Adiabatic Quantum Algorithms for the NP-Complete MIS, Exact Cover and 3SAT Problems

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Outline

1. NP-Complete Problems: Exact Cover, MIS, Positive 1-in-3SAT
2. Adiabatic Quantum Algorithm
3. Two Adiabatic Algorithms for EC3
   - Clause-violation based
   - MIS-based
4. Avoid FQPT: Change Problem Hamiltonian

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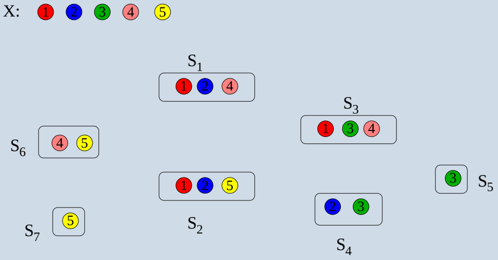
Exact Cover

- **Input:** A set of m elements, $X = \{c_1, c_2, \ldots, c_m\}$, a family of n subsets of X, $\mathcal{S} = \{S_1, S_2, \ldots, S_n\}$, where $S_i \subset X$
- **Question:** Is there an exact cover of X? That is, is there a subset $I \subseteq \{1, \ldots, n\}$ such that $\cup_{i \in I} S_i = X$, where $S_i \cap S_j = \emptyset$ for $i \neq j \in I$?

Example



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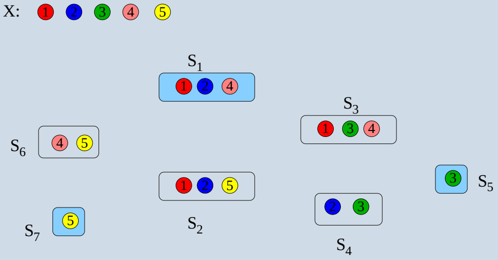

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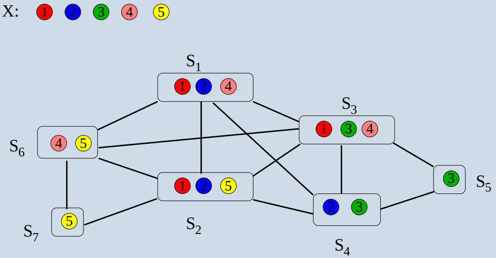

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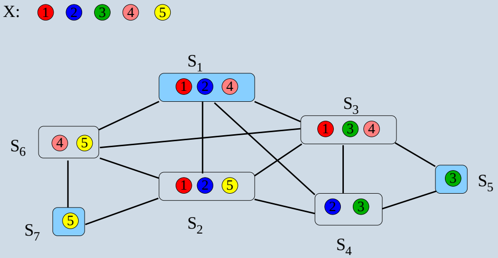

Maximum-weight Independent Set(MIS) Problem

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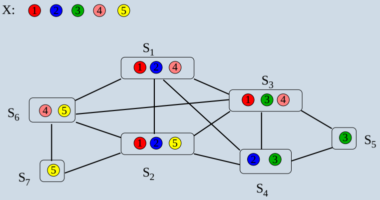
Maximum-weight Independent Set Problem

- **Input:** A graph $G(= (\mathrm{V}(G), \mathrm{E}(G)))$, B_i is the weight of vertex $i \in \mathrm{V}(G)$
- **Output:** A subset $S \subseteq \mathrm{V}(G)$ such that S is independent and the total weight of S $(= \sum_{i \in S} B_i)$ is maximized.

independent: for $i, j \in mis(G)$, $ij \notin \mathrm{E}(G)$

Example



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Positive 1-in-3SAT

- **Input:** A 3CNF boolean formula $\Psi(x_1, \ldots, x_n) = C_1 \wedge \ldots \wedge C_m$, n variables $x_i \in \{0, 1\}$ and m clauses C_k
- **Question:** Is there an assignment such that there is exactly one variable in each clause is true?

Example

$\Psi(x_1, \ldots, x_7) = C_1 \wedge C_2 \wedge C_3 \wedge C_4 \wedge C_5$

- $C_1 = x_1 \vee x_2 \vee x_3$, $C_2 = x_1 \vee x_2 \vee x_4$, $C_3 = x_3 \vee x_4 \vee x_5$
- $C_4 = x_1 \vee x_3 \vee x_6$, $C_5 = x_2 \vee x_6 \vee x_7$

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$x_1 = x_5 = x_7 = 1$

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EC3: A Special Case of Exact Cover

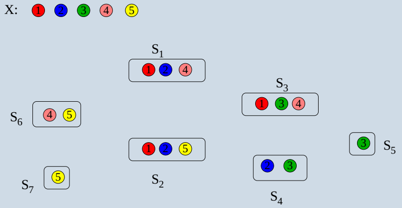
Recall: Exact Cover

Input: A set of m elements, $X = \{c_1, c_2, \ldots, c_m\}$, a family of n subsets of X, $\mathcal{S} = \{S_1, S_2, \ldots, S_n\}$, where $S_i \subset X$

Question: Is there an exact cover of X?

EC3: each element $c_i \in X$ appears exactly in three subsets

Example



- Associate each set S_i with a binary variable x_i ($S_i \leftrightarrow x_i$)
- For each element $c_i \in X$, let S_{i_1}, S_{i_2}, S_{i_3} be the three sets that consist of c_i. Define the corresponding clause $C_i = x_{i_1} \vee x_{i_2} \vee x_{i_3}$. ($c_i \leftrightarrow C_i$)

c_1 appears in S_1, S_2, S_3

$C_1 = x_1 \vee x_2 \vee x_3$

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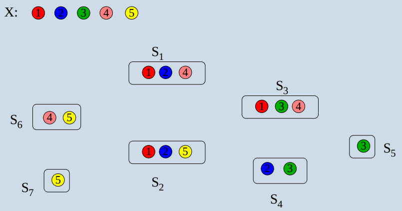

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Example (Positive 1-in-3SAT $\leq_P$ EC3 $\leq_P$ MIS)

- $\Psi(x_1, \ldots, x_7) = C_1 \wedge C_2 \wedge C_3 \wedge C_4 \wedge C_5$ where
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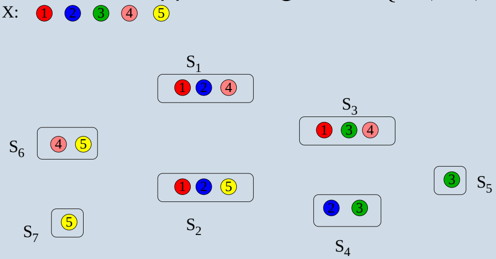

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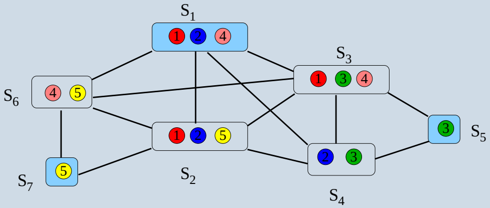
X: 1 2 3 4 5



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Adiabatic Quantum Algorithm

System Hamiltonian:

$$\mathcal{H}(t) = (1 - s(t))\mathcal{H}_{\text{init}} + s(t)\mathcal{H}_{\text{problem}}$$

for $t \in [0, T]$, $s(0) = 0$, $s(T) = 1$.

1. Initial Hamiltonian: $\mathcal{H}(0) = \mathcal{H}_{\text{init}}$ ground state known (easy to construct)
2. Problem Hamiltonian: $\mathcal{H}(T) = \mathcal{H}_{\text{problem}}$ ground state encodes the answer to the desired optimization problem
3. Evolution path: $s : [0, T] \longrightarrow [0, 1]$, e.g., $s(t) = \frac{t}{T}$

T: running time of the algorithm

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Example

1. Initial Hamiltonian: $\mathcal{H}_{\text{init}} = -(\sigma_1^x + \sigma_2^x + \sigma_3^x)$
2. Evoluation Path : $s(t) = \frac{t}{T}$
3. Problem Hamiltonian:
   $\mathcal{H}_{\text{problem}} = 5\sigma_1^z + 10\sigma_2^z + \sigma_3^z + 7\sigma_1^z\sigma_2^z + 7\sigma_2^z\sigma_3^z$

$\mathcal{E}(s_1, s_2, s_3) = 5s_1 + 10s_2 + s_3 + 7s_1s_2 + 7s_2s_3$, spin $s_i \in \{-1, +1\}$

state	energy
101	-18
100	-14
010	-10
001	-6
000	-2
110	6
011	14
111	30

- $|\psi(0)\rangle = \frac{1}{8}\sum_{x_i \in \{0,1\}} |x_1x_2x_3\rangle$
- $|\psi(T)\rangle = |101\rangle$

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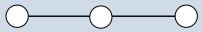

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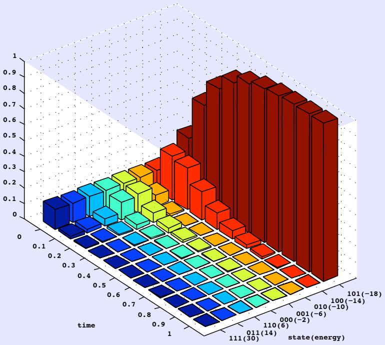
Decomposed State Evolution Visualization (DeSEV)

- Decompose ground state:

$$|\psi(s)\rangle = \sum_{x\in\{0,1\}^n} \alpha_x(s)|x\rangle, \sum_{x\in\{0,1\}^n} |\alpha_x(s)|^2 = 1$$



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Adiabatic Running Time (ART)

Adiabatic Theorem

For $s(t) = t/T$. If T is "large" enough:

$$T = O\left(\frac{\text{poly(n)}}{g_{\min}^2}\right)$$

where minimum spectral gap

$$g_{\min} = \min_{0 \le t \le T} (E_1(t) - E_0(t)),$$

$E_0(t) < E_1(t) < \ldots$ are the energy levels of $\mathcal{H}(t)$. Then the system remains "close" to the ground state of $\mathcal{H}(t)$.

"Traditional" version:

$$\text{ART}(\mathcal{H}) = \frac{\max_{0 \le s \le 1} |\langle E_1(s)| \frac{d\mathcal{H}}{ds} |E_0(s)\rangle|}{g_{\min}^2} \max_{0 \le s \le 1} ||\mathcal{H}(s)||$$

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Throughout this talk, we fix the initital Hamiltonian and evolution path, and vary the problem Hamiltonian:

1. Initial Hamiltonian: $\mathcal{H}_{\text{init}} = -\sum_{i \in \mathrm{V}(G)} \sigma_i^x$
2. Evoluation Path : $s(t) = \frac{t}{T}$
3. Problem Hamiltonian

Different problem Hamiltonians $\Rightarrow$ different adiabatic algorithms for the same problem.

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Given an instance of EC3: $\Psi(x_1, \ldots, x_n) = C_1 \wedge \ldots \wedge C_m$

- Algorithm 1: Clause-violation based problem Hamiltonian $\mathcal{H}_A$:

$$\mathcal{H}_A = \sum_{i \in V(G_{EC})} B_i \sigma_i^z + \sum_{ij \in E(G_{EC})} I_{ij} \sigma_i^z \sigma_j^z \quad (1)$$

B_i: #clauses that contains variable x_i
I_{ij}: #clauses that contains both x_i and x_j (was called $J_{ij} = \frac{1}{2}(J_{ij} + J_{ji})$)

- Algorithm 2: MIS-reduction based problem Hamiltonian $\mathcal{H}_C$:

$$\mathcal{H}_C = \sum_{i \in V(G_{EC})} \left(\sum_{j \in \mathrm{nbr}(i)} J_{ij} - 2B_i \right) \sigma_i^z + \sum_{ij \in E(G_{EC})} J_{ij} \sigma_i^z \sigma_j^z \quad (2)$$

where $J_{ij} > \min\{B_i, B_j\}$.

Question: ART(Algorithm 1) ⇒ ART(Algorithm 2)?

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Algorithm 1: Altshuler et al.

Energy function:

$$\mathcal{E}_\Psi(x_1, \ldots, x_n) = \sum_{i=1}^{m} (x_{i_1} + x_{i_2} + x_{i_3} - 1)^2$$

penalizes each violating clause $C_i = x_{i_1} \vee x_{i_2} \vee x_{i_3}$

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"While our argument immediately implies that a particular quantum adiabatic algorithm for EC3 will fail, it is important to note that it also applies to more general cases. In particular, it does not rely on the specific form of the problem Hamiltonian, but rather on its general statistical properties, so that it should extend to other NP-complete problems such as 3-SAT. "

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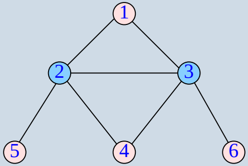
Algorithm 2: MIS-based

Recall: Maximum Independent Set (unweighted) Problem

- Input: a graph G, $\mathrm{V}(G) = \{1, 2, \ldots, n\}$,
- Output: $mis(G) \subseteq \mathrm{V}(G)$, independent, $|mis(G)|$ is maximized

independent: for $i, j \in mis(G)$, $ij \notin \mathrm{E}(G)$

Example



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Quadratic Pseudo-boolean Function

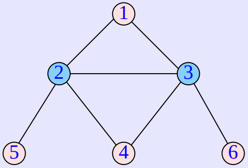
For $i \in \mathrm{V}(G)$, associate it with a binary variable $x_i \in \{0, 1\}$. Define

$$\mathcal{Y}(x_1, \ldots, x_n) = \sum_{i \in \mathrm{V}(G)} x_i - \sum_{ij \in \mathrm{E}(G)} J_{ij} x_i x_j$$

J_{ij} – penalty for the edge ij

Example: for $J_{ij} = 2$

- $\mathcal{Y}(1, 0, 0, 0, 0, 1) = 2$
- $\mathcal{Y}(1, 1, 0, 0, 0, 1) = 1 + 1 - 2 + 1 = 1$
- $\mathcal{Y}(1, 0, 0, 1, 1, 1) = 4$



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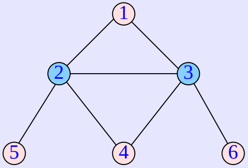

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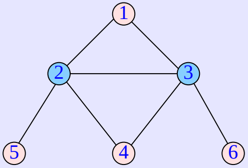
$$\mathcal{Y}(x_1, \ldots, x_n) = \sum_{i \in \mathrm{V}(G)} x_i - \sum_{ij \in \mathrm{E}(G)} J_{ij} x_i x_j$$

J_{ij} – penalty for the edge ij

Example: for $J_{ij} = 2$

- $\mathcal{Y}(1, 0, 0, 0, 0, 1) = 2$
- $\mathcal{Y}(1, 1, 0, 0, 0, 1) = 1 + 1 - 2 + 1 = 1$
- $\mathcal{Y}(1, 0, 0, 1, 1, 1) = 4$



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Theorem

If $J_{ij} > 1$ for all $ij \in \mathrm{E}(G)$, then

$$|\mathrm{mis}(G)| = \max \mathcal{Y}(x_1, \ldots, x_n).$$

and $\mathrm{mis}(G) = \{i \in \mathrm{V}(G) : x_i^* = 1\}$, *where* $(x_1^*, \ldots, x_n^*) = \mathrm{argmax}_{(x_1,\ldots,x_n) \in \{0,1\}^n} \mathcal{Y}(x_1, \ldots, x_n)$.

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Generalize to weighted MIS problem

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Theorem

If $J_{ij} > \min\{B_i, B_j\}$ *for all* $ij \in \mathrm{E}(G)$*, then the maximum value of*

$$\mathcal{Y}(x_1, \ldots, x_n) = \sum_{i \in \mathrm{V}(G)} B_i x_i - \sum_{ij \in \mathrm{E}(G)} J_{ij} x_i x_j \qquad (3)$$

is the total weight of the MIS, and $\mathrm{mis}(G) = \{i \in \mathrm{V}(G) : x_i^* = 1\}$*, where* $(x_1^*, \ldots, x_n^*) = \arg\max_{(x_1,\ldots,x_n)\in\{0,1\}^n} \mathcal{Y}(x_1, \ldots, x_n)$.

Change variables: $x_i = \frac{1+s_i}{2}$ $(x_i = 0 \Leftrightarrow s_i = -1,\ x_i = 1 \Leftrightarrow s_i = +1)$

$$\text{Min} \quad \mathcal{E}(s_1, \ldots, s_n) = \sum_{i \in \mathrm{V}(G)} \Big(\sum_{j \in \mathrm{nbr}(i)} J_{ij} - 2B_i \Big) s_i + \sum_{ij \in \mathrm{E}(G)} J_{ij} s_i s_j$$

$$\mathcal{H} = \sum_{i \in \mathrm{V}(G)} \left(\sum_{j \in \mathrm{nbr}(i)} J_{ij} - 2B_i \right) \sigma_i^z + \sum_{ij \in \mathrm{E}(G)} J_{ij} \sigma_i^z \sigma_j^z$$

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Theorem

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Comparison: Algorithm 1 vs. Algorithm 2

- Algorithm 1:

$$\mathcal{H}_A = \sum_{i \in \mathrm{V}(G_{\mathrm{EC}})} B_i \sigma_i^z + \sum_{ij \in \mathrm{E}(G_{\mathrm{EC}})} I_{ij} \sigma_i^z \sigma_j^z$$

- Algorithm 2:

$$\mathcal{H}_C = \sum_{i \in \mathrm{V}(G_{\mathrm{EC}})} \left(\sum_{j \in \mathrm{nbr}(i)} J_{ij} - 2B_i \right) \sigma_i^z + \sum_{ij \in \mathrm{E}(G_{\mathrm{EC}})} J_{ij} \sigma_i^z \sigma_j^z$$

where $J_{ij} > \min\{B_i, B_j\}$

Recall: $2B_i = \sum_{j \in \mathrm{nbr}(i)} I_{ij}$
Write $J_{ij} = 2I_{ij} + D_{ij}$, for $D_{ij} > \min\{B_i, B_j\} - 2I_{ij}$

$$\mathcal{H}_C = 2\mathcal{H}_A + \sum_{i \in \mathrm{V}(G_{\mathrm{EC}})} \sum_{j \in \mathrm{nbr}(i)} D_{ij} \sigma_i^z + \sum_{ij \in \mathrm{E}(G_{\mathrm{EC}})} D_{ij} \sigma_i^z \sigma_j^z$$

Does it matter if we choose different D_{ij}?

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Computing spectral gap by perturbation

- Require computing the energy difference $E_{12}(s)$ – depends on the energy function of the problem Hamiltonian.
- While the energy function for $\mathcal{H}_A$ only depends on B_i and I_{ij}, the energy function for $\mathcal{H}_C$ also depends on J_{ij} whose values have a range to choose.
- "E_{12}^4 is given by a sum of $\theta(N)$ random terms with zero mean" no longer applies here as J_{ij} are not random.

Example (2nd order correction)

- using $\mathcal{H}_A$: $E_x^{(2)} = -\sum_{i=1}^{n} 1/B_i$
- using $\mathcal{H}_C$:

$$E_x^{(2)} = -\sum_{\{i:x_i=0\}} \frac{1}{B_i - \sum_{\{j\in nbr(i):x_j=1\}} J_{ij}} + \sum_{\{i:x_i=1\}} \frac{1}{B_i}$$

– depend on the connectivity of the graph, and the non-random choice of J_{ij}

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– depend on the connectivity of the graph, and the non-random choice of J_{ij}

Outline

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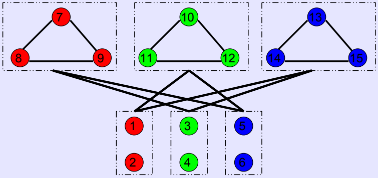
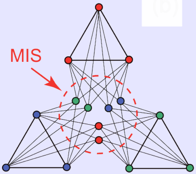
15-Vertex CK Graph





- $V_A = \{1, \ldots, 6\}$: $\bullet$, $w_A = 1$
- $V_B = \{7, \ldots, 15\}$: $\triangle$, $1 \leq w_B < 2$

The corresponding Hamiltonian:

$$\mathcal{H}_1 = \sum_{i \in V_A} (6J - 2)\sigma_i^z + \sum_{i \in V_B} (6J - 2w_B)\sigma_i^z + J \sum_{ij \in \mathrm{E}(G)} \sigma_i^z \sigma_j^z$$

Here we fix $J_{ij} = J = 2 > w_B$ for all $ij \in \mathrm{E}(G)$.

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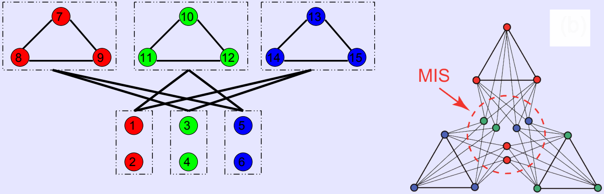
15-Vertex CK Graph



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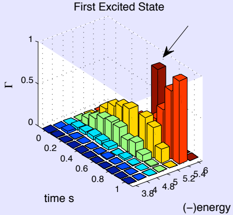
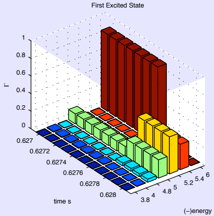
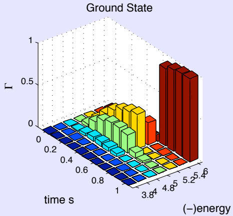
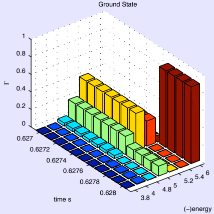
FQPT

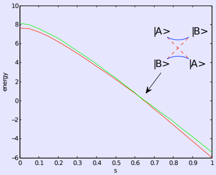
(Zoom:$s = 0.627 \ldots 0.628$)











$s^* = 0.6276$, $g_{\min} = 1.04 \times 10^{-5}$

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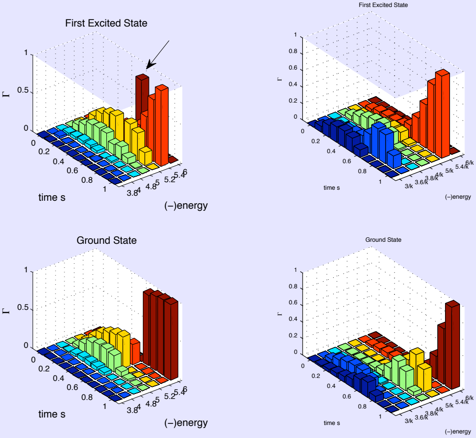
Change Parameter... Avoid FQPT: $g_{\min} = 10^{-5} \rightarrow 10^{-1}$

$J = 2$ $\qquad$ $J = 20$



$s^* = 0.627637, g_{\min} = 1.04 \times 10^{-5}$ $\qquad$ $s^* = 0.667731, g_{\min} = 0.145$

$J = 2$	$\lvert \bullet\bullet\bullet\bullet\bullet\rangle + \lvert \triangle\triangle\triangle\triangle\triangle\rangle$	$\lvert \triangle\triangle\triangle\triangle\rangle$	$\lvert \triangle\triangle\triangle\rangle$	$\lvert \bullet\bullet\bullet\bullet\bullet\bullet\rangle$
$J = 20$	$\lvert \bullet\bullet\bullet\bullet\rangle$	$\lvert \bullet\bullet\bullet\bullet\bullet\rangle$	$\lvert \triangle\triangle\triangle\rangle$	$\lvert \bullet\bullet\bullet\bullet\bullet\bullet\rangle$

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