

# QB Metrics Documentation

## 1. System Metrics

- (a) **Number of electrons**  $\eta$
- (b) **Number of natural orbitals**  $N_{\text{nao}}$
- (c) **Number of qubits**  $n$
- (d) **Log FCI Size**  $\log_{10} \left( \binom{N}{N_{\uparrow}} \binom{N}{N_{\downarrow}} \right)$

## 2. One-norm

$$\lambda(H) = \sum_{ij} |h_{ij}^{(1)}| + \frac{1}{2} \sum_{\ell=1}^L |\lambda_{\ell}| \left( \sum_{pq} |g_{pq}^{(\ell)}| \right)^2 \quad (1)$$

## 3. Double Factorization Metrics

- (a) **Rank**  $L$
- (b) **Eigenvalues**  $\{\lambda_{\ell}\}_{\ell=1}^L$

## 4. Hypergraph Metrics

Let  $G_{\text{Interaction}}(H) = (V, E)$  where  $V = [n]$  for an  $n$ -qubit Hamiltonian  $H$  where the edge set contains hyperedges  $e_i = (i_1, \dots, i_{k(i)}) \in E$  where  $i_1, \dots, i_{k(i)} \in \{X, Y, Z\}$  are all those non-identity Pauli string terms. The graph has edge weights  $w(e) = h_e$  where  $h_e$  is the coefficient of Pauli string  $e \in E$  where  $H = \sum_{e \in E} h_e P_e$ . We take statistics (max, min, mean, std. dev.) on edge order (Pauli weight), vertex degree, and edge weights.

- (a) **Number of Pauli Strings**

$$|E| = \left| \left\{ P : |h_P| > 0, H = \sum_P h_P P \right\} \right| \quad (2)$$

- (b) **Edge Order**

$$\text{ord}(e_i) = k(i) \quad (3)$$

- (c) **Vertex Degree**

$$\deg(v) = |\{v \in e : e \in E\}| \quad (4)$$

## 5. Other Graphs

- (a) **Frustration Graph**  $G_{\text{frus}}$
- (b) **Fermionic Graph**  $G_F = (V = [N], E = E_F)$  comes from which terms appear in the one-body terms of the Hamiltonian  $\sum_{ij} h_{ij}^{(1)} \hat{a}_i^{\dagger} \hat{a}_j$ , two orbital are connected by an edge  $e = (i, j) \in E_F$  if  $|h_{ij}^{(1)}| > 0$

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