

Accurate 100+ site Kagome Lattice Ground State Energy (GSE) by Perturbing Hamiltonian on the defect triangles

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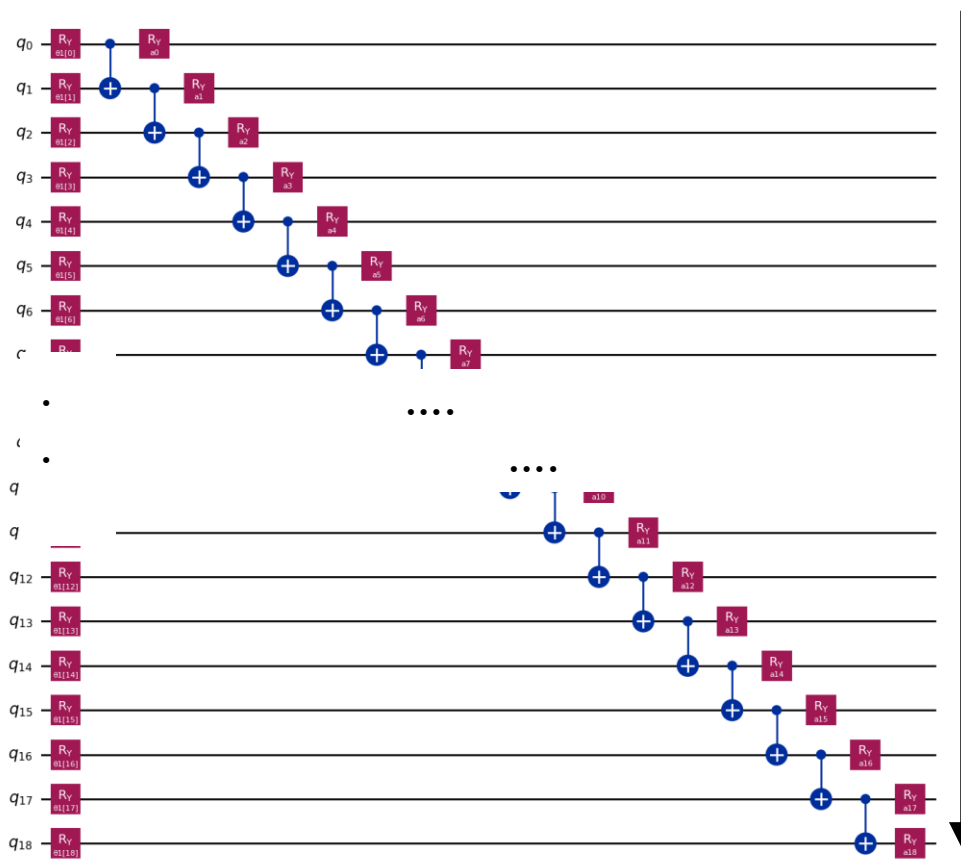
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IBM Researcher program 2023, IBM Credit Program 2024

Key insights from the credits program experiment and study (1) Success of ODR Method for 100x100 circuit



Problem:
Higher error in observable (qubits) at higher circuit depth !

Increasing Circuit Depth

Truncated circuit qubits range [a-b]	Segmented original $\langle obs \rangle: x$	Segmented Ref $\langle obs \rangle: y$	Noise mitigated Segmented $\langle obs \rangle = 10x/r$
[1-20]	-6.50±0.15	8.45±0.10	-7.7
[21-40]	-6.64±0.27	6.6±0.42	-10.06
[41-60]	-5.58±0.36	3.83±0.52	-14.6
[61-80]	-3.99±0.06	3.16±0.16	-12.62
[81-100]	-3.64±0.30	3.09±0.32	-11.78
Complete Circuit	$\langle obs \rangle = -26.53$ Original error in the $\langle obs \rangle$: 47%	25.13	$\langle obs \rangle = -52.76$ Mitigated Error in the $\langle obs \rangle$: 5.2%

Torino jobs: crhgpgvut4r4kjefe2mg & crhgphaji5oi10mnb9ng

Solution: With operator Decoherence Renormalization (ODR) method, noise at higher depths was effectively mitigated !

Qiskit101-qubit Real Amplitude ansatz for KAFM Ground State Energy (GSE) problem

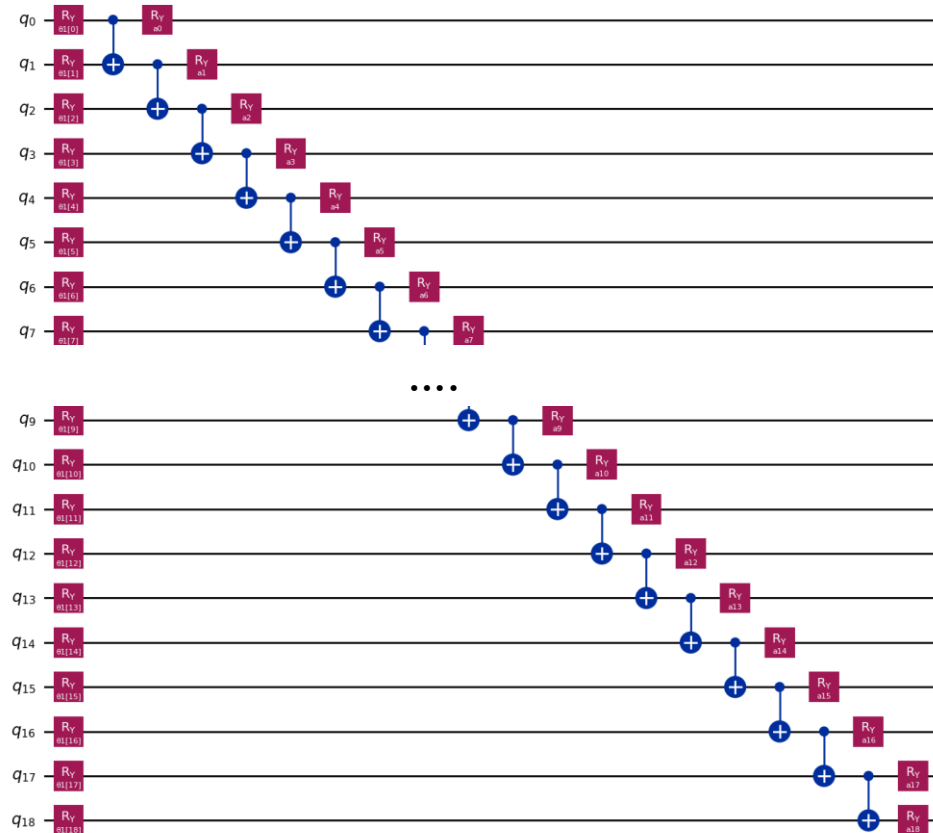
Key insights from the last year credits program experiments and study (2) Hamiltonian Perturbation method needs revision

- Dimer covering: takes us close to the GSE, but not close enough. The gap can't be bridged without dealing with **DEFECT TRIANGLES**
- Qiskit 100x100 single layer Real Amplitude ansatz: is good at generating dimer cover, but can it address **DEFECT TRIANGLE** problem?
- Exploit Defect Triangles (new strategy):
 - Extract defect triangle from dimer covering generated by the ansatz
 - Focus Hamiltonian perturbation on defect triangle and update edge weights
 - Recompute GSE by VQE with the same ansatz

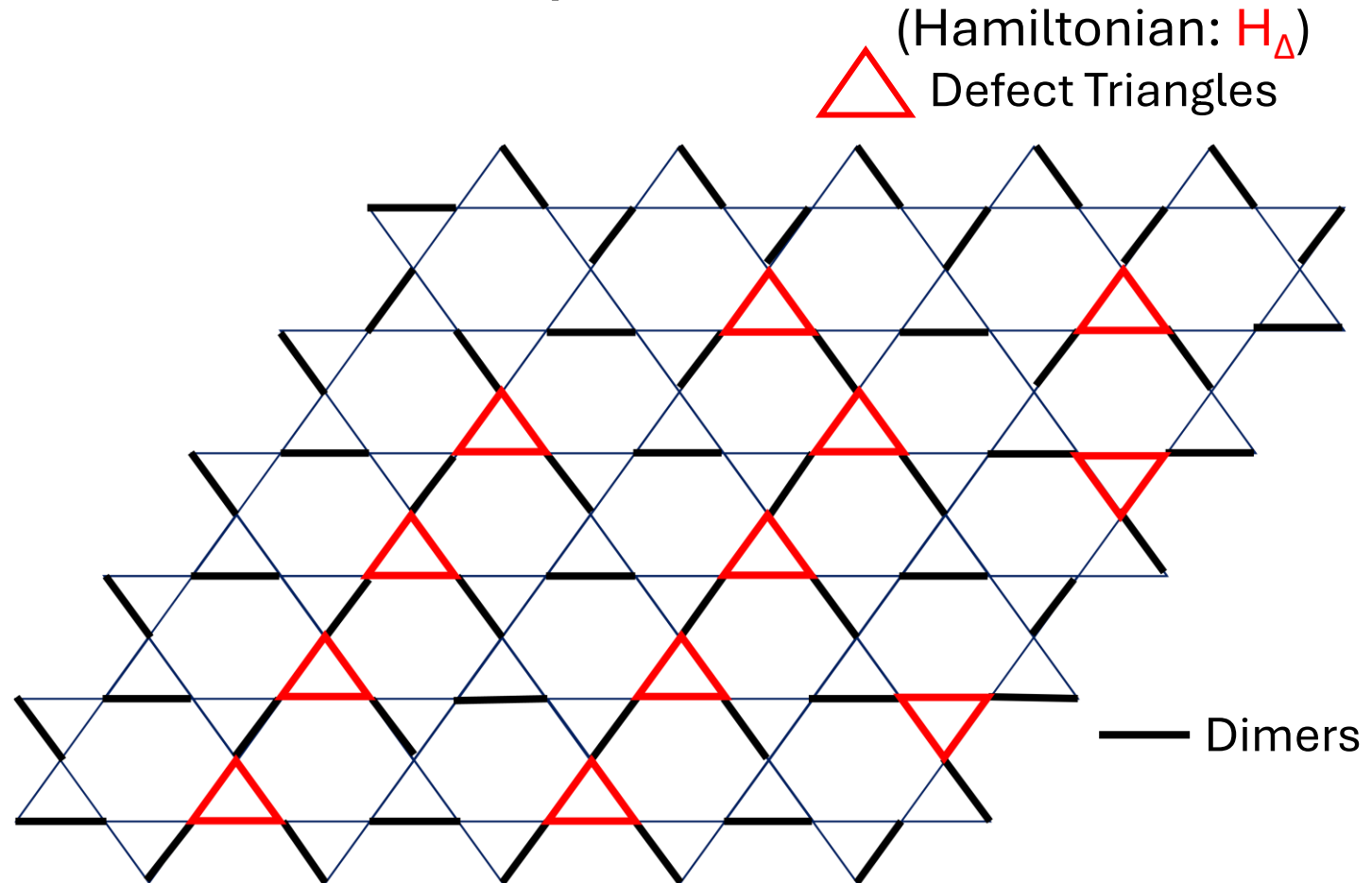
Existing IBM cloud quantum simulators can only simulate up to 64-qubit 100x100 real-amplitude ansatz !

Modified (new) proposal:

100-qubit quantum compute: $\min_{\varphi} \langle \varphi | H_{pert} | \varphi \rangle$



100x100 real amplitude ansatz: $|\varphi\rangle$



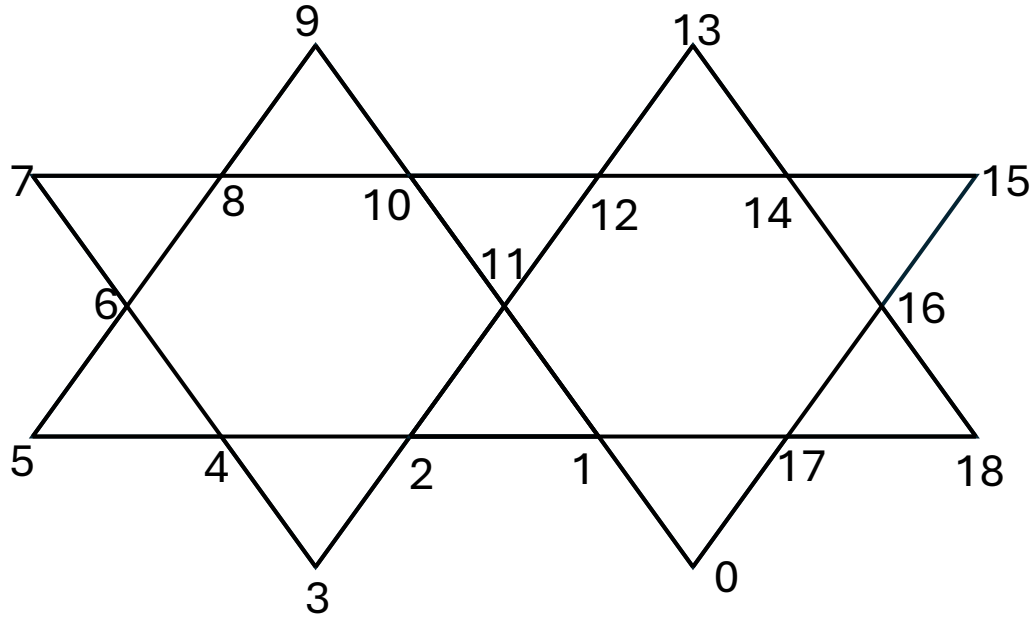
Hamiltonian perturbation on defect triangles

$$H_{pert} = H_{orig} + 0.5 H_{\Delta}$$

Proof of concept

GSE with two-unit cell Kagome lattice

Two unit-cell Kagome Lattice GSE Example

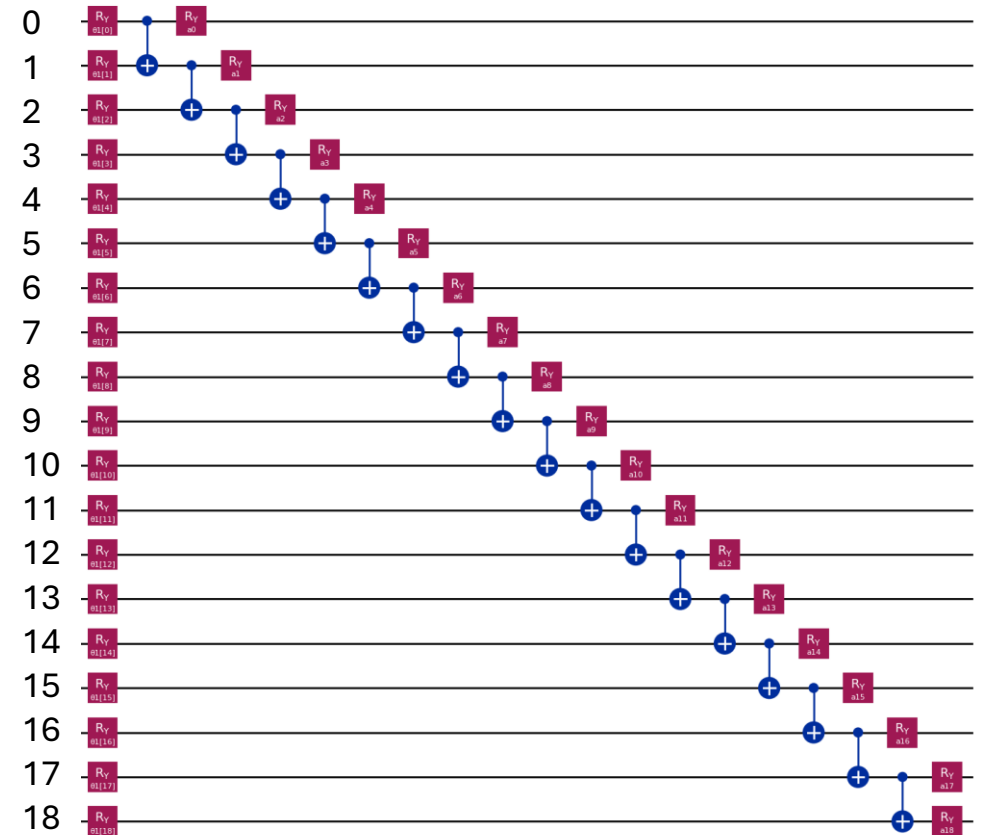


Two unit-cell Kagome lattice

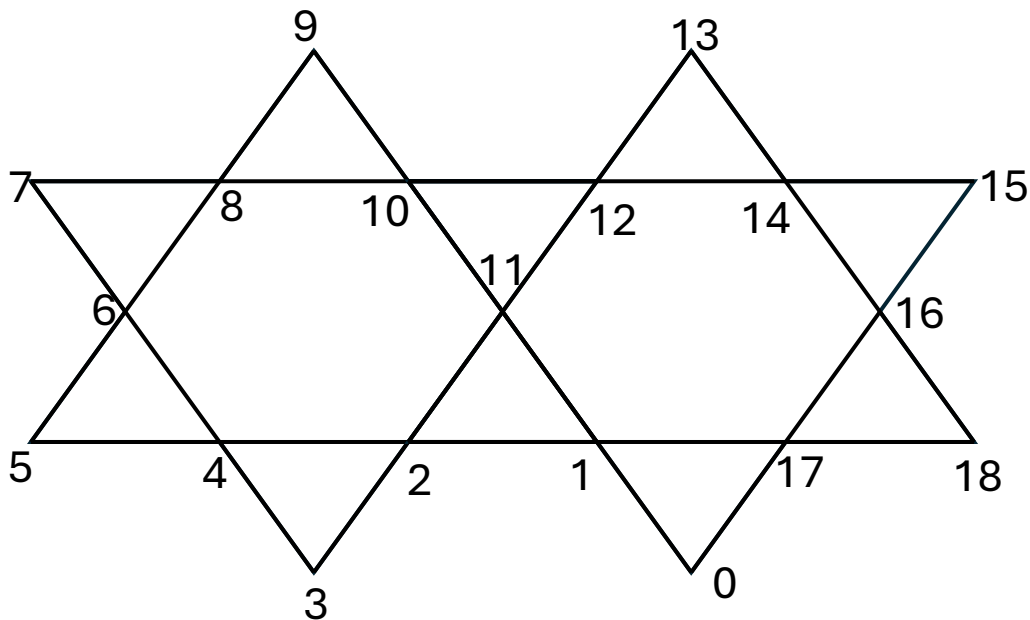
- 19 sites [0,1,2,...,18]
- 30 edges :

$E = \{ [0,1], [1,2], [1,11], [2,11], [2,3], [3,4], [2,4], [4,6], [4,5], [5,6], [6,7], [6,8], [7,8], [8,9], [9,10], [8,10], [10,11], [11,12], [10,12], [12,13], [13,14], [12,14], [14,15], [15,16], [14,1], [16,17], [17,1], [16,18], [17,0], [17,1] \}$

All edges have weight = 1,
i.e., $\forall_{i,j} \text{weight}[i,j] = 1$



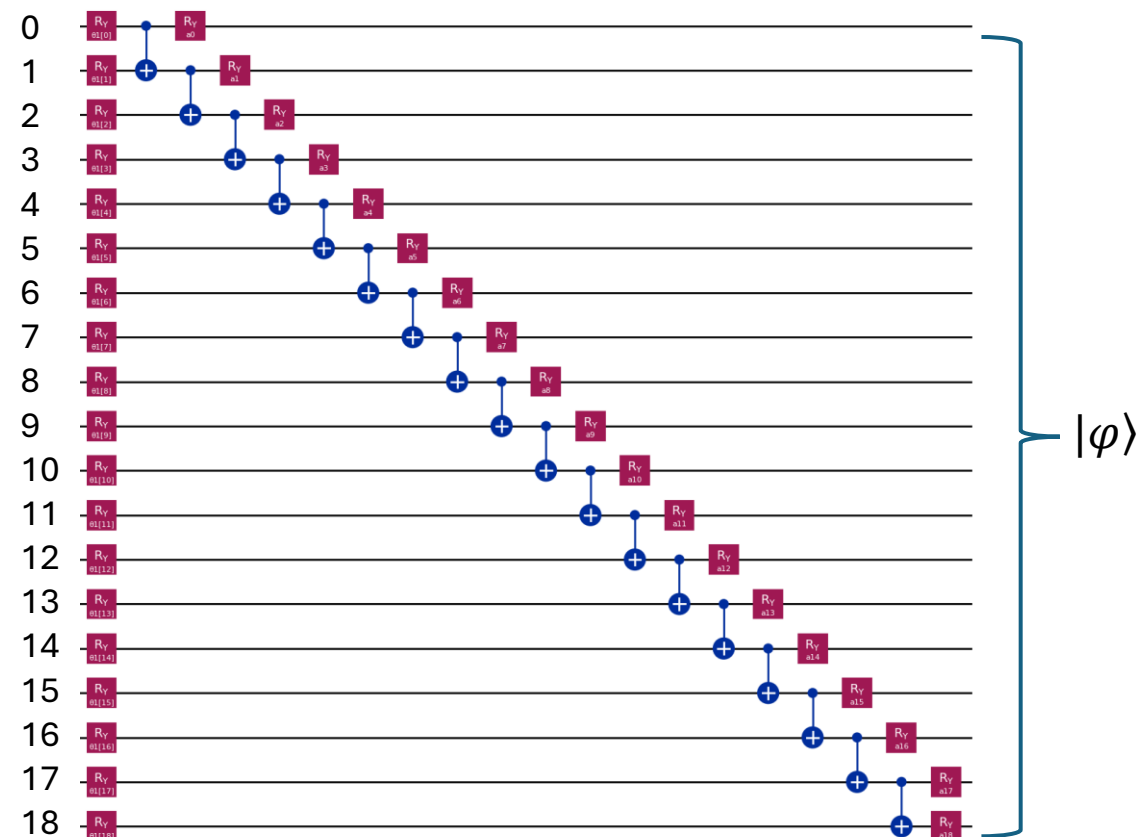
Qiskit:19-qubit Real Amplitude
Single-layer ansatz



Heisenberg KAFM Hamiltonian

$$H = \sum_{[i,j] \in E} X_i X_j + Y_i Y_j + Z_i Z_j$$

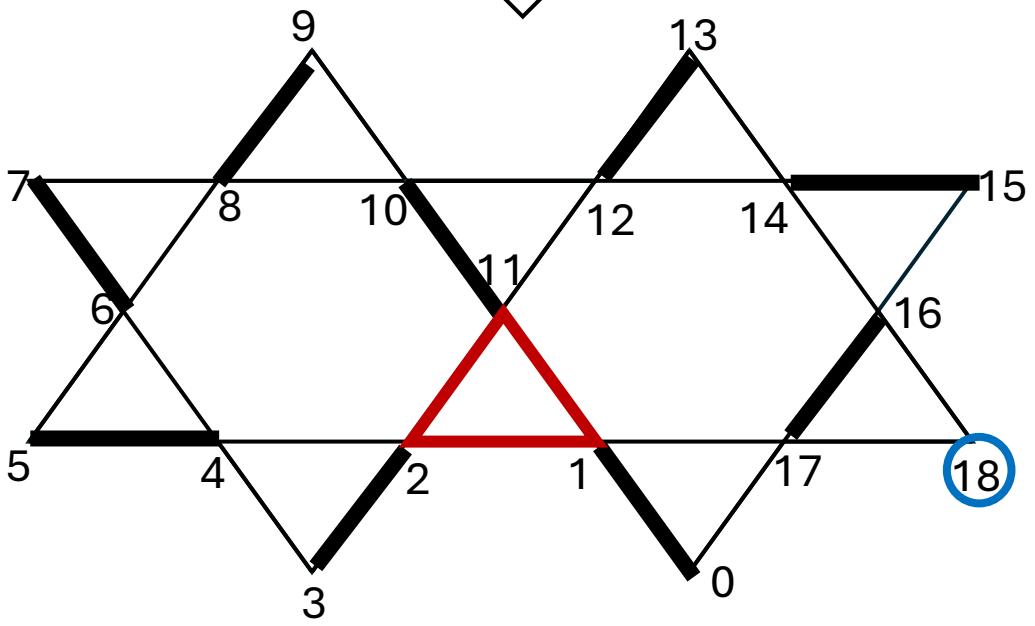
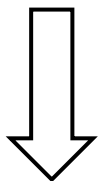
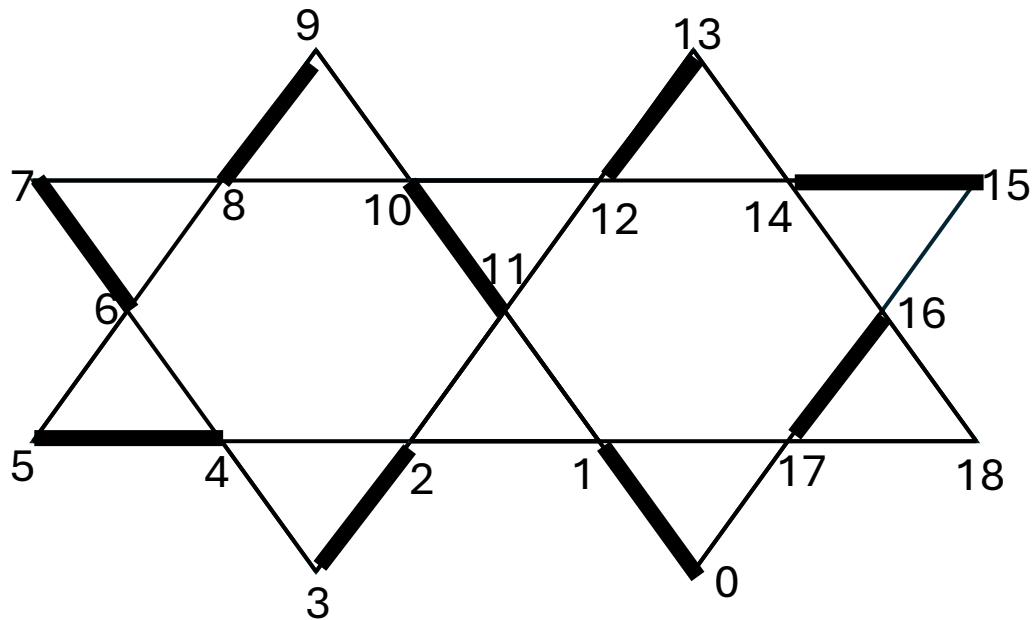
True GSE = -29.14



Qiskit: 19-qubit Real Amplitude
Single-layer ansatz

The ansatz's lowest estimate of
GSE: $\langle \varphi | H | \varphi \rangle = -27.2$

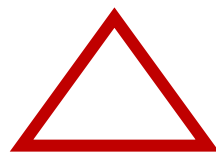
Error = 6.7%



Lattice with dimer covering
 $C = \{[0,1],[2,3],[4,5],[6,7],[8,9],$
 $[10,11],[12,13],[14,15],[16,17]\}$



Dimer



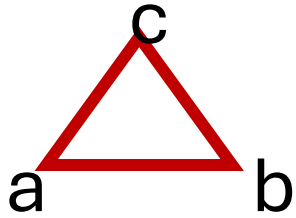
Defect Triangle



Spinion

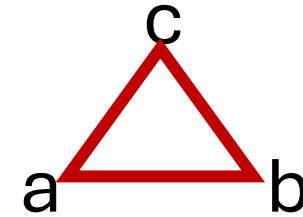
Dimer covering C resulting in
 defect triangle and spinion

Perturbed Hamiltonian of the Defect Triangle



Original Hamiltonian: H

$$H_{\text{orig}} = X_a X_b + Y_a Y_b + Z_a Z_b + \\ X_b X_c + Y_b Y_c + Z_b Z_c + \\ X_c X_a + Y_c Y_a + Z_c Z_a$$



Perturbed Hamiltonian: H_{pert}

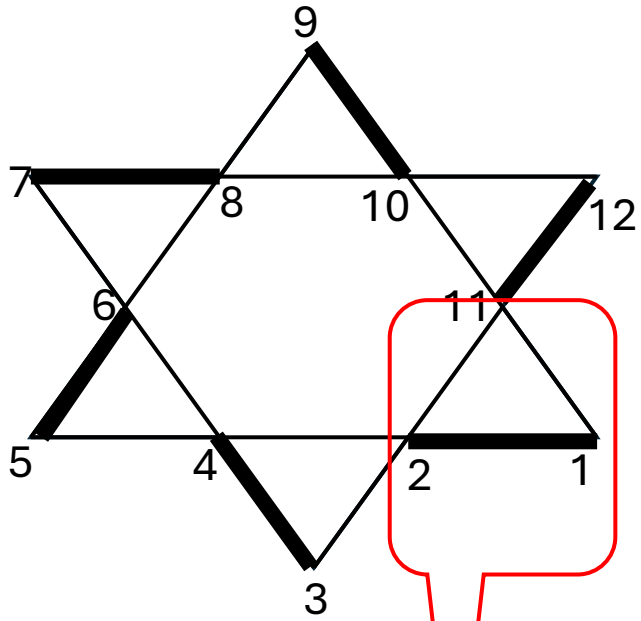
$$H_{\text{pert}} = (1+wt) (X_a X_b + Y_a Y_b + Z_a Z_b) + \\ (1+wt)(X_b X_c + Y_b Y_c + Z_b Z_c) + \\ (1+wt) (X_c X_a + Y_c Y_a + Z_c Z_a)$$

where $wt \approx 0.5$ (WHY?)

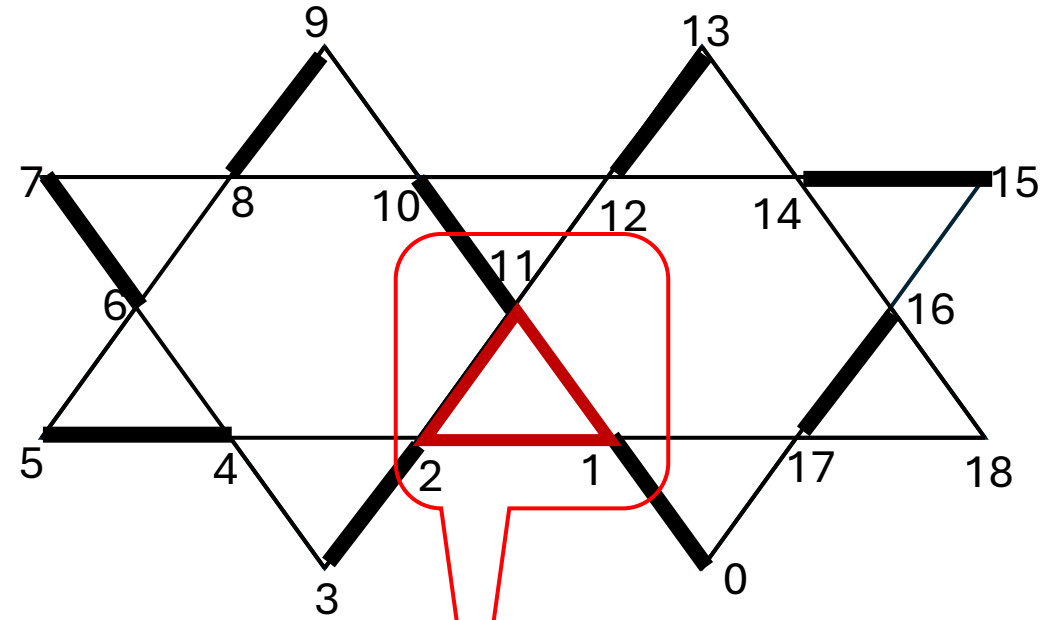
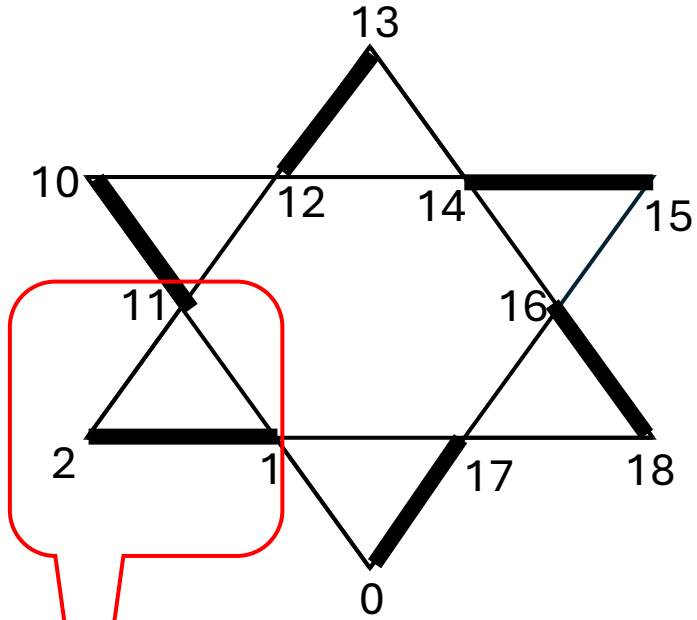
Calculating additional weight: wt

- $N \rightarrow$ Number of Kagome unit cells, mapped by the ansatz circuit, whose dimer covering creates the DEFECT TRIANGLE (DT)
- $K (\leq 3) \rightarrow$ Number of individual Kagome unit cells, each separately mapped by respective ansatz circuit, whose dimer covering places a dimer in DT
- $wt = N/(N + k)$

Example

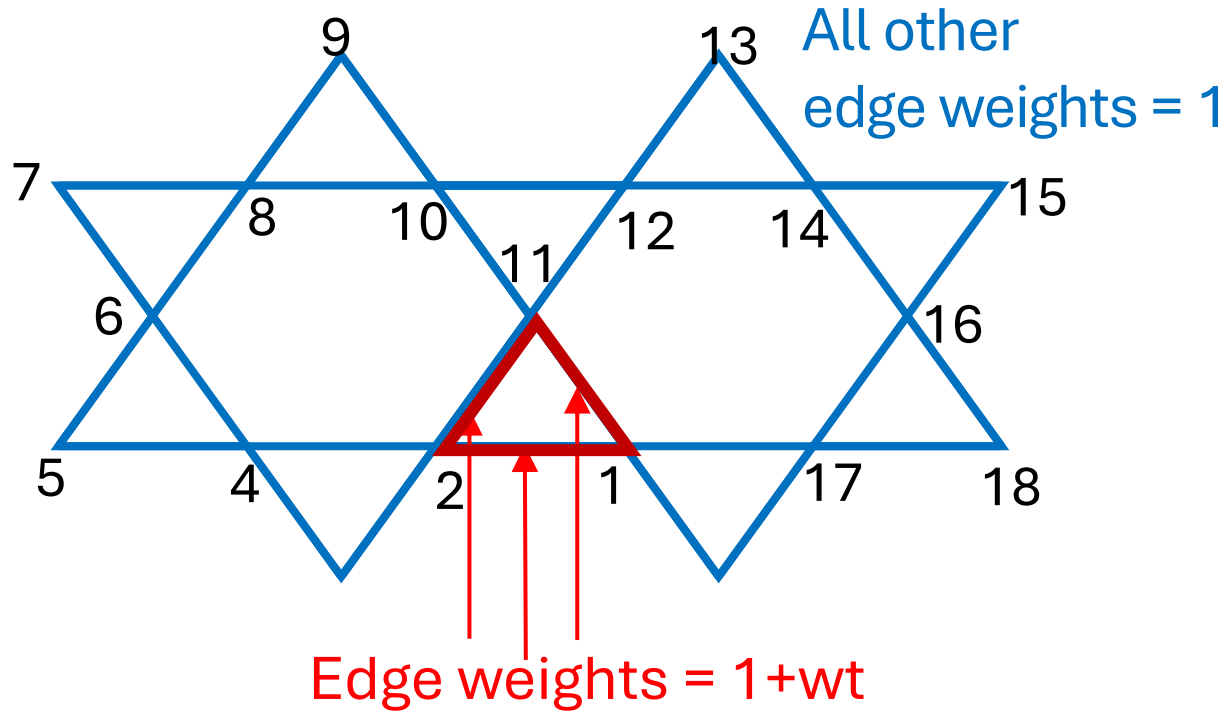


Dimer present in DT
 $k = 1 + 1 = 2$



Dimer absent in DT
 $N = 2$

Example (contd...)



$U = \{ [0,1], [2,3], [3,4], [2,4], [4,6], [4,5], [5,6], [6,7], [6,8], [7,8], [8,9], [9,10], [8,10], [10,11], [11,12], [10,12], [12,13], [13,14], [12,14], [14,15], [15,16], [14,1], [16,17], [17,1], [16,18], [17,0], [17,1] \}$

weight = 1

$S = \{ [1,2], [1,11], [2,11] \}$

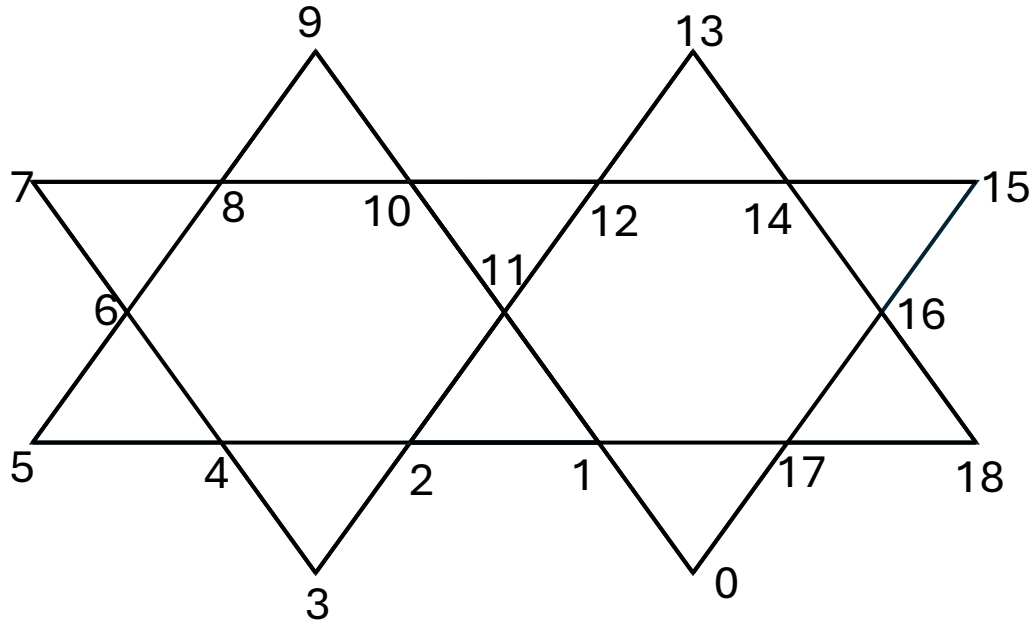
weight = 1+wt

$$H_{\text{pert}} = \sum_{[i,j] \in U} X_i X_j + Y_i Y_j + Z_i Z_j +$$

$$(1 + wt) \sum_{[i,j] \in S} X_i X_j + Y_i Y_j + Z_i Z_j$$

← H_{pert} : Perturbed Hamiltonian

Example (contd...)

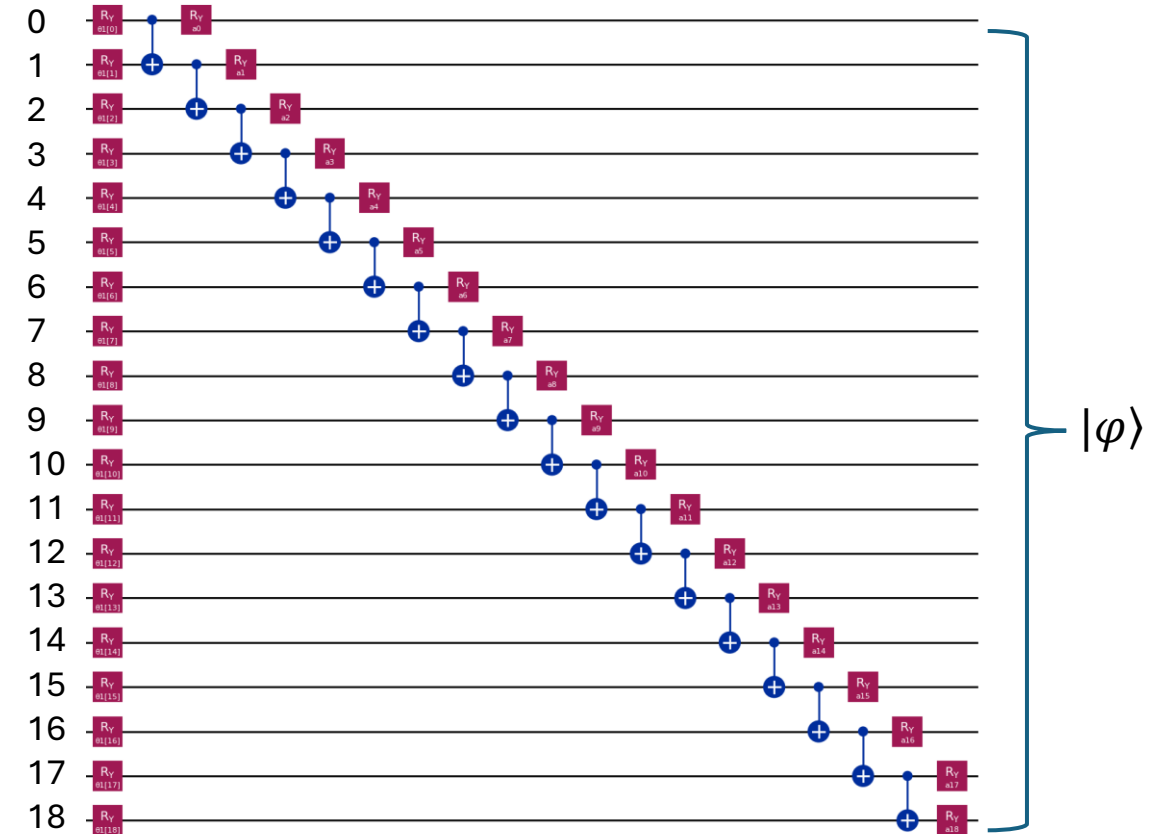


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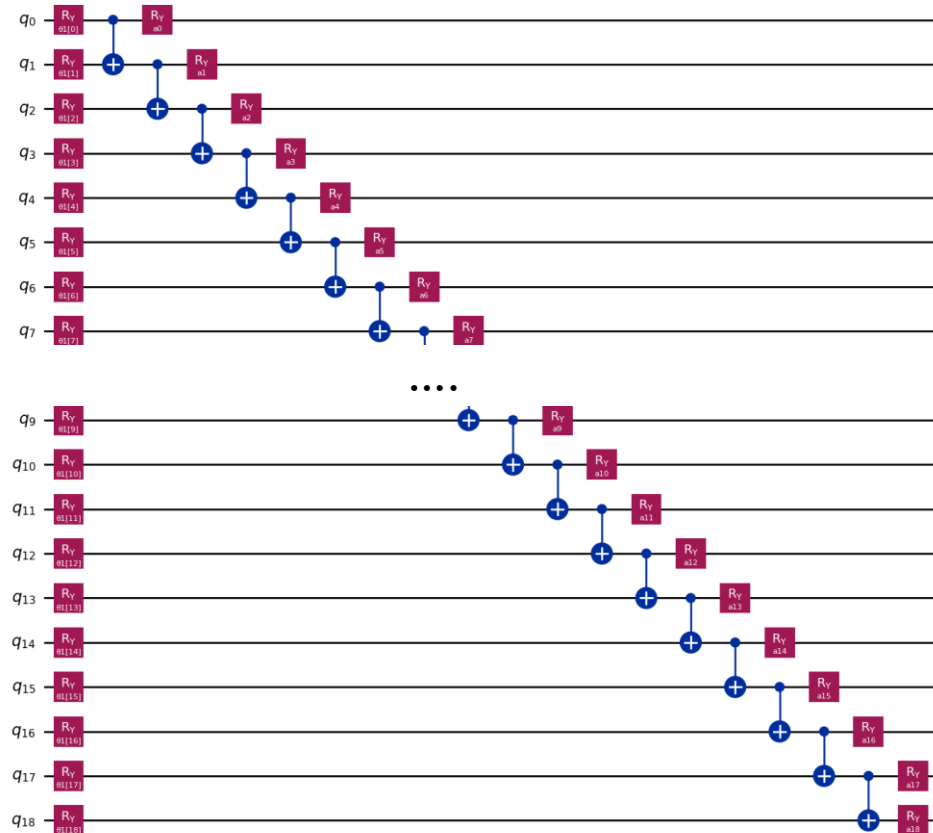


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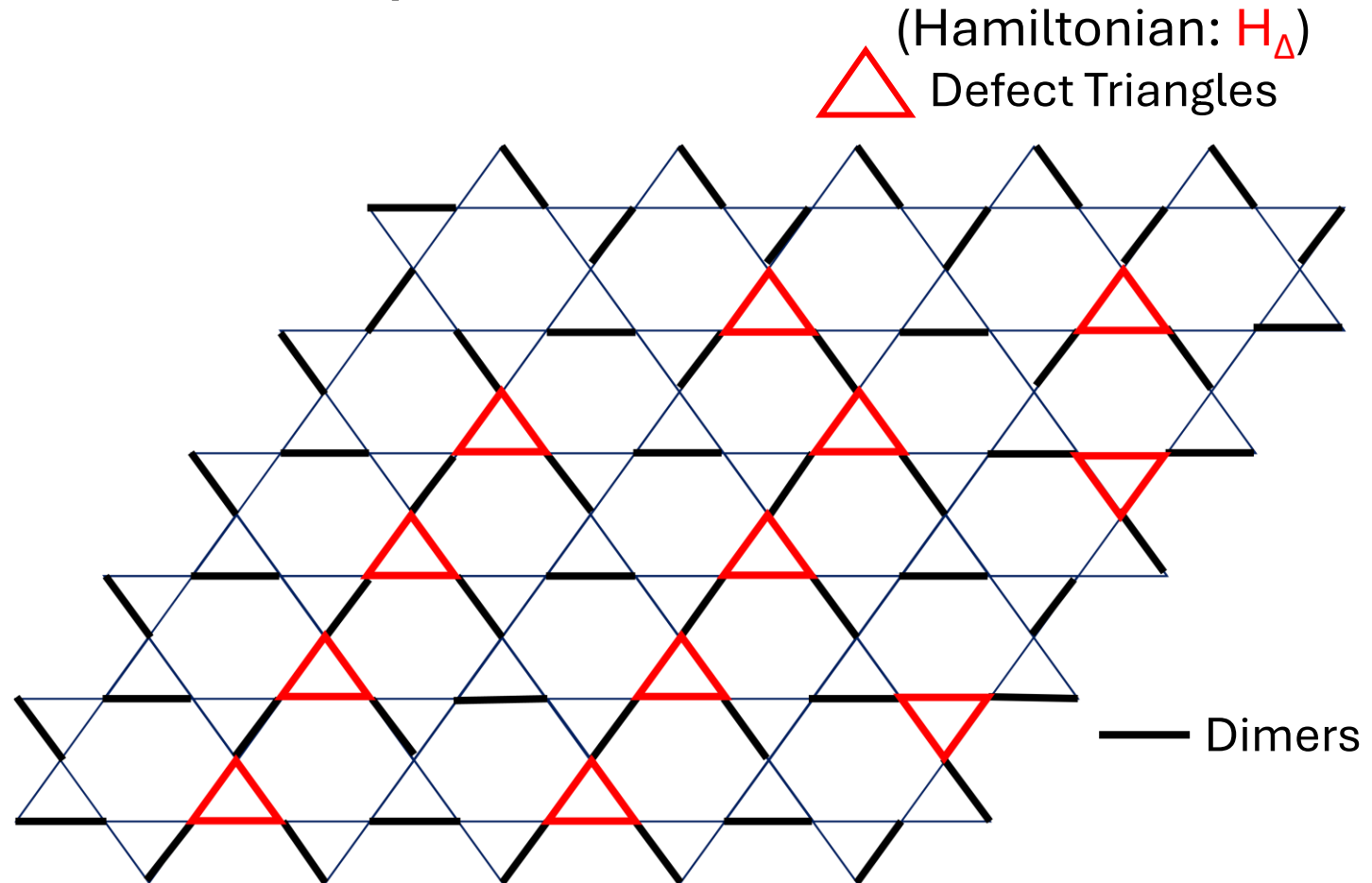
With perturbed Hamiltonian same ansatz lowers the GSE error to 0.9% ($\ll 6.7\%$)

Modified (new) proposal:

To quantum compute: $\min_{\varphi} \langle \varphi | H_{pert} | \varphi \rangle$



100x100 real amplitude ansatz: $|\varphi\rangle$



Hamiltonian perturbation on defect triangles

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