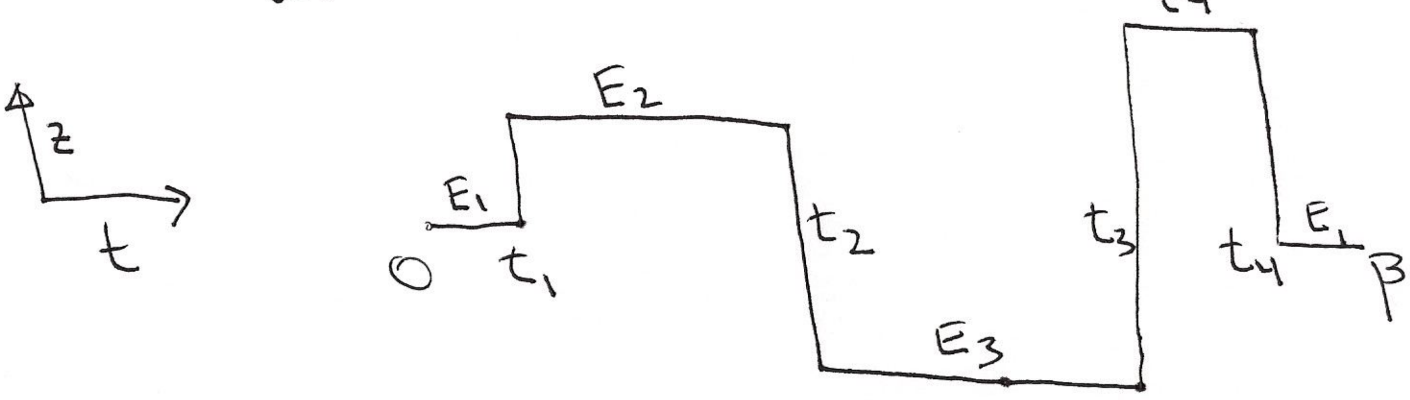
Stoquastic

Math $\quad Z(\beta) = \mathrm{Tr}\left[e^{-\beta H}\right]$

$$= \sum_{m=0}^{\infty} (-\lambda)^m \sum_{z_1 \ldots z_m} \langle z_1|V|z_m\rangle \langle z_m|V|z_{m-1}\rangle \cdots \langle z_2|V|z_1\rangle$$

$$\times \int_0^{\beta} dt_m \int_0^{t_m} dt_{m-1} \cdots \int_0^{t_2} dt_1 \, e^{-(E_1 t_1 + E_2(t_2 - t_1) + \ldots E_1(\beta - t_m))}$$

where $E_i = \langle z_i|H_0|z_i\rangle$



$$\text{path } z(t) = \begin{cases} z_1 & 0 \le t < t_1 \\ z_2 & t_1 \le t < t_2 \\ \vdots & \end{cases}$$

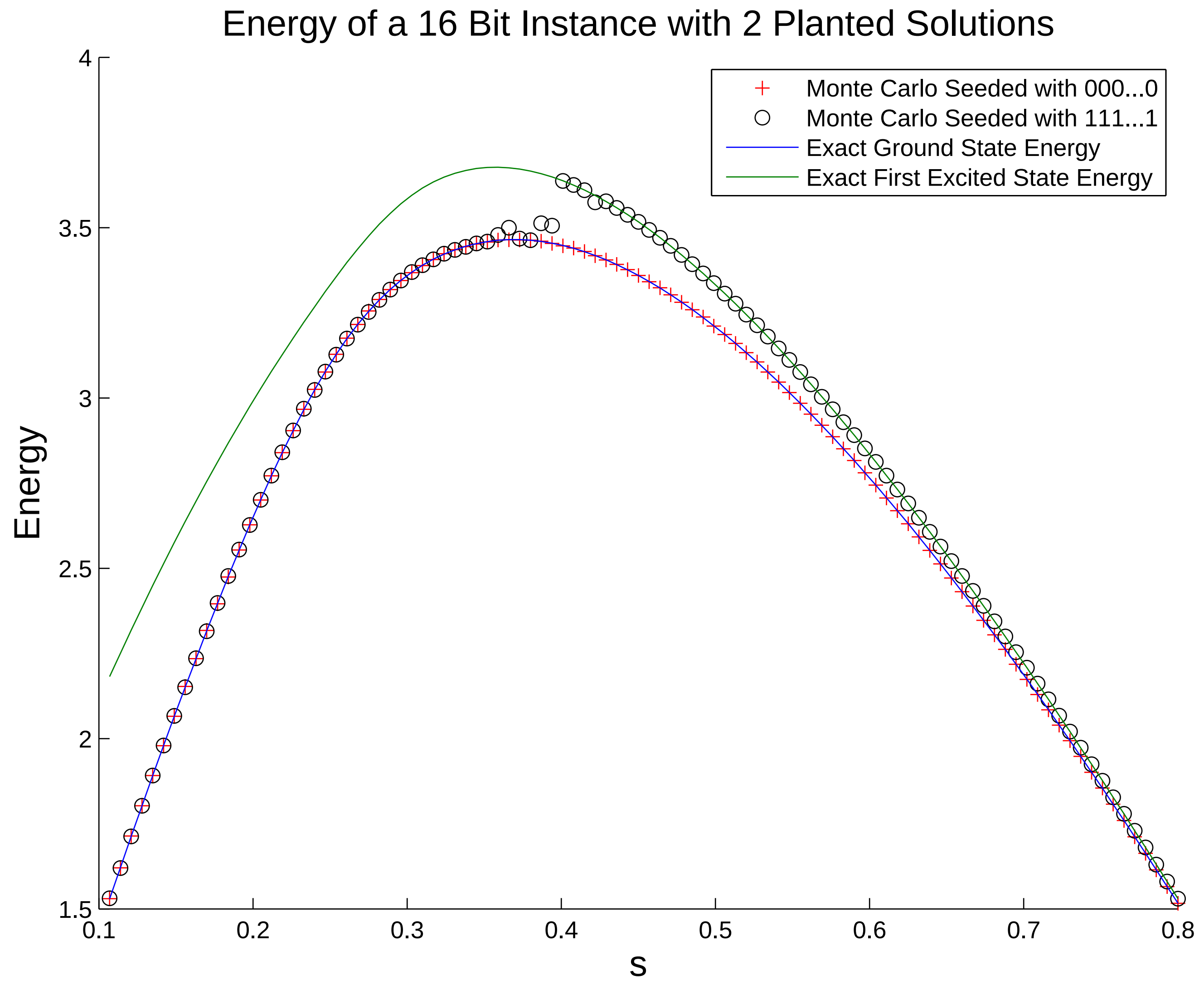
Probability (measure) of a path

$$\rho(z) = \frac{1}{Z(\beta)} (-\lambda)^m \langle z_1 | V | z_m \rangle \langle z_m | V | z_{m-1} \rangle \cdots \langle z_2 | V | z_1 \rangle$$

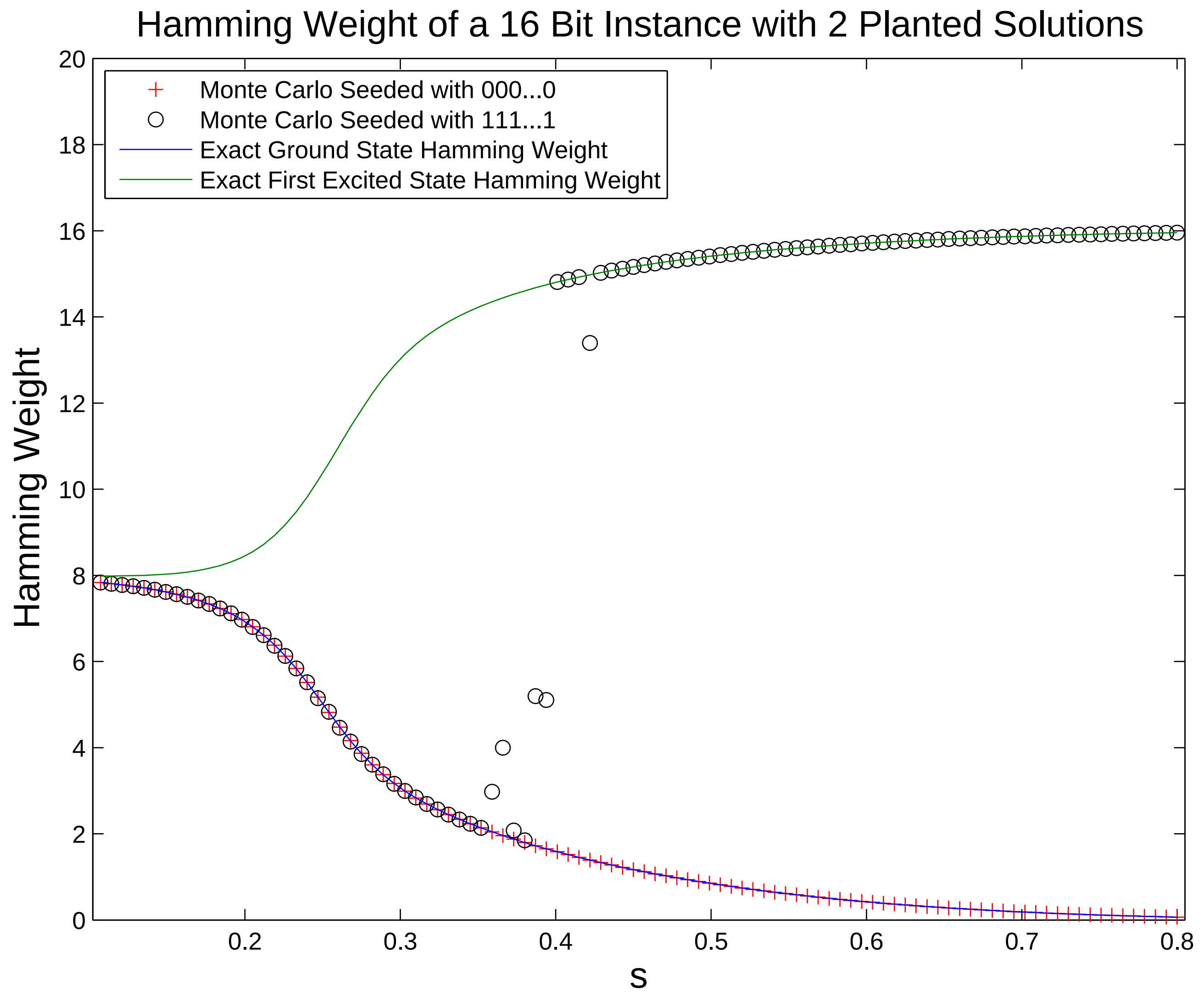
$$\cdot\, e^{-(E_1 t_1 + E_2 (t_2 - t_1) + \ldots E_1 (\beta - t_m))} \qquad dt_1\, dt_2 \ldots dt_m$$

We can efficiently sample from these paths and do continuous time quantum Monte Carlo

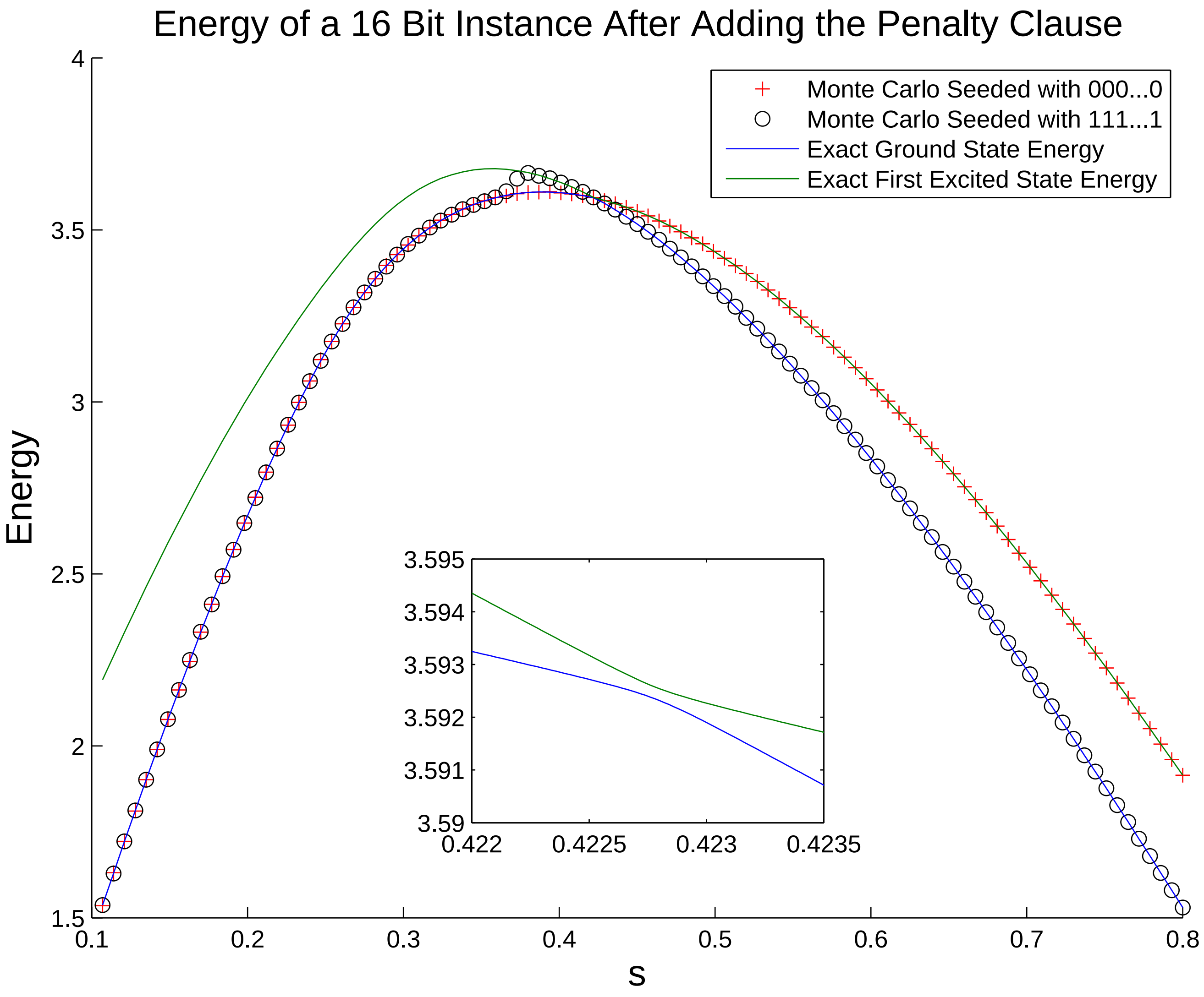
No Trotter Error Only Statistical Error



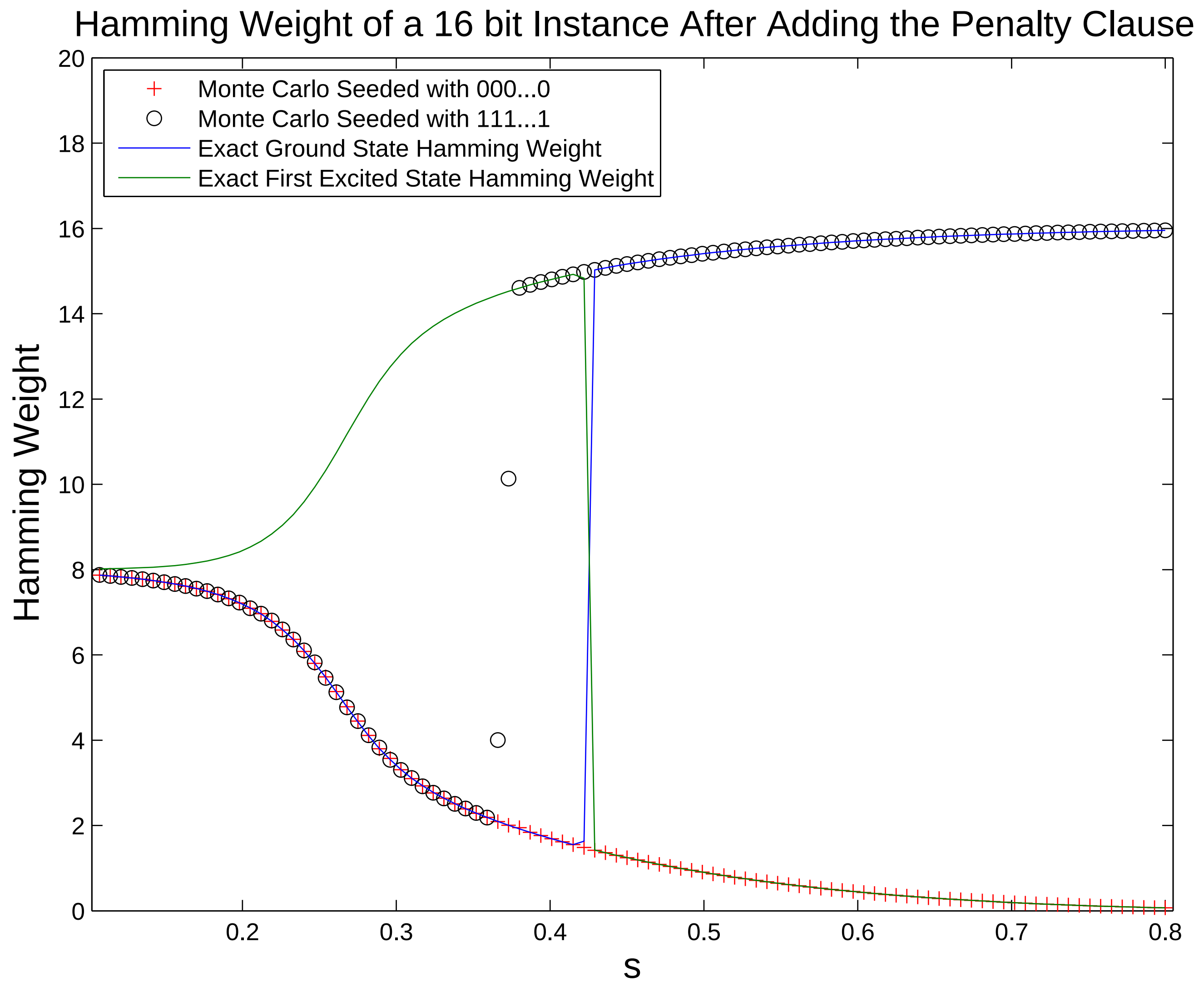
Energy of a 16 Bit Instance with 2 Planted Solutions
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Exact Ground State Energy
Exact First Excited State Energy
Energy
s
4
3.5
3
2.5
2
1.5
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8



Hamming Weight of a 16 Bit Instance with 2 Planted Solutions
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Exact Ground State Hamming Weight
Exact First Excited State Hamming Weight
Hamming Weight
s
0
2
4
6
8
10
12
14
16
18
20
0.2
0.3
0.4
0.5
0.6
0.7
0.8



Energy of a 16 Bit Instance After Adding the Penalty Clause
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Exact Ground State Energy
Exact First Excited State Energy
Energy
s
4
3.5
3
2.5
2
1.5
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
3.595
3.594
3.593
3.592
3.591
3.59
0.422
0.4225
0.423
0.4235



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Monte Carlo Seeded with 111...1
Exact Ground State Hamming Weight
Exact First Excited State Hamming Weight
Hamming Weight
s
0
2
4
6
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10
12
14
16
18
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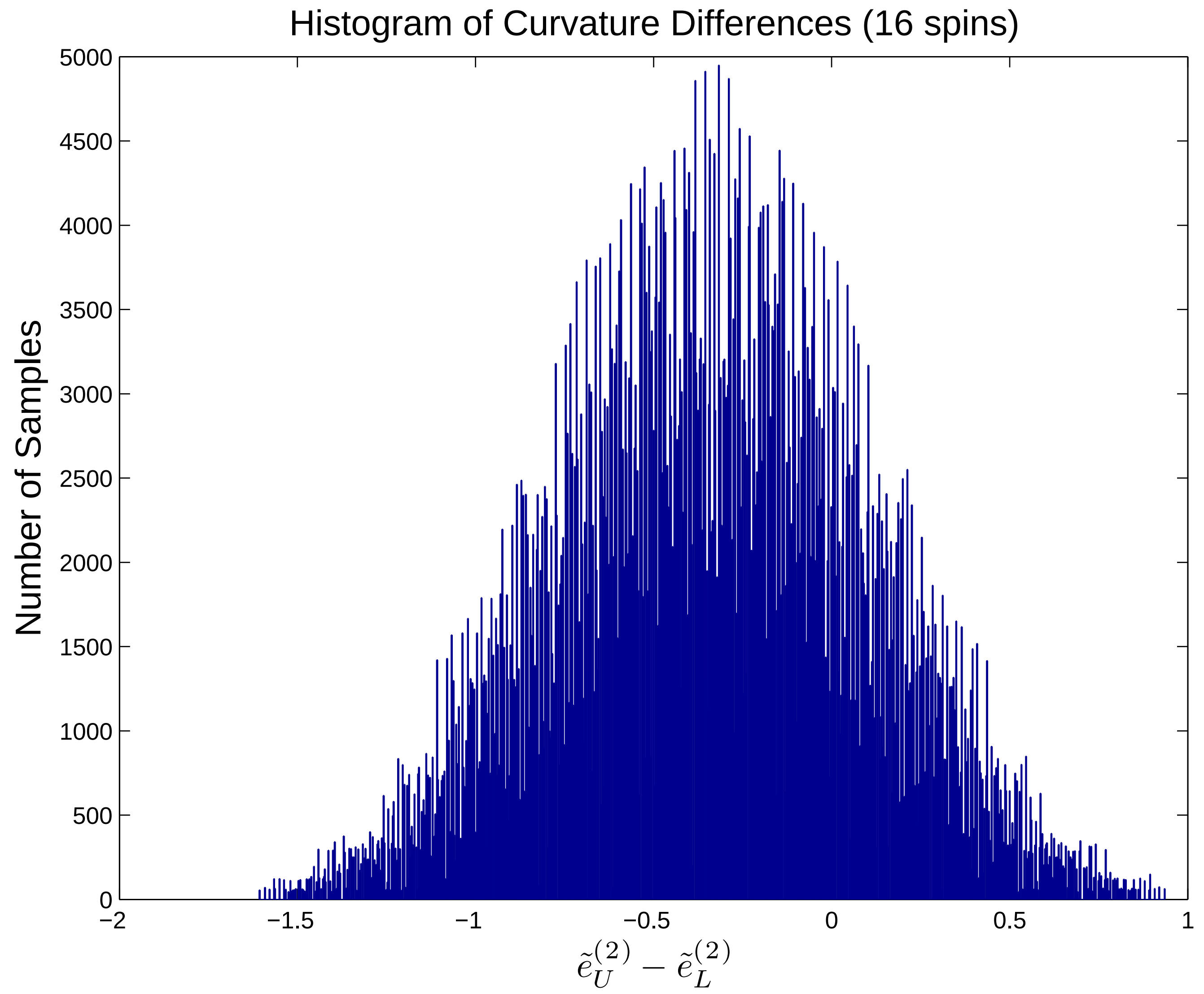
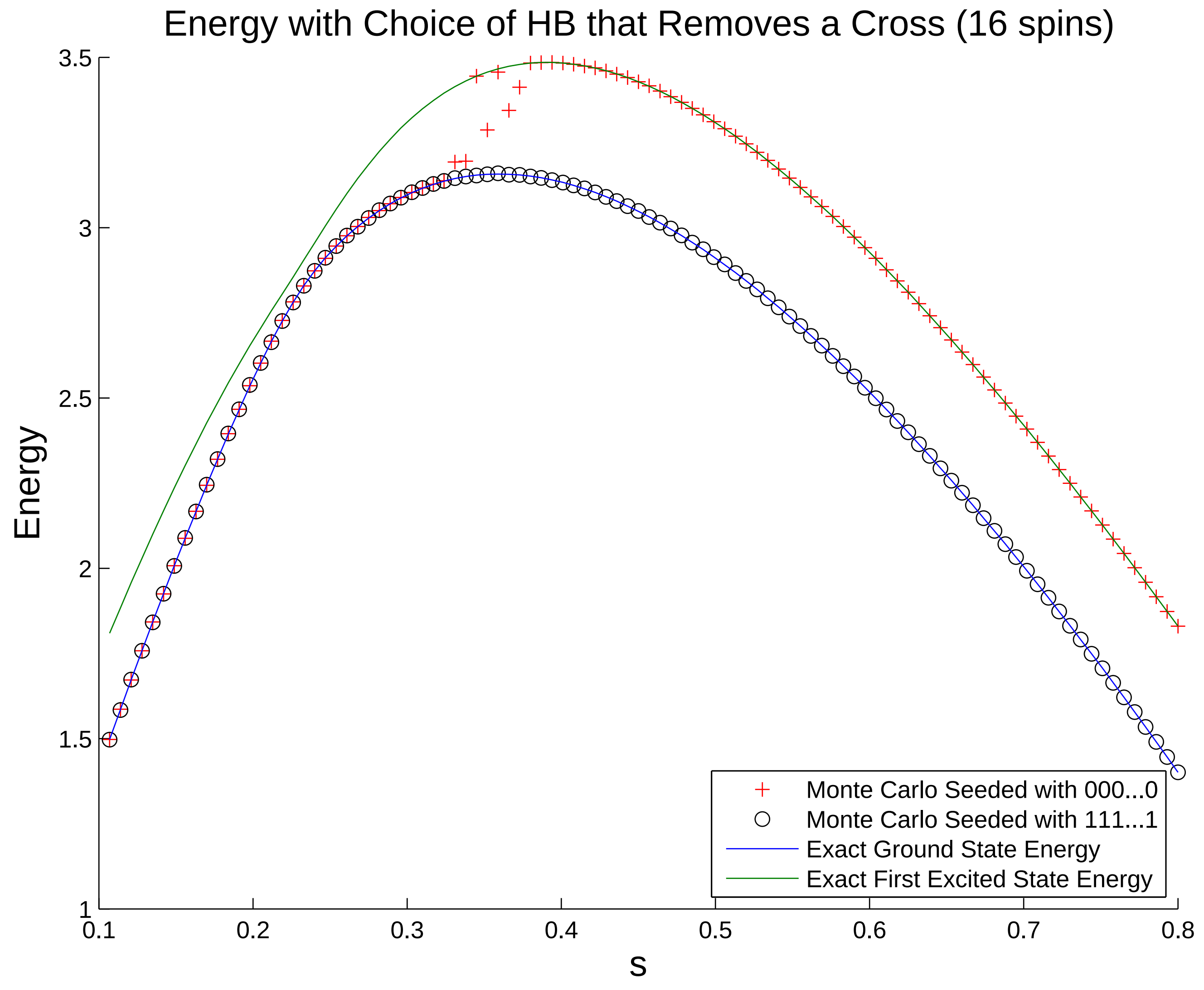
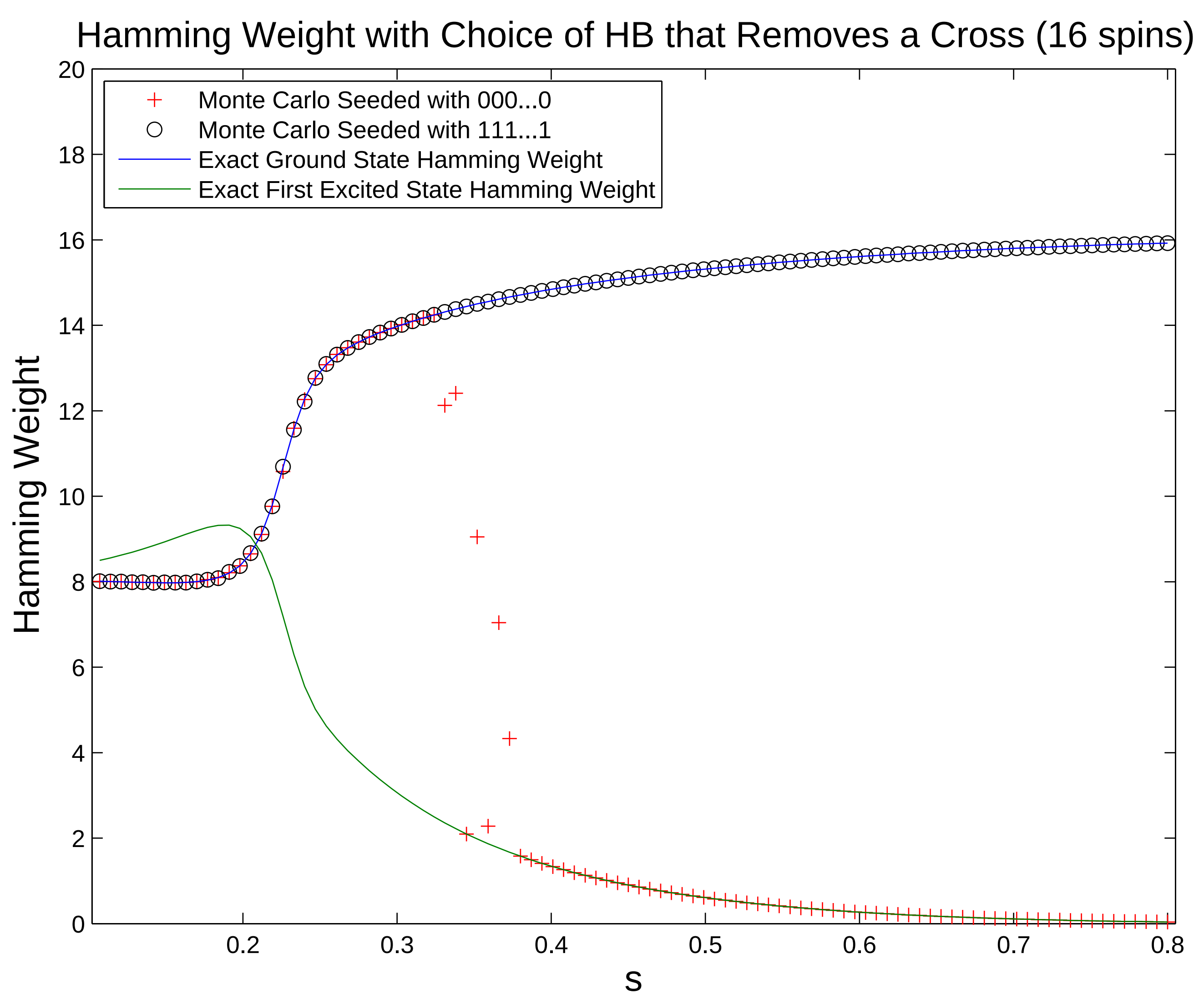
0.2
0.3
0.4
0.5
0.6
0.7
0.8

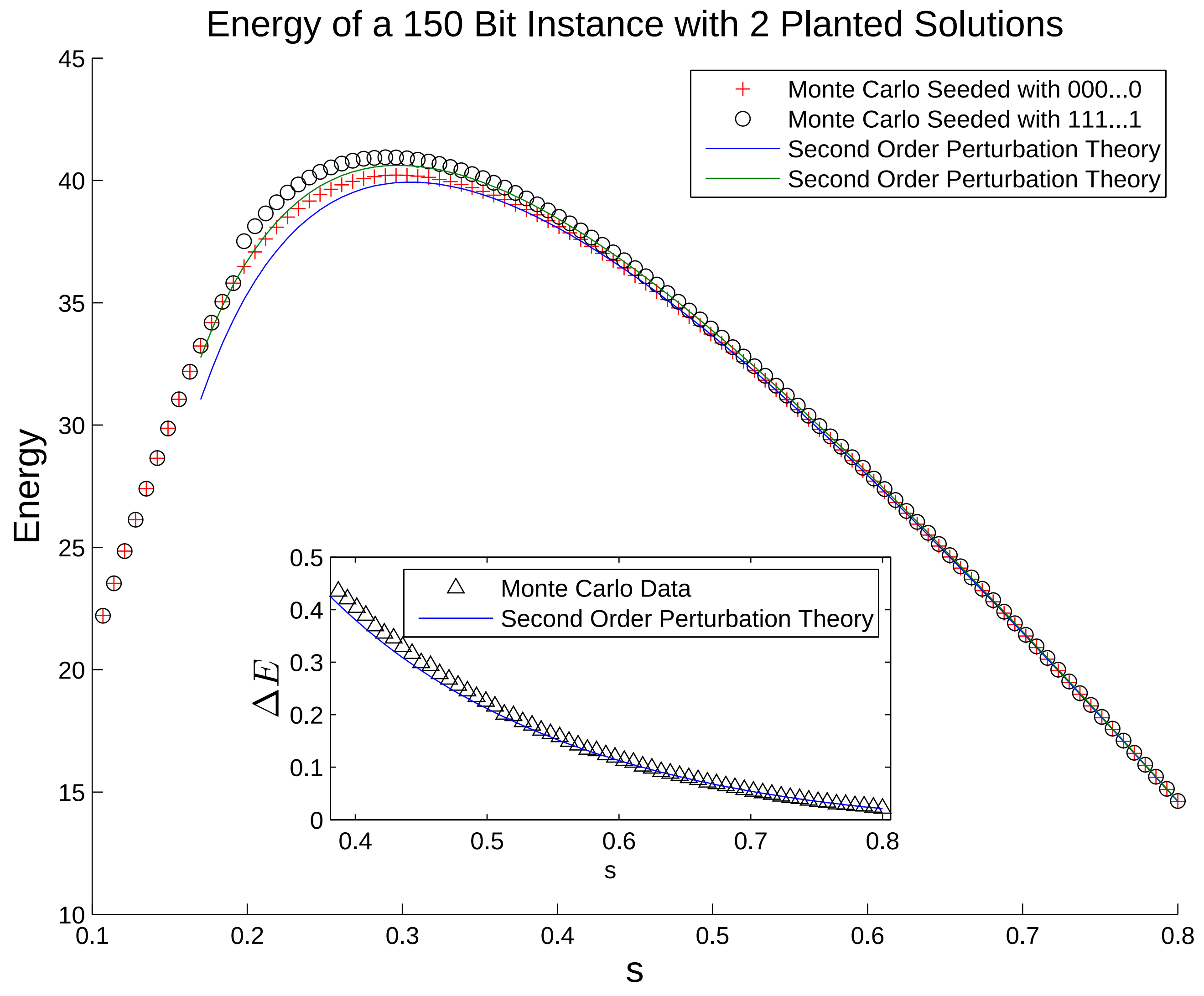


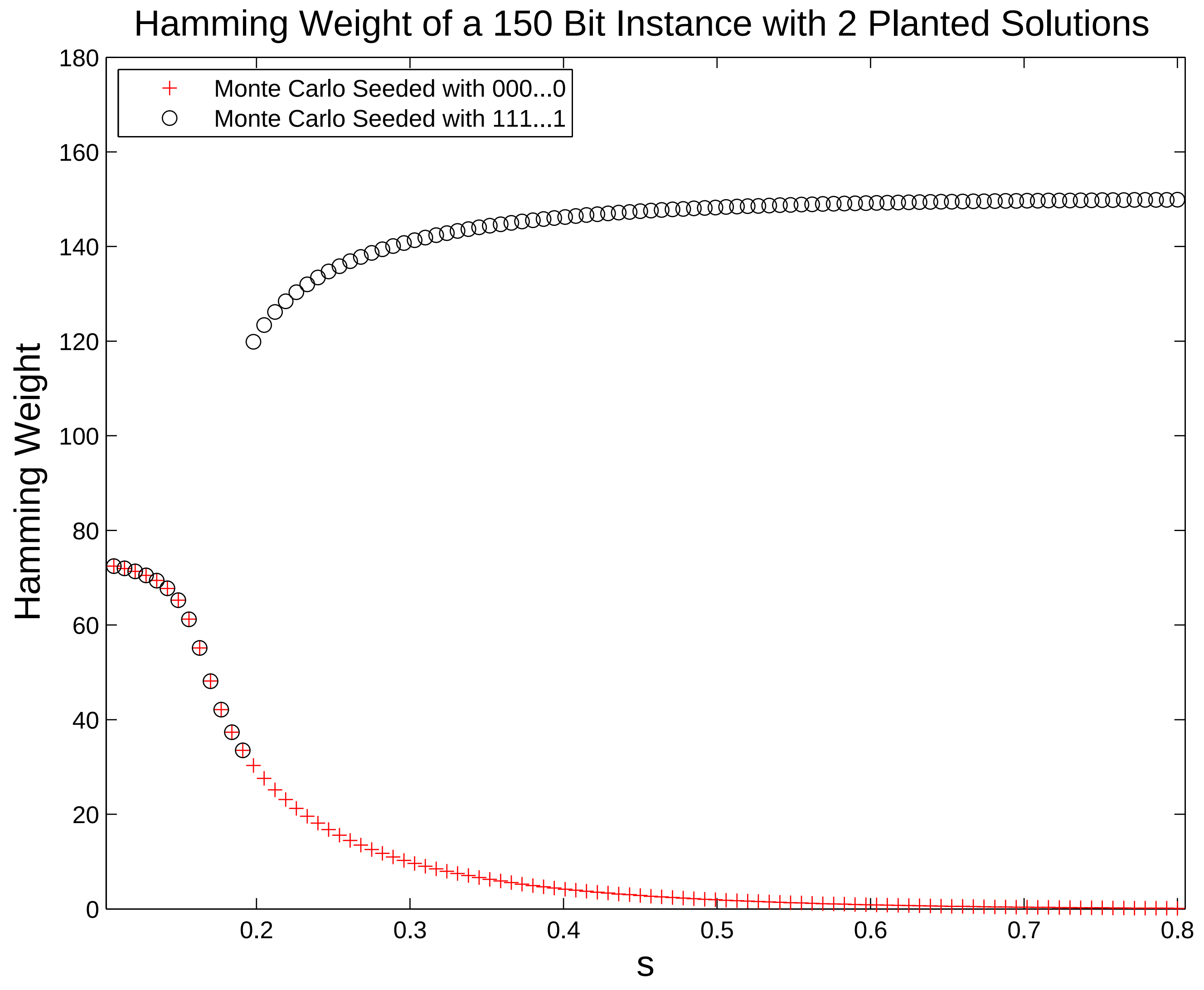
Histogram of Curvature Differences (16 spins)
Number of Samples
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
−2
−1.5
−1
−0.5
0
0.5
1
$\tilde{e}_U^{(2)} - \tilde{e}_L^{(2)}$

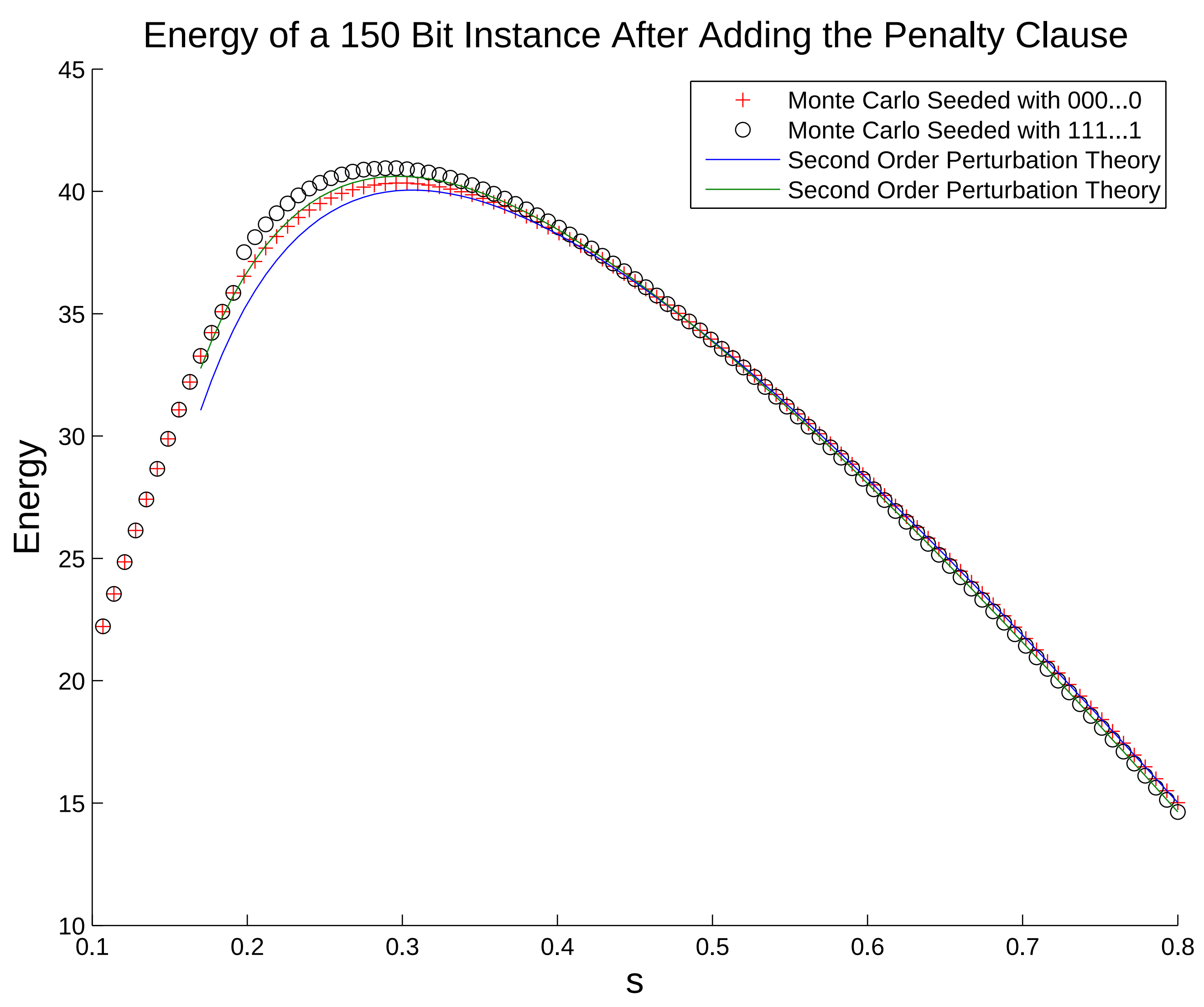

Energy with Choice of HB that Removes a Cross (16 spins)
Energy
s
3.5
3
2.5
2
1.5
1
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Exact Ground State Energy
Exact First Excited State Energy

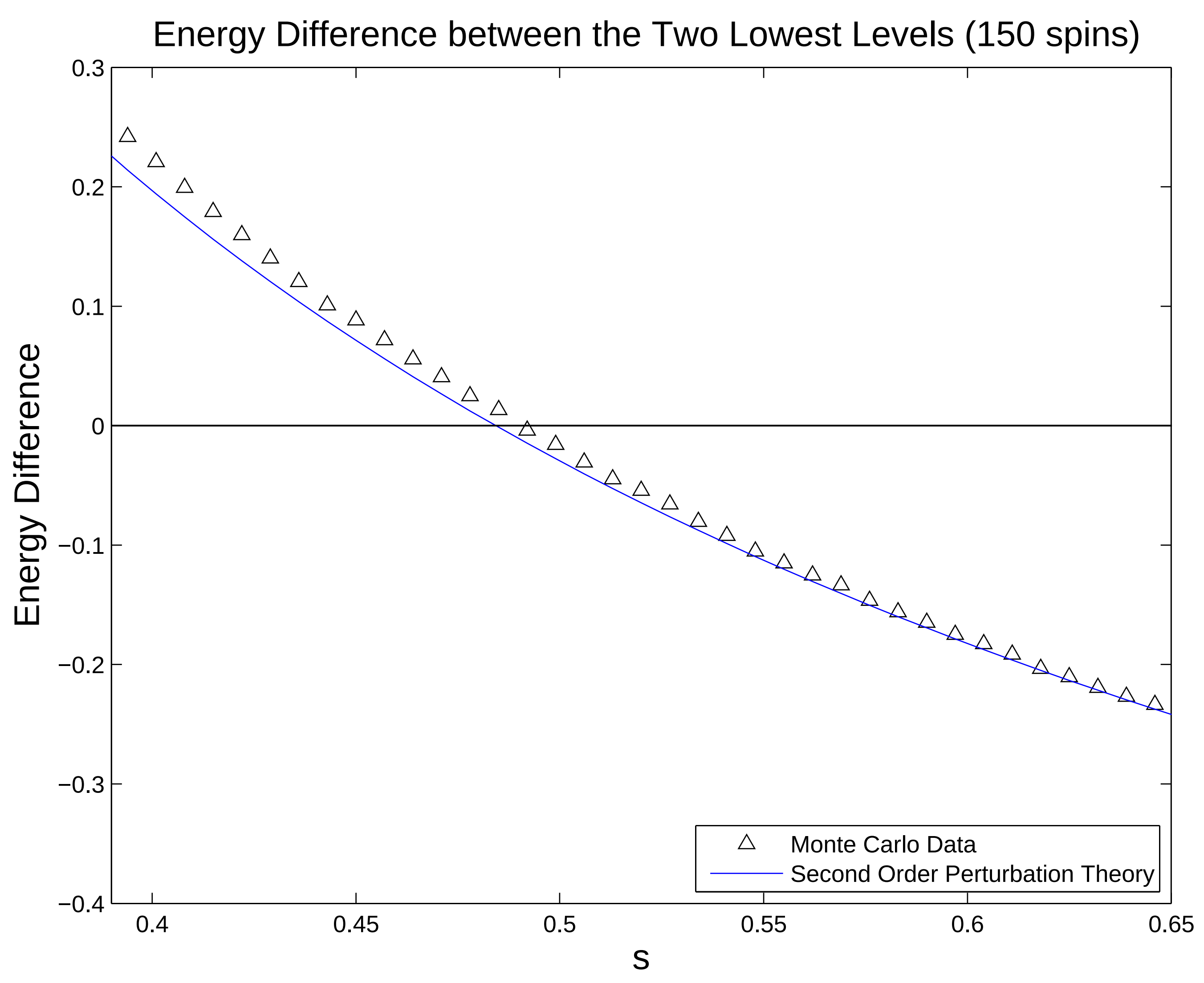


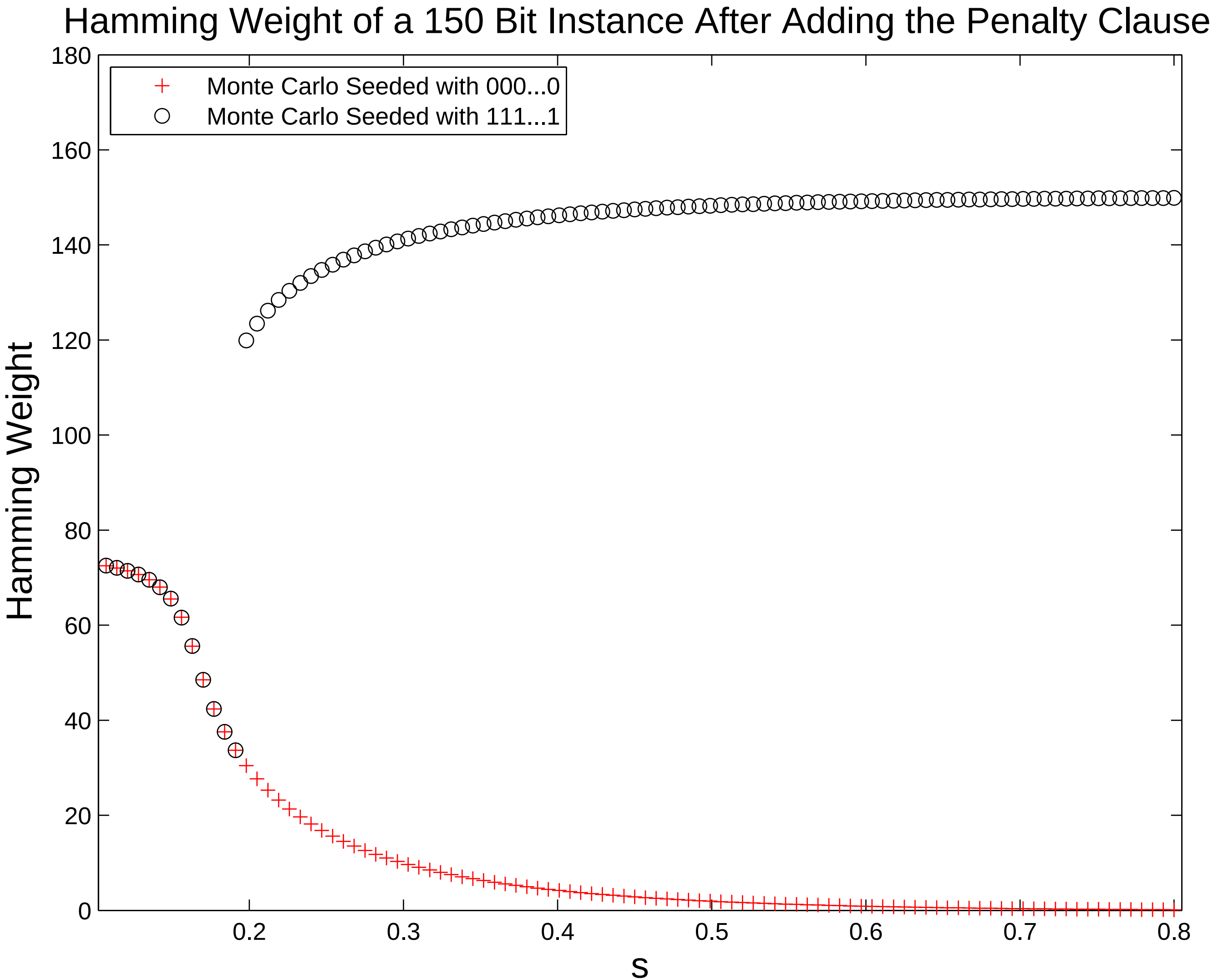
Hamming Weight with Choice of HB that Removes a Cross (16 spins)
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Exact Ground State Hamming Weight
Exact First Excited State Hamming Weight
Hamming Weight
s
0
2
4
6
8
10
12
14
16
18
20
0.2
0.3
0.4
0.5
0.6
0.7
0.8


Energy of a 150 Bit Instance with 2 Planted Solutions
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Second Order Perturbation Theory
Second Order Perturbation Theory
Energy
s
45
40
35
30
25
20
15
10
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Monte Carlo Data
Second Order Perturbation Theory
ΔE
s
0.5
0.4
0.3
0.2
0.1
0
0.4
0.5
0.6
0.7
0.8


Hamming Weight of a 150 Bit Instance with 2 Planted Solutions
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Hamming Weight
s
0
20
40
60
80
100
120
140
160
180
0.2
0.3
0.4
0.5
0.6
0.7
0.8


Energy of a 150 Bit Instance After Adding the Penalty Clause
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Second Order Perturbation Theory
Second Order Perturbation Theory
Energy
s
45
40
35
30
25
20
15
10
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8


Energy Difference between the Two Lowest Levels (150 spins)
Energy Difference
s
0.3
0.2
0.1
0
−0.1
−0.2
−0.3
−0.4
0.4
0.45
0.5
0.55
0.6
0.65
Monte Carlo Data
Second Order Perturbation Theory


Hamming Weight of a 150 Bit Instance After Adding the Penalty Clause
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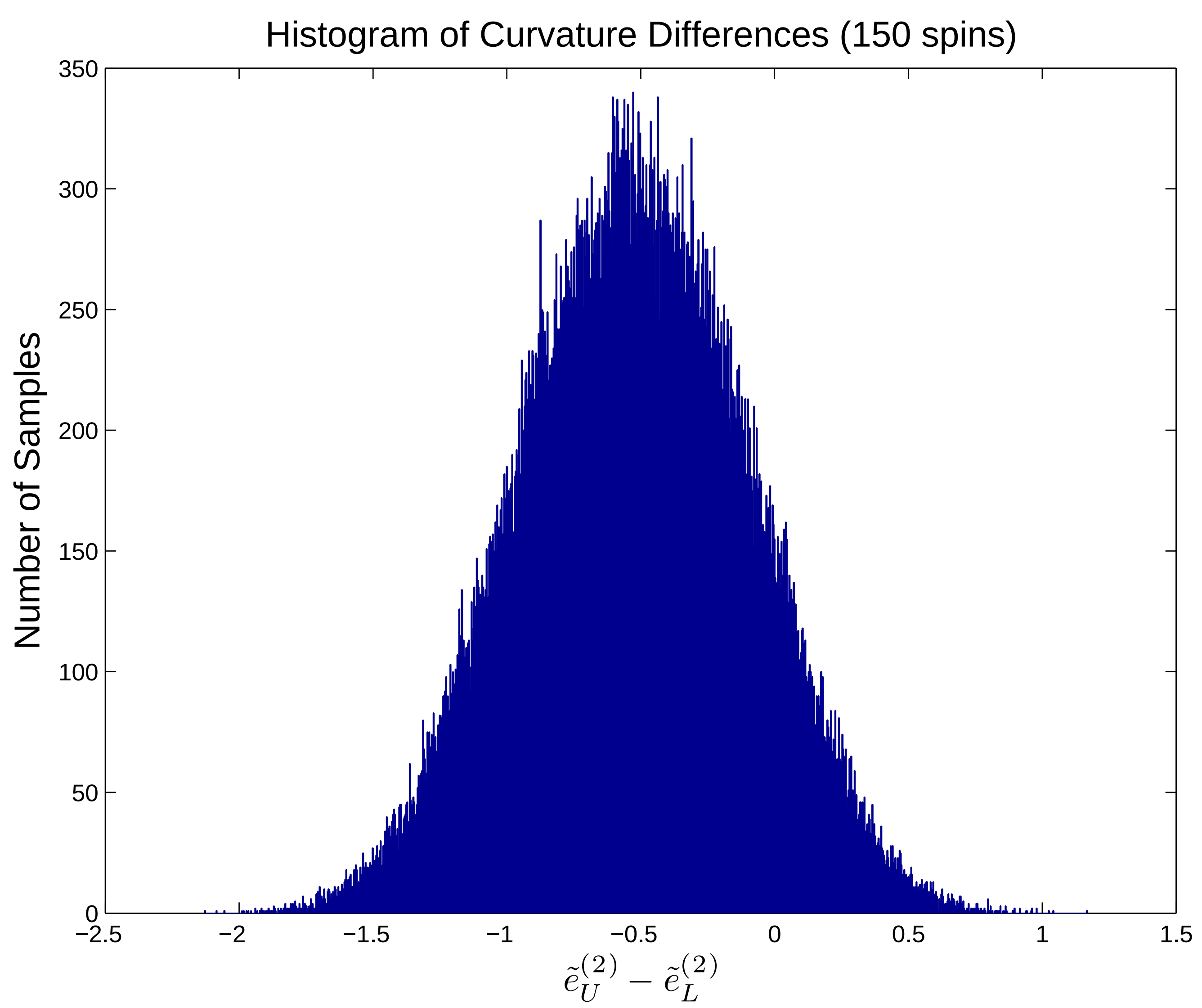
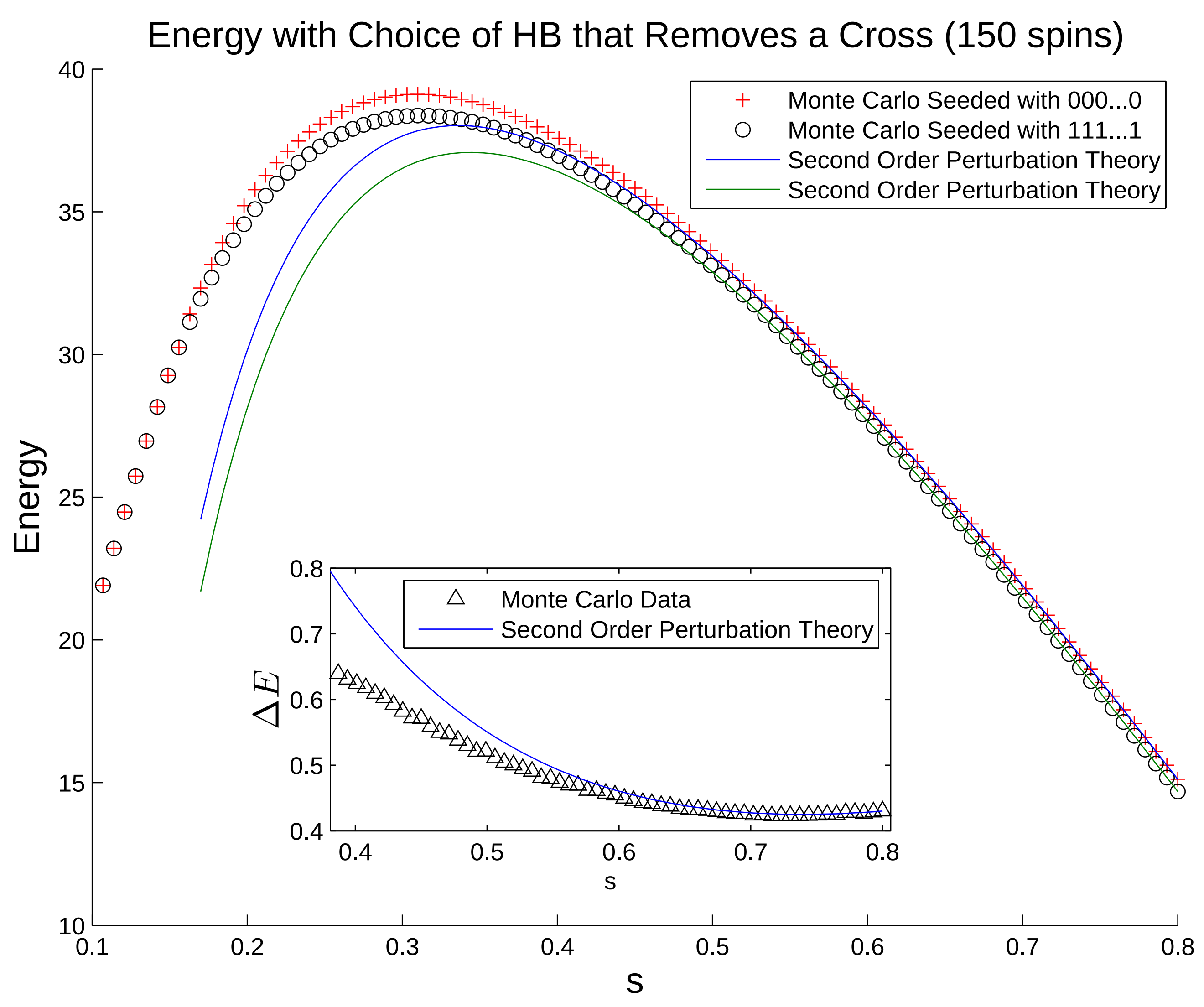
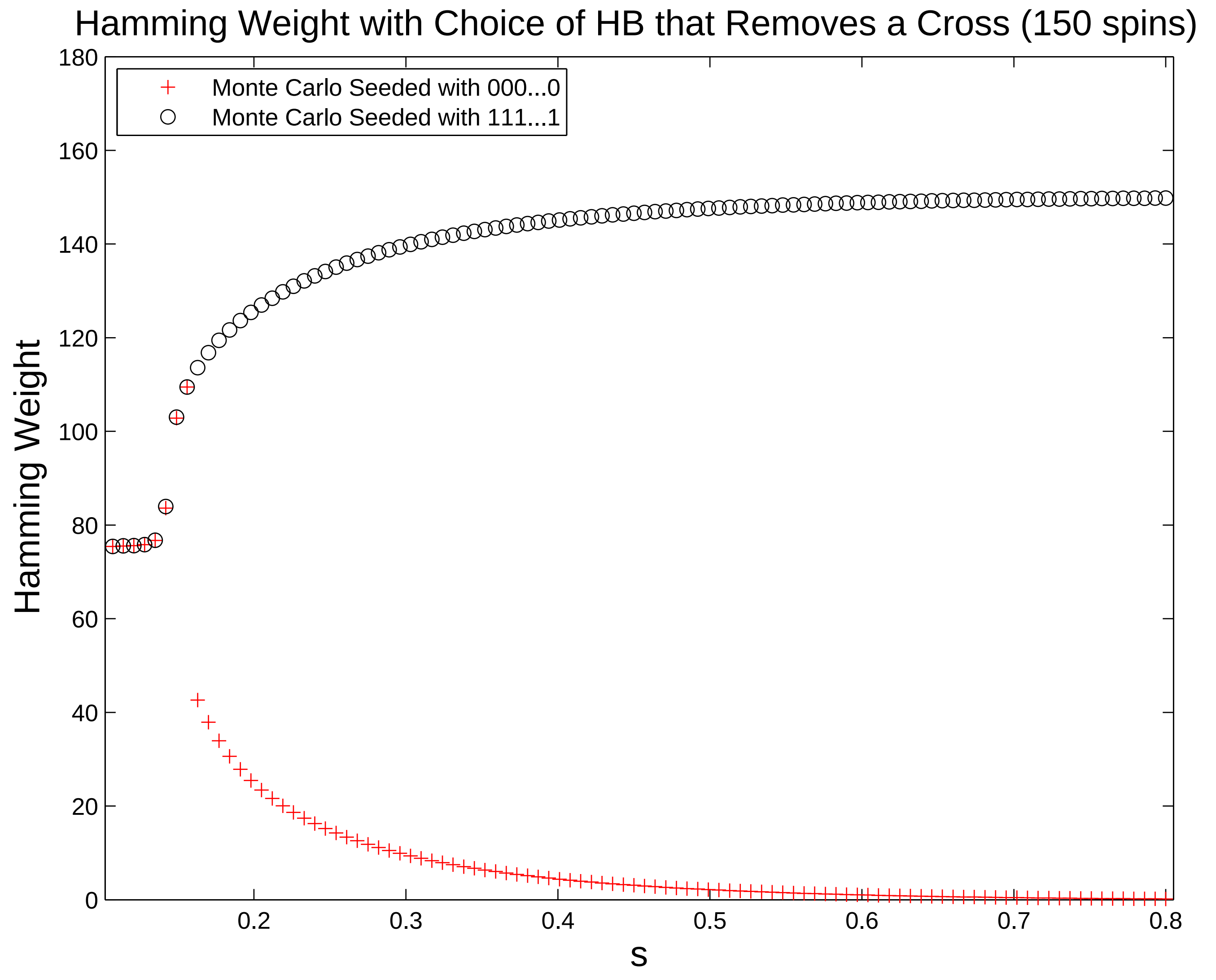
Monte Carlo Seeded with 111...1
Hamming Weight
s
0
20
40
60
80
100
120
140
160
180
0.2
0.3
0.4
0.5
0.6
0.7
0.8


Histogram of Curvature Differences (150 spins)
Number of Samples
350
300
250
200
150
100
50
0
−2.5
−2
−1.5
−1
−0.5
0
0.5
1
1.5
$\tilde{e}_U^{(2)} - \tilde{e}_L^{(2)}$



Energy with Choice of HB that Removes a Cross (150 spins)
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Second Order Perturbation Theory
Second Order Perturbation Theory
Energy
s
40
35
30
25
20
15
10
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Monte Carlo Data
Second Order Perturbation Theory
ΔE
0.8
0.7
0.6
0.5
0.4
0.4
0.5
0.6
0.7
0.8
s



Hamming Weight with Choice of HB that Removes a Cross (150 spins)
Monte Carlo Seeded with 000...0
Monte Carlo Seeded with 111...1
Hamming Weight
s
0
20
40
60
80
100
120
140
160
180
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Altshuler Krovi Roland

studied essentially the same issue!

Us They did not consider path change.

Unique Satisfying Assignment

K other assignments which are far from the winner which violate few clauses

In this case path change will succeed with

$$\boxed{\text{probability} > \frac{1}{\text{poly}(K)}}$$

What if K is exponential in n???