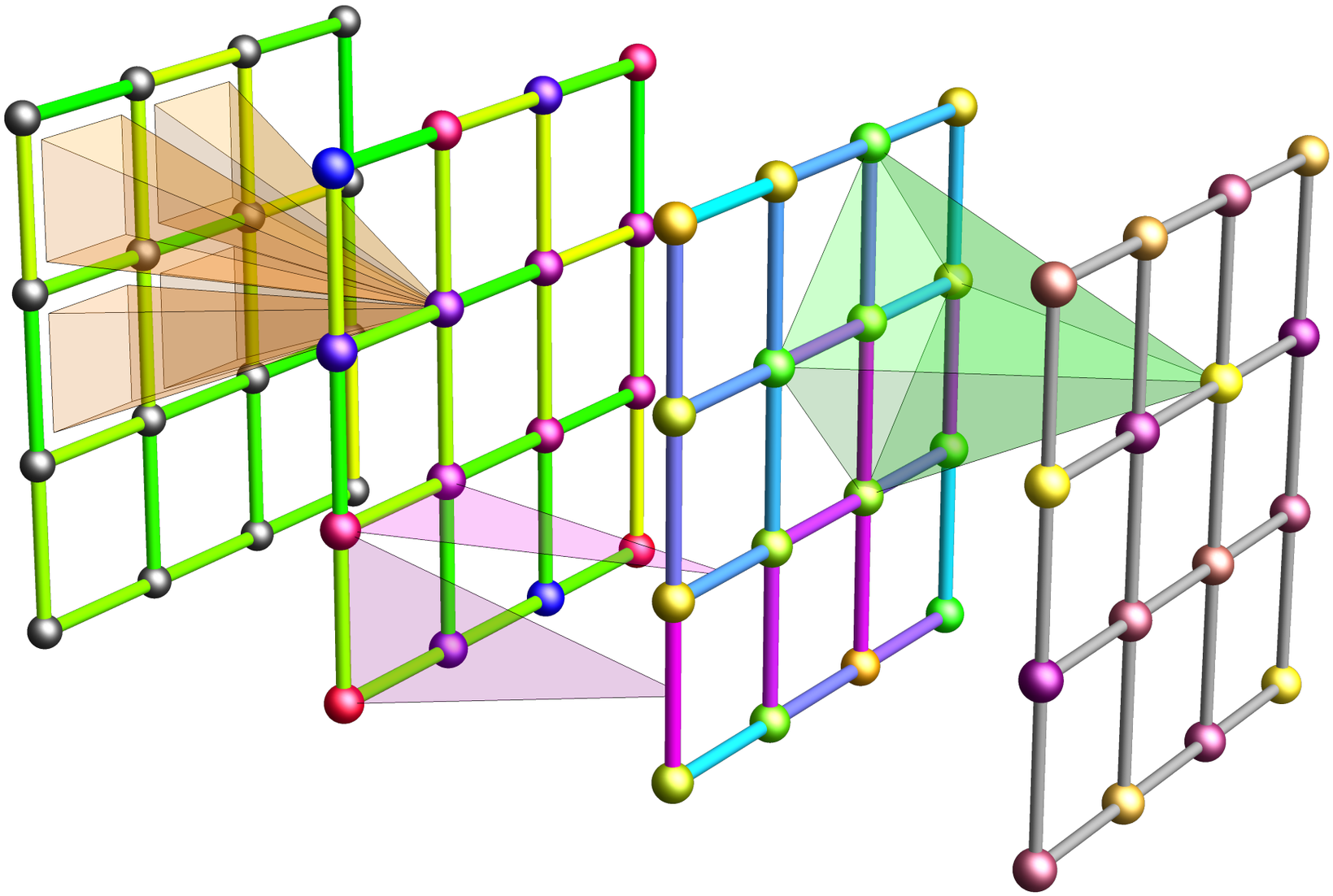
# Gauge-Equivariant GNN for Lattice Gauge Theories

arXiv:2604.20797



Ali Rayat, Yaohang Li, **Gia-Wei Chern**

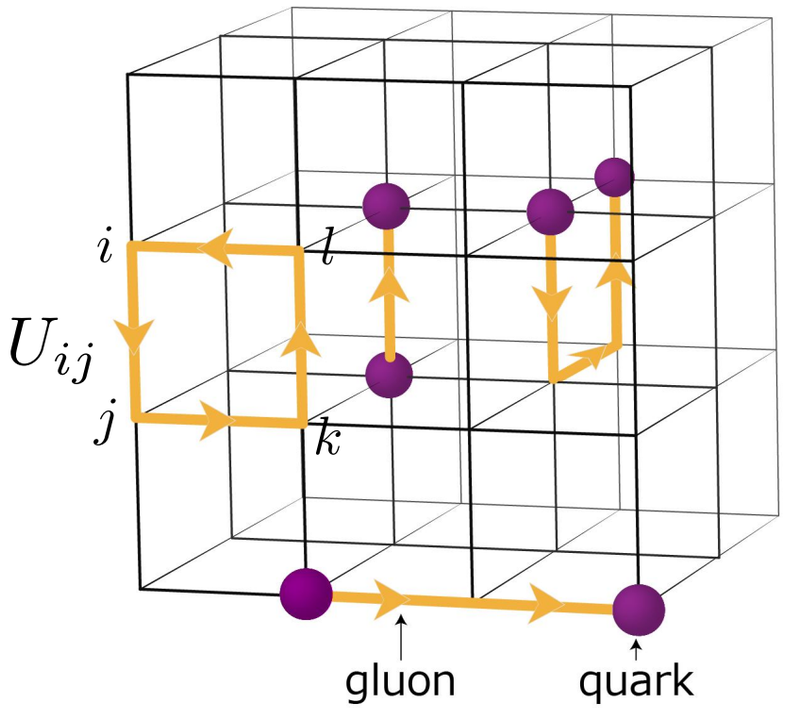
Digital Twins for Nuclear and Particle Physics
Trento 5/12/2026

U.S. DEPARTMENT OF ENERGY

# ML model for Lattice Gauge systems

- "Structure-property" mapping: $U_{ij} \in \mathrm{SU(N)}$

$$\mathcal{F}_{\boldsymbol{\theta}}: \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$



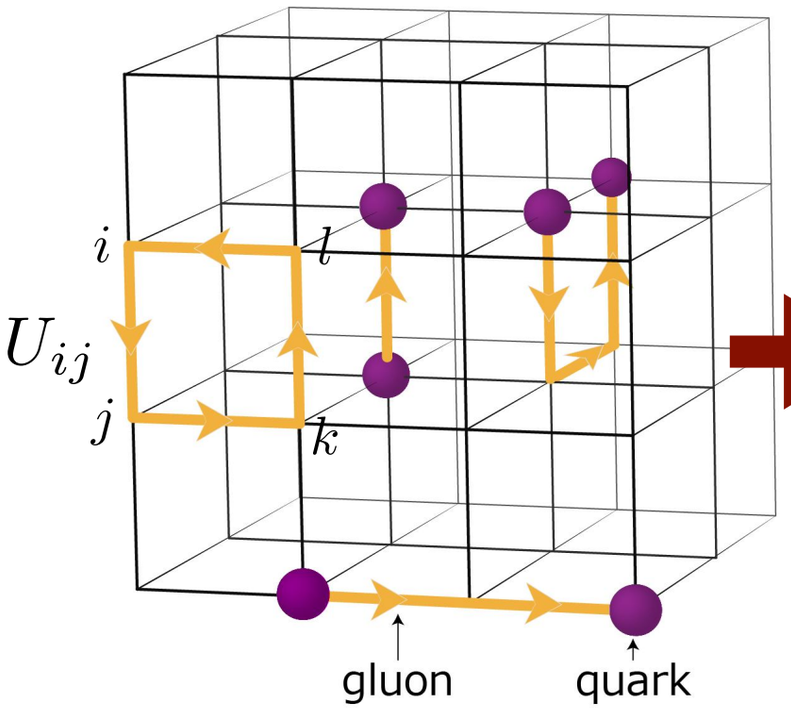

- Wilson action
- System energy
- Topological change
- 2-point correlates

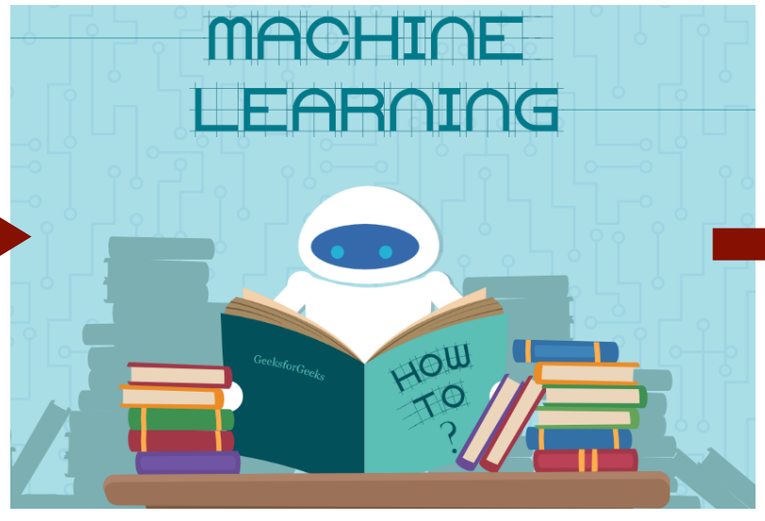
...

# ML model for Lattice Gauge systems

- "Structure-property" mapping: $U_{ij} \in \mathrm{SU(N)}$

$$\mathcal{F}_{\boldsymbol{\theta}}: \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$



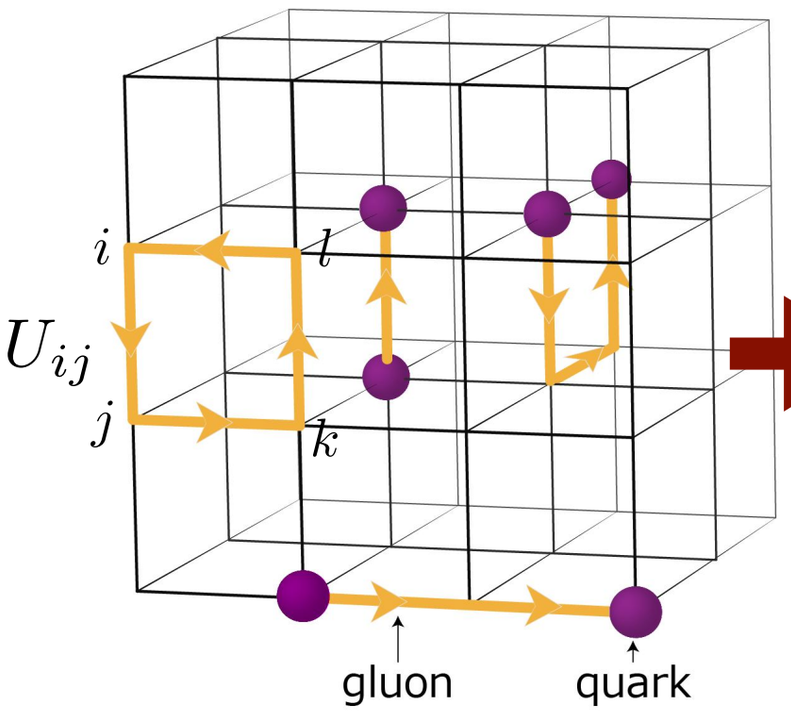

- Wilson action
- System energy
- Topological change
- 2-point correlates

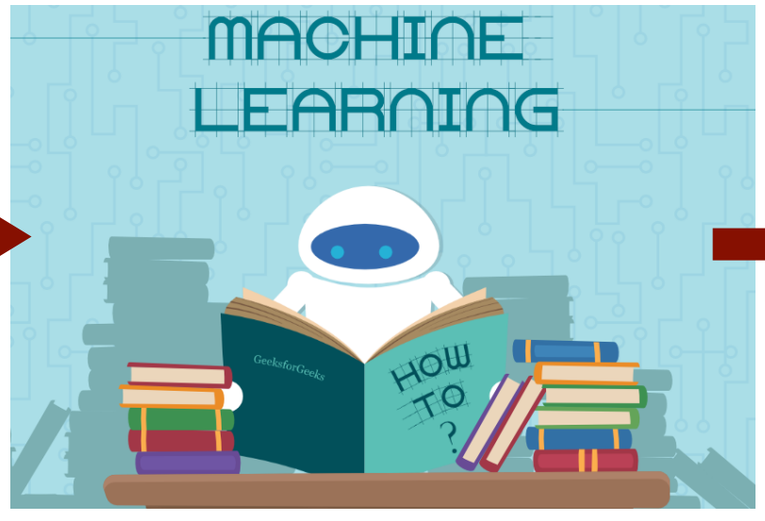
...

# ML model for Lattice Gauge systems

- "Structure-property" mapping: $U_{ij} \in \mathrm{SU(N)}$

$$\mathcal{F}_{\boldsymbol{\theta}}: \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$




- Wilson action
- System energy
- Topological change
- 2-point correlates

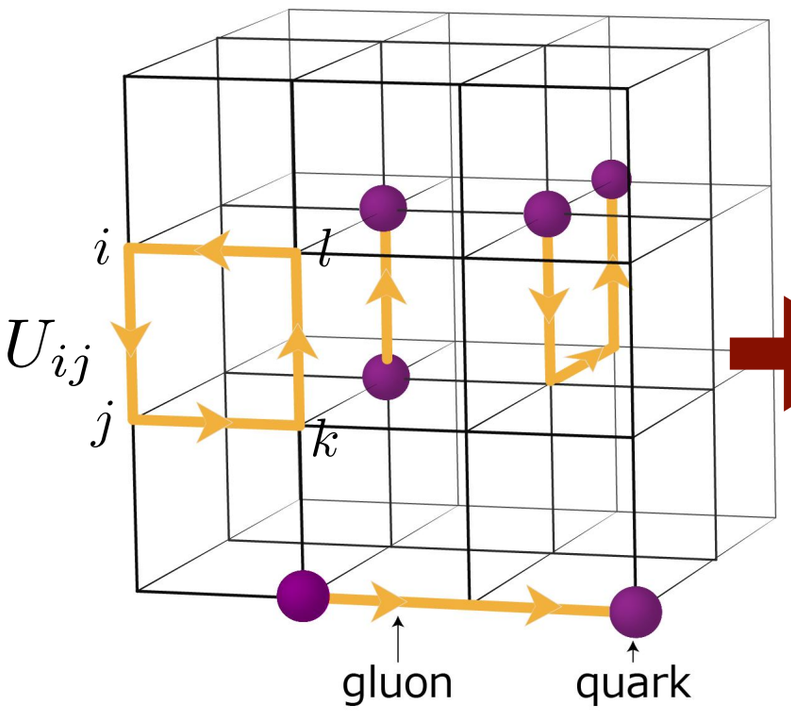
...

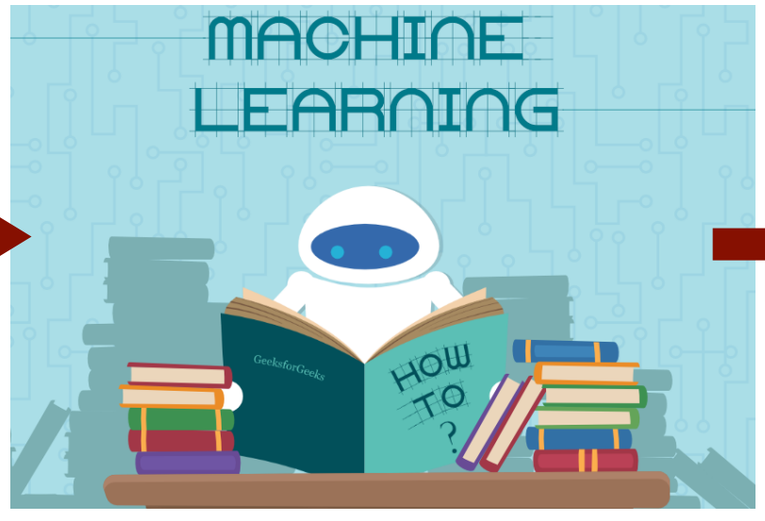
- Gauge Symmetry: $U_{ij} \Rightarrow g_i U_{ij} g_j^{\dagger} \qquad g_i \in \mathrm{SU(N)}$

# ML model for Lattice Gauge systems

- "Structure-property" mapping: $U_{ij} \in \mathrm{SU(N)}$

$$\mathcal{F}_{\boldsymbol{\theta}}: \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$




- Wilson action
- System energy
- Topological change
- 2-point correlates

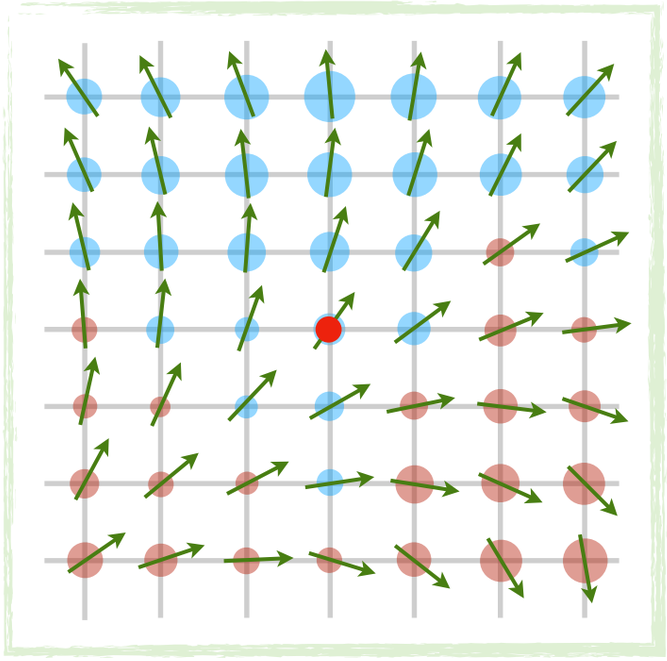
...

- Gauge Symmetry: $U_{ij} \Rightarrow g_i U_{ij} g_j^\dagger \qquad g_i \in \mathrm{SU(N)}$

How to incorporate gauge symmetry into ML model?

# Global symmetry in ML surrogate models

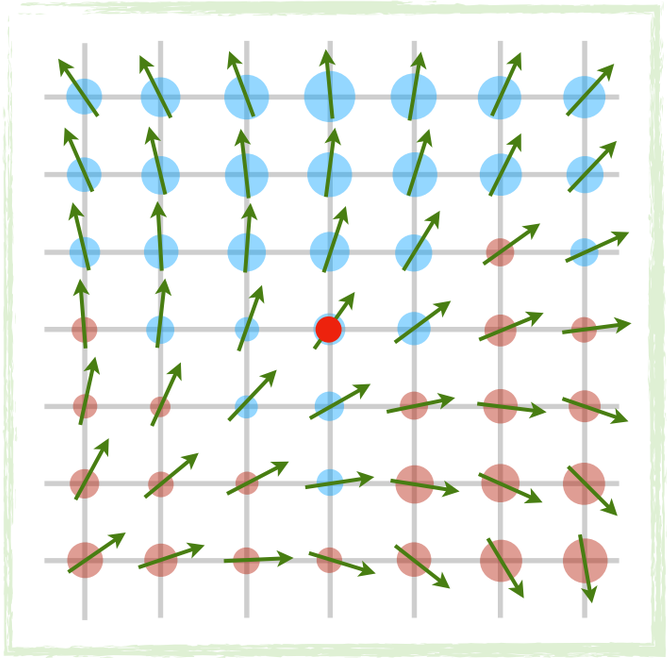
$\mathcal{C}_1$



$$\mathcal{F}_{\boldsymbol{\theta}}: \ \mathcal{C} \implies E$$

# Global symmetry in ML surrogate models

$\mathcal{C}_1$

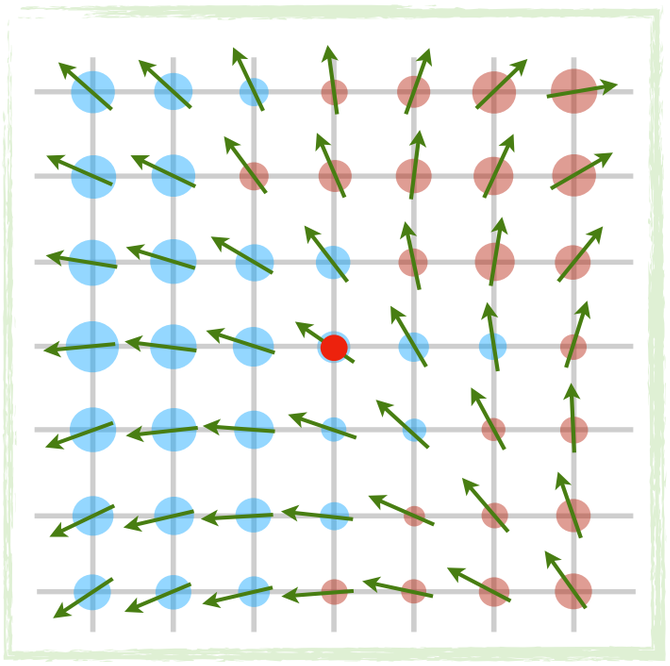


$$\mathcal{F}_{\boldsymbol{\theta}}: \ \mathcal{C} \implies E$$

90° rotation

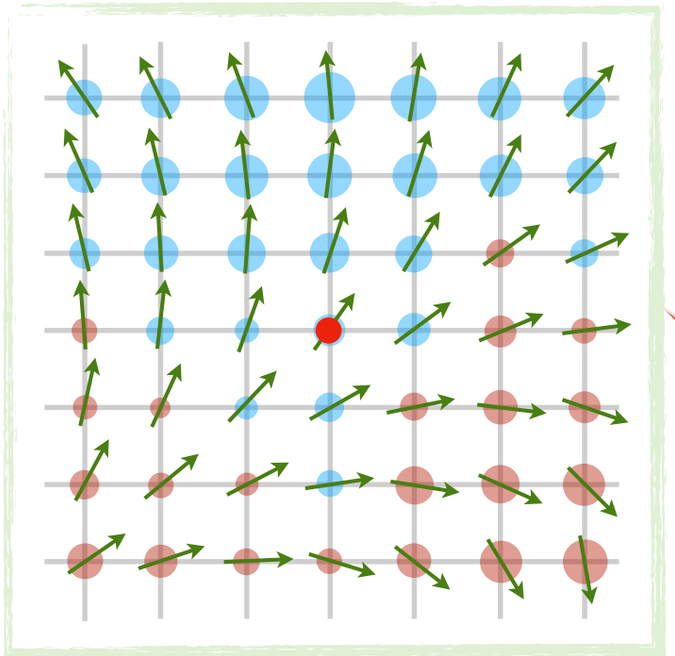


$\mathcal{C}_2$



# Global symmetry in ML surrogate models

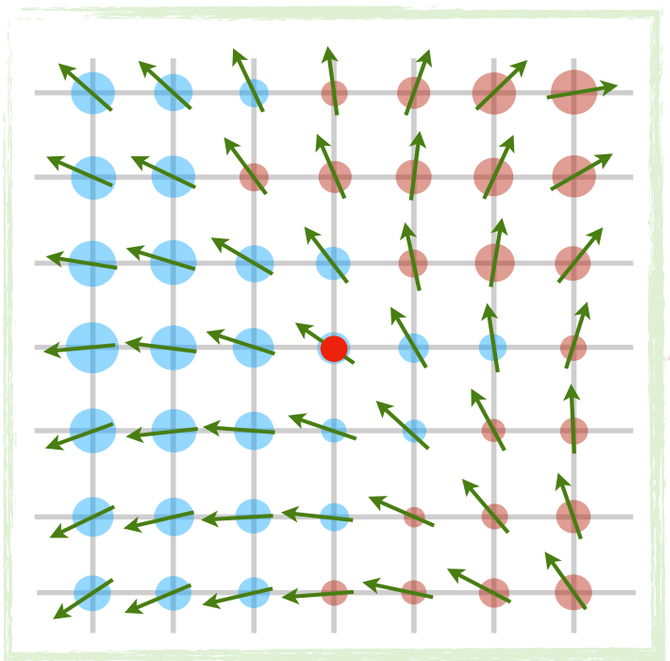
$\mathcal{C}_1$

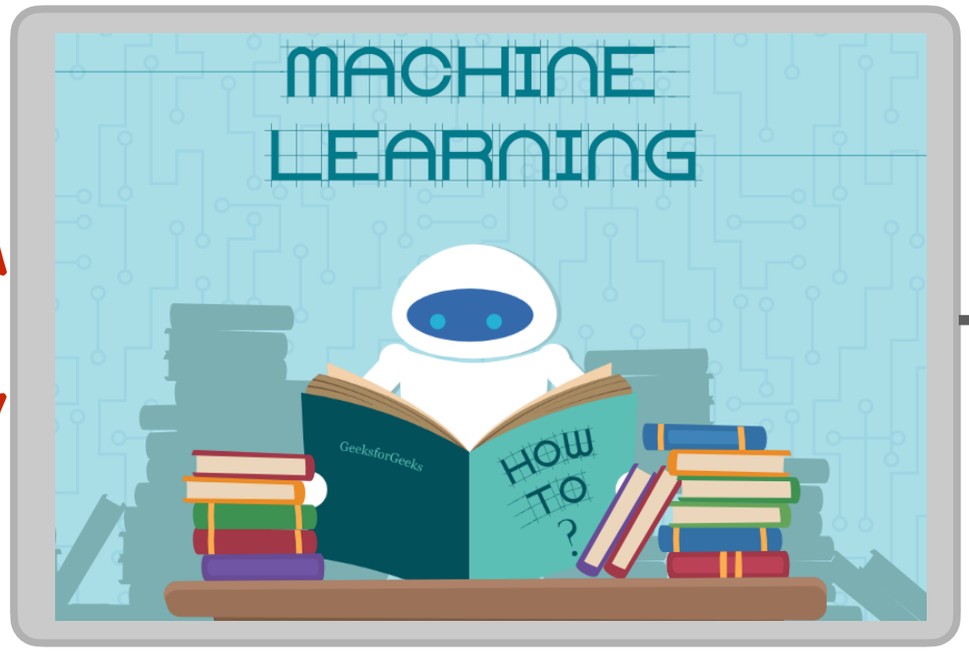


$$\mathcal{F}_{\boldsymbol{\theta}}: \ \mathcal{C} \implies E$$

90° rotation

$\mathcal{C}_2$

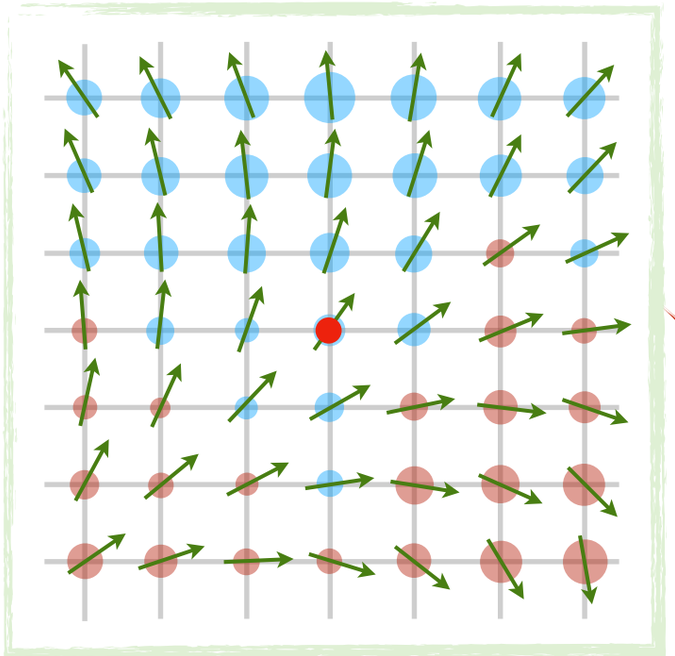





$E$

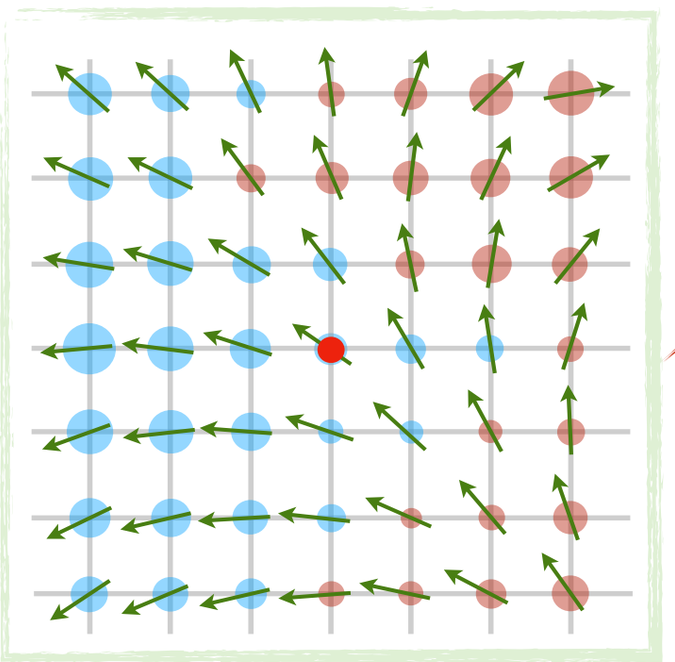
# Global symmetry in ML surrogate models

$\mathcal{C}_1$



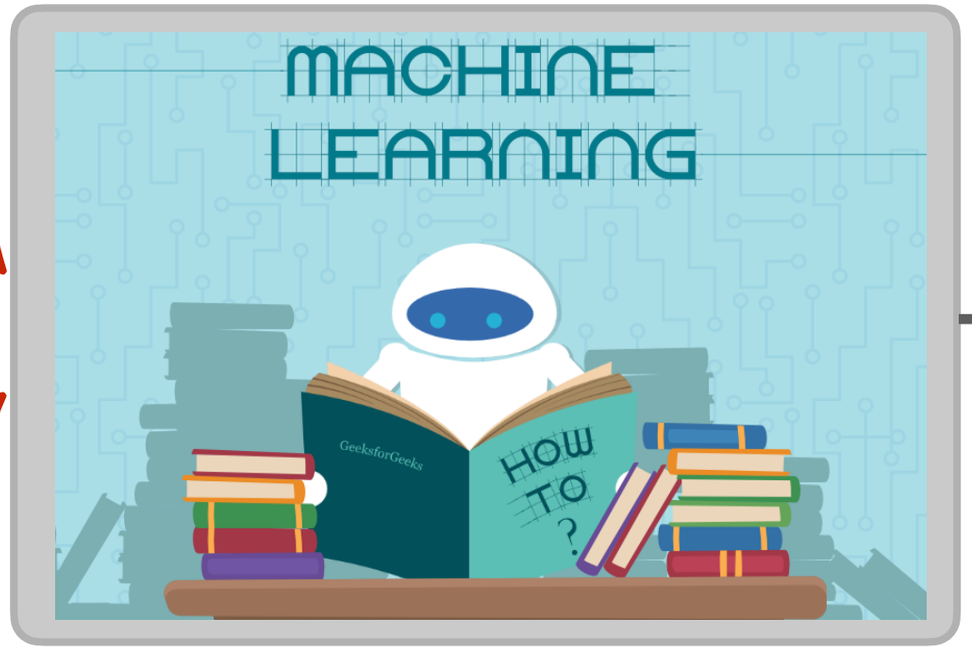
90° rotation

$\mathcal{C}_2$



$$\mathcal{F}_{\boldsymbol{\theta}}: \mathcal{C} \Longrightarrow E$$

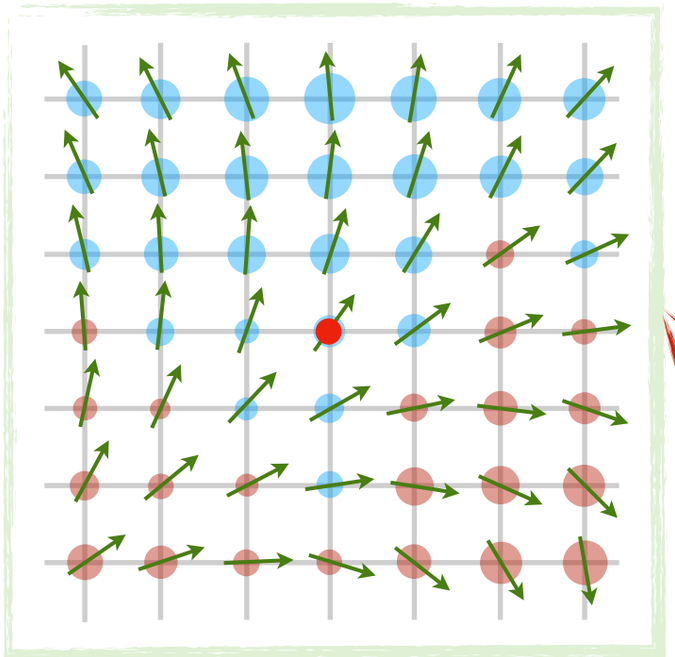
$$\overset{?}{E_1 = E_2}$$




$E$

# Global symmetry in ML surrogate models

$\mathcal{C}_1$

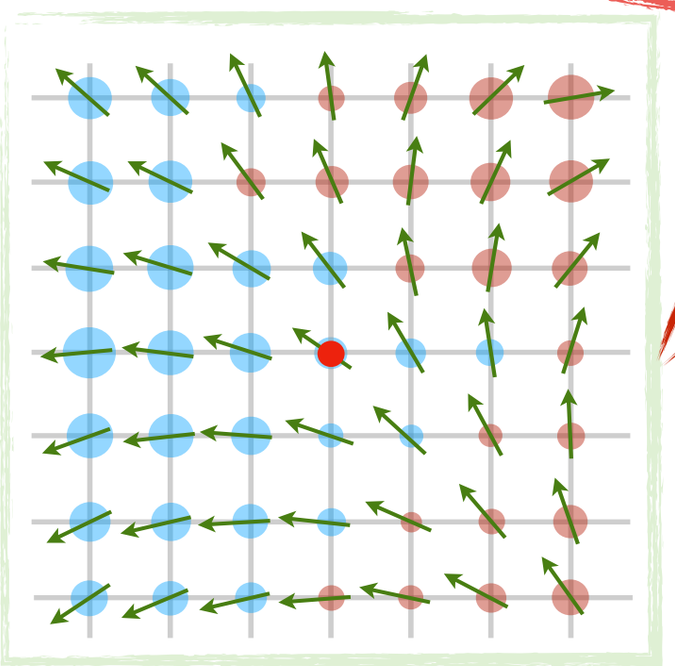


$\mathcal{F}_{\boldsymbol{\theta}}: \mathcal{C} \Longrightarrow E$

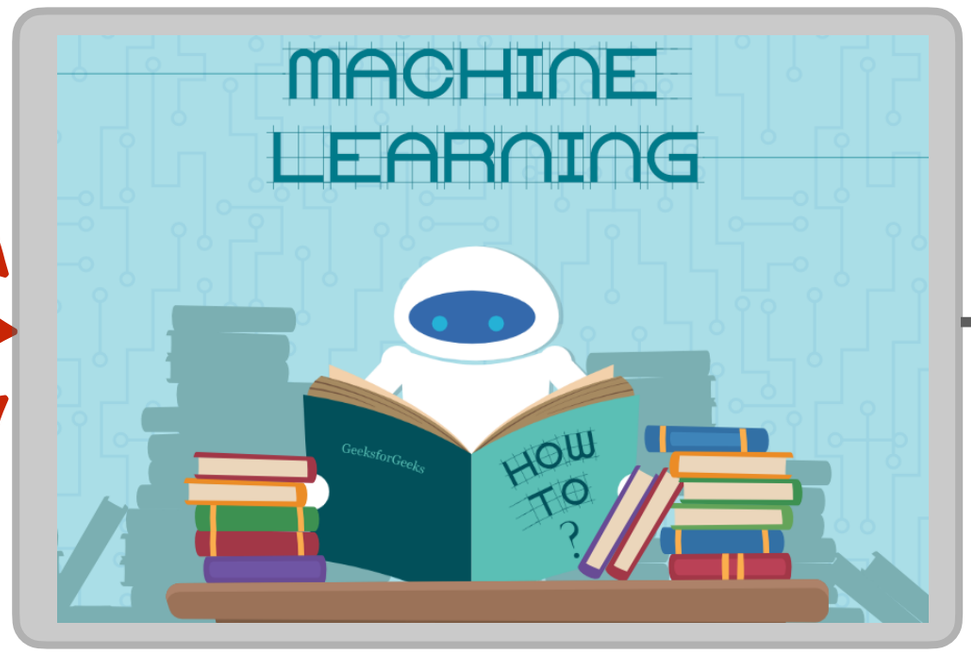
? $E_1 = E_2$

90° rotation

$\mathcal{C}_2$



$G_1, G_2, G_3, \cdots$

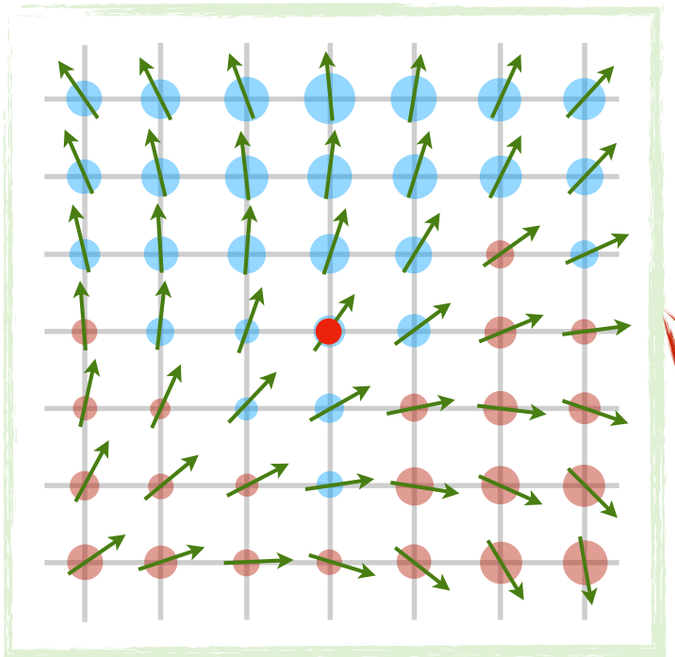



$E$

- Feature variables which are already invariant under symmetry transformations

# Global symmetry in ML surrogate models

$\mathcal{C}_1$

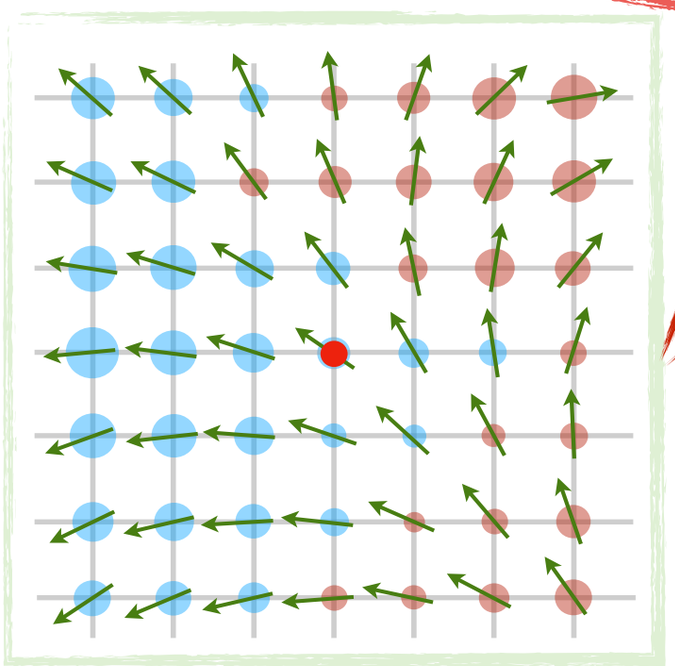


$\mathcal{F}_{\boldsymbol{\theta}}: \mathcal{C} \Longrightarrow E$

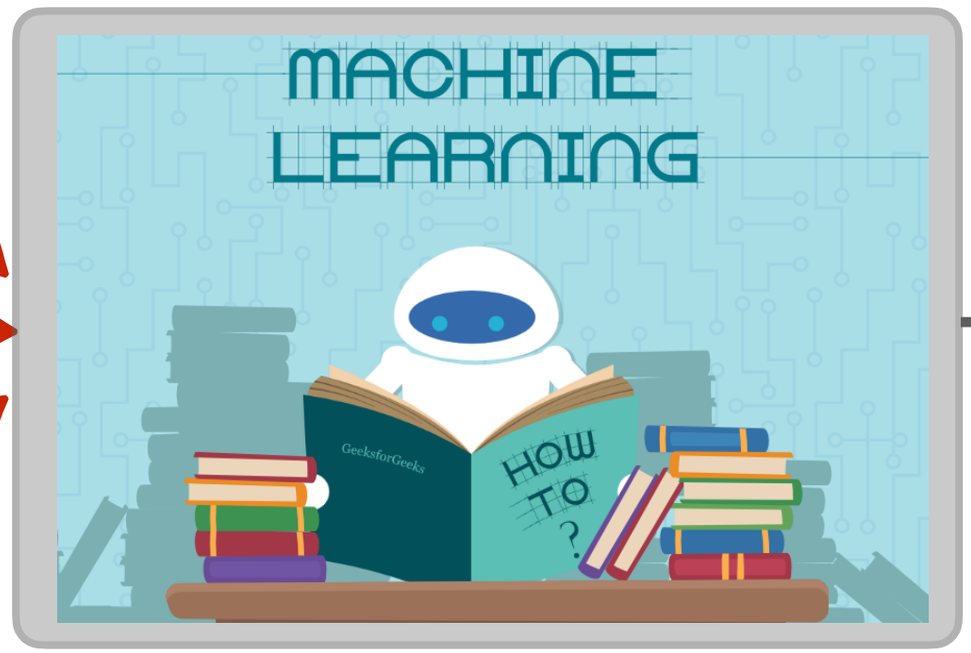
$$\overset{?}{E_1 = E_2}$$

90° rotation

$\mathcal{C}_2$



$G_1, G_2, G_3, \cdots$



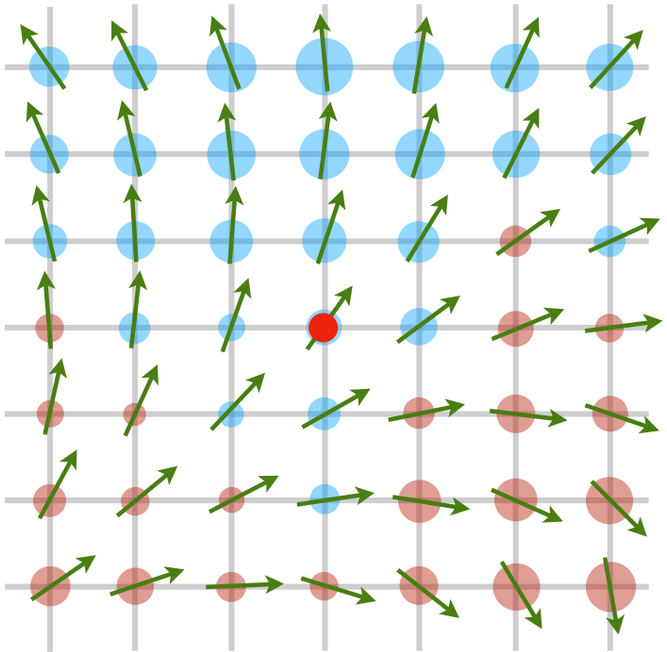

$E$

- Feature variables which are already invariant under symmetry transformations
- Feature Engineering / Symmetry-Aware Descriptor often combined with simple MLP

# Equivariant Neural Network

- Example: Discrete D4 point group

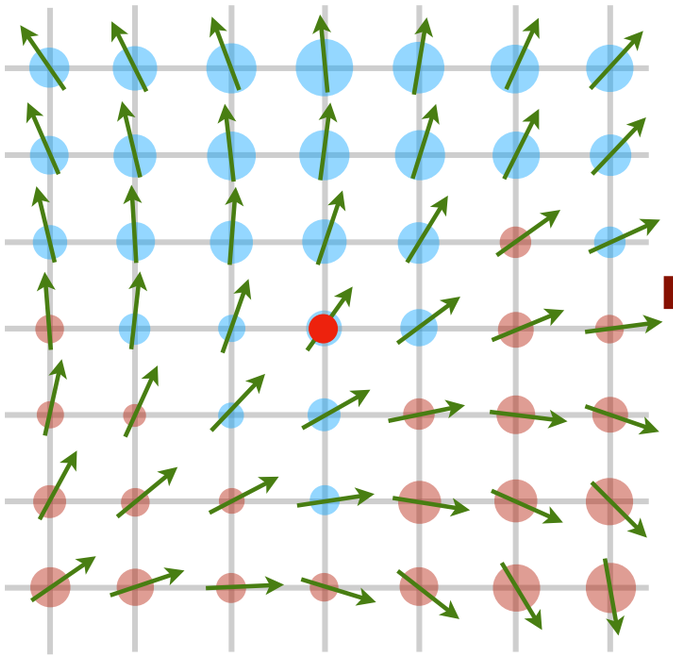
$$\mathcal{F}_{\boldsymbol{\theta}} : \mathcal{C} \implies E$$

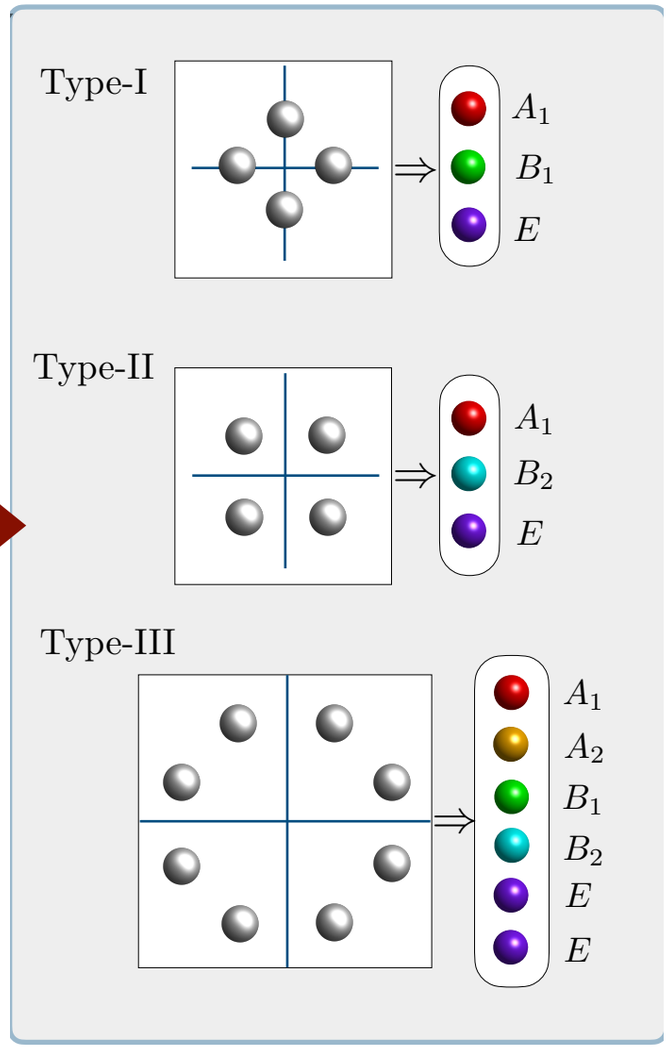


# Equivariant Neural Network

- Example: Discrete D4 point group

$$\mathcal{F}_{\boldsymbol{\theta}} : \mathcal{C} \Longrightarrow E$$

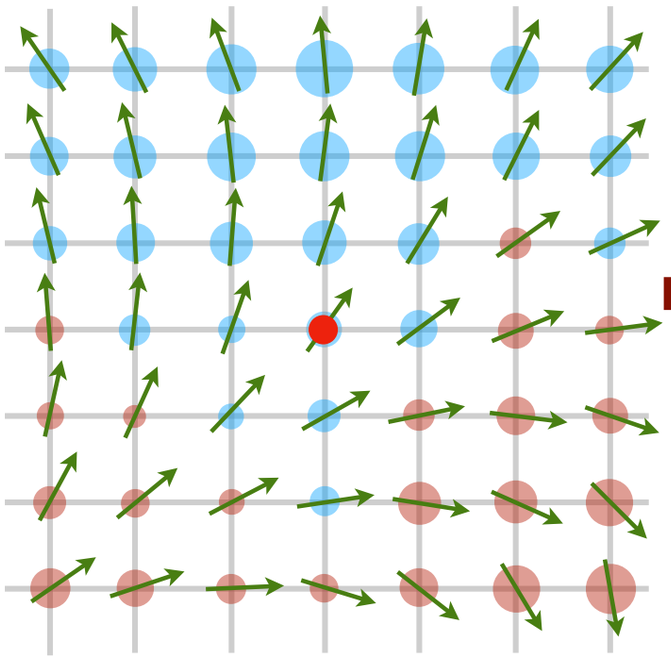


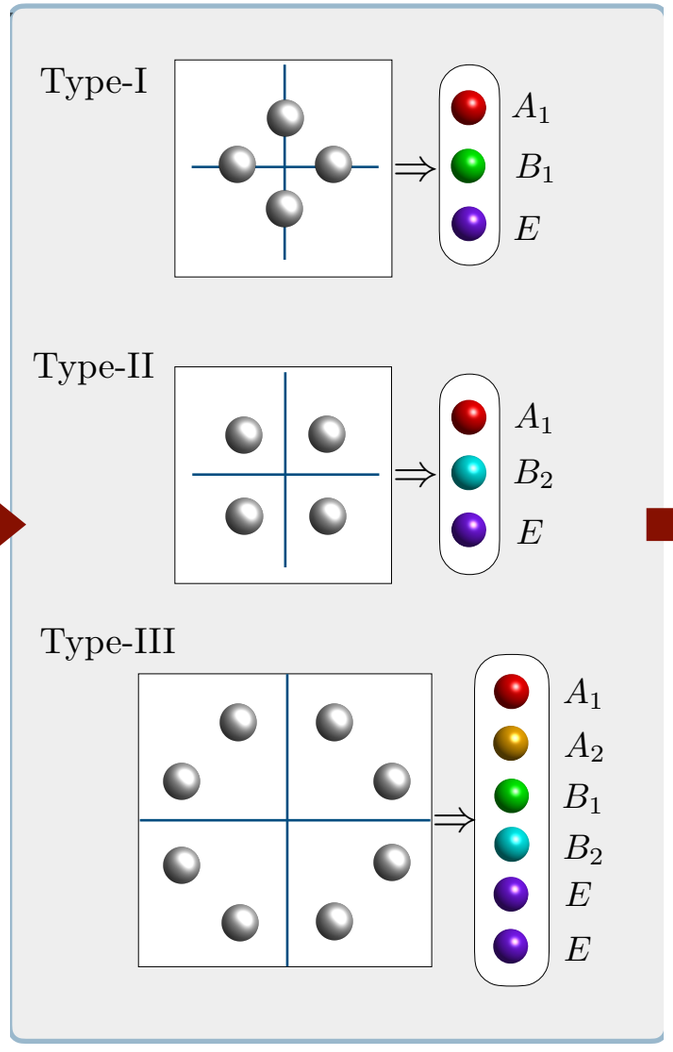


# Equivariant Neural Network

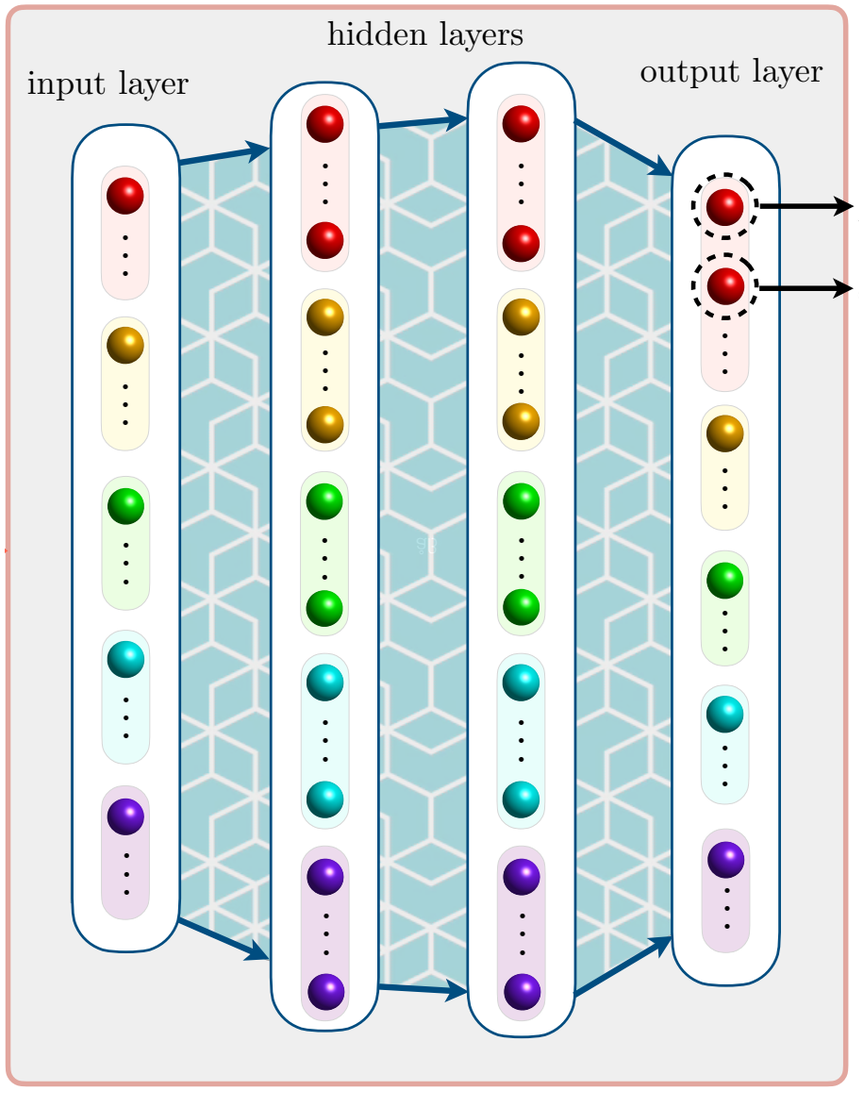
- Example: Discrete D4 point group

$$\mathcal{F}_{\boldsymbol{\theta}}: \mathcal{C} \Longrightarrow E$$





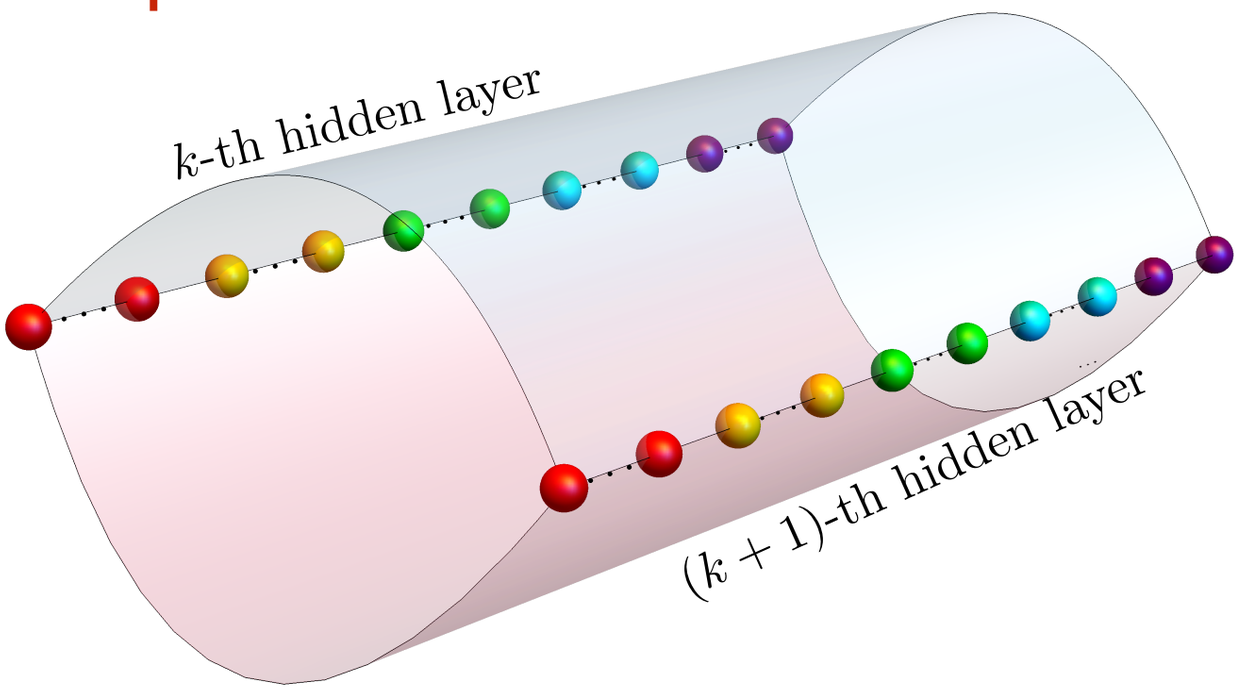

- Equivariant NN




- Each neuron (embedded features) belongs to a Irreducible Representation IR of the group:
  (A1, A2, B1, B2, E, …) for finite group, $\ell = 0, 1, 2, 3, \cdots$ for SO(3)

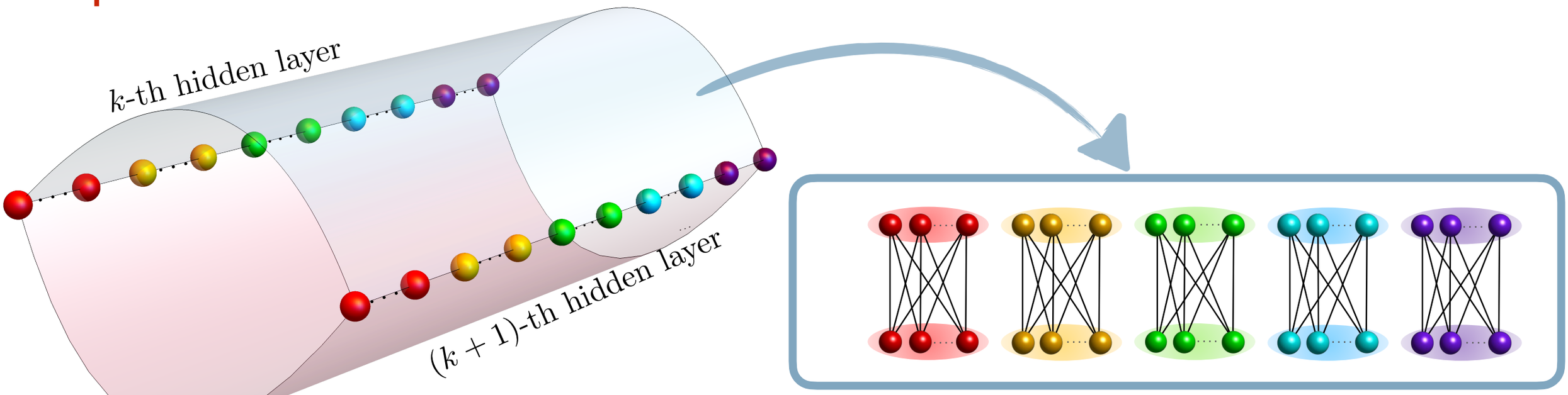
# Equivariant Neural Networks

## Implementations



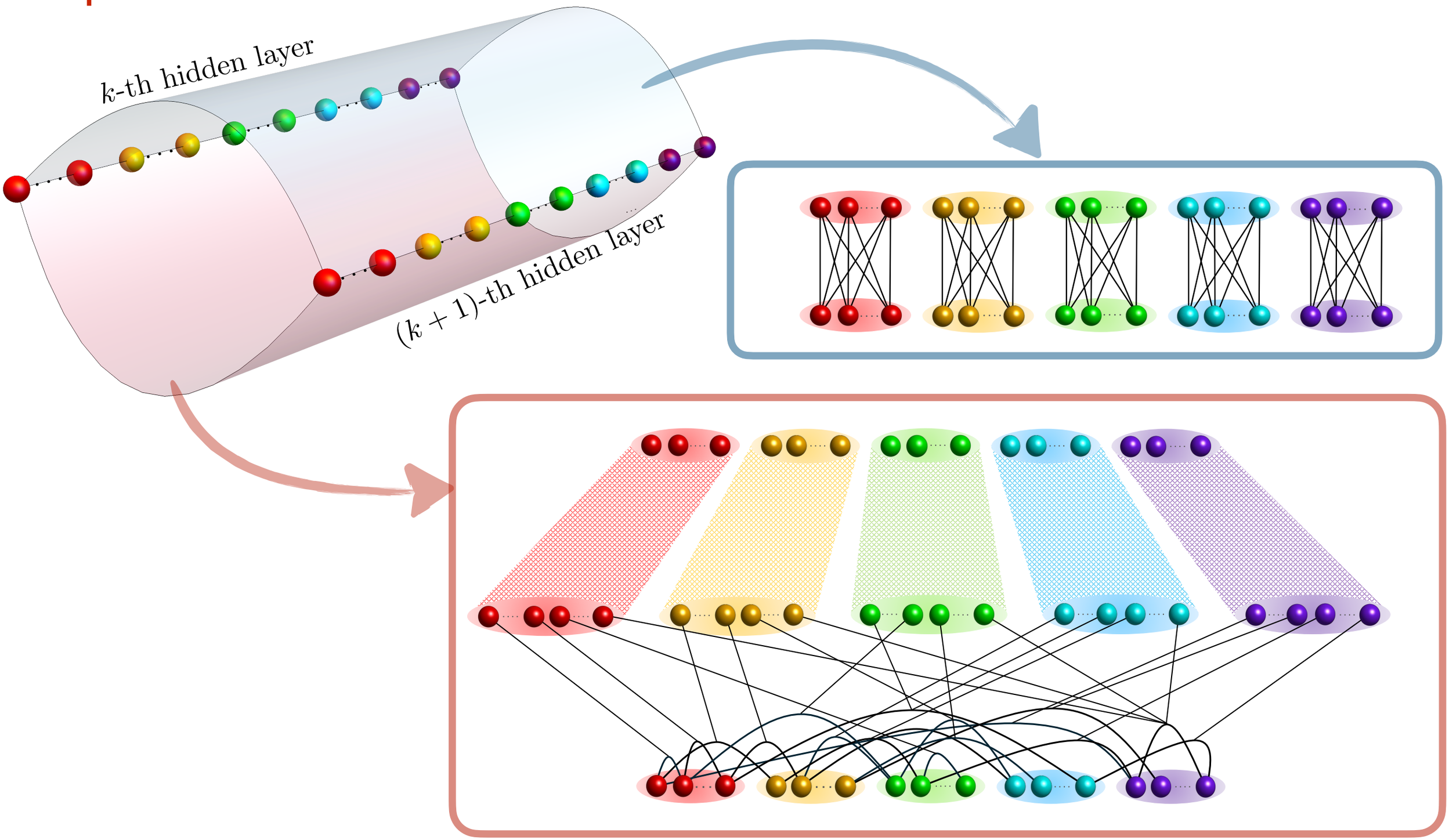
# Equivariant Neural Networks

## Implementations



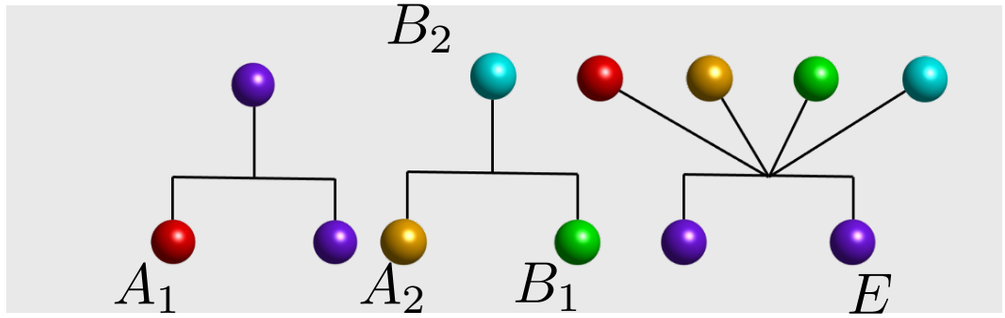
# Equivariant Neural Networks

## Implementations

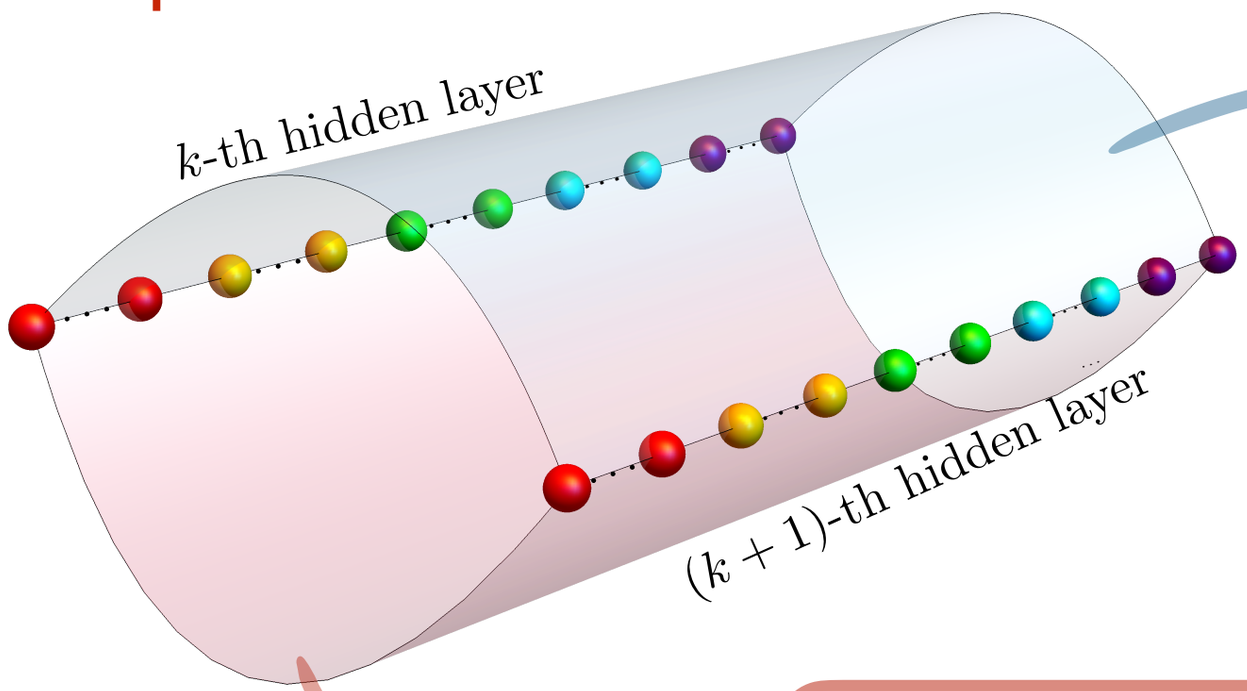


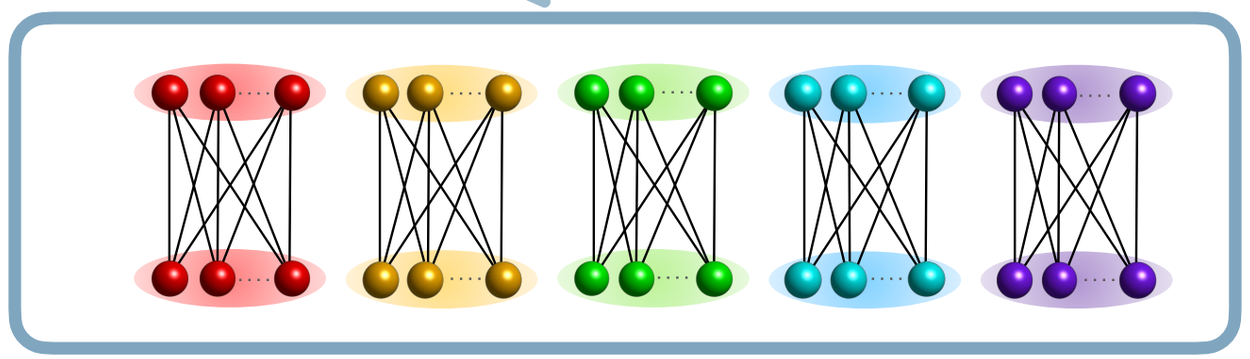
# Equivariant Neural Networks

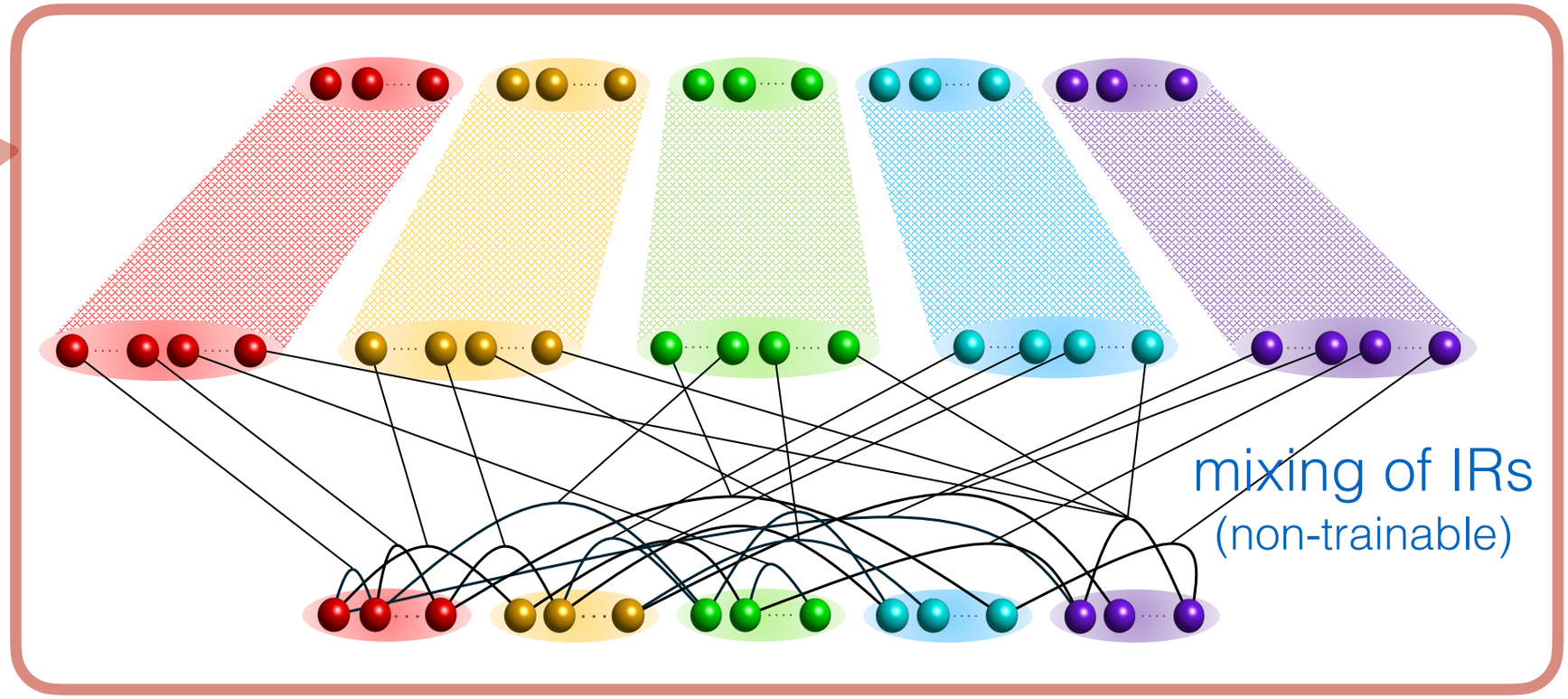
## Implementations




multiplication table of IRs

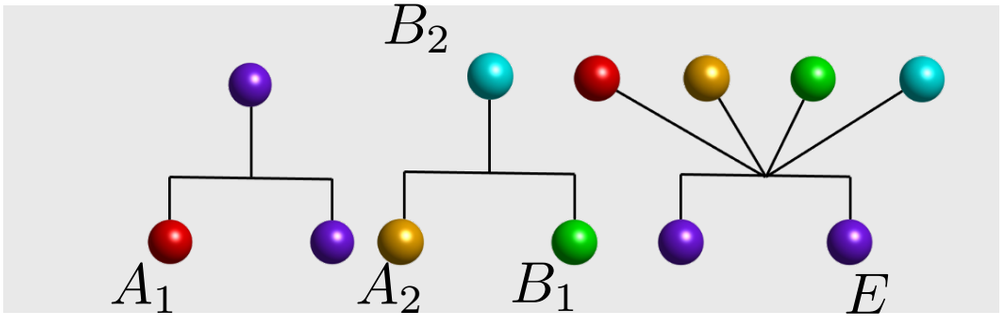


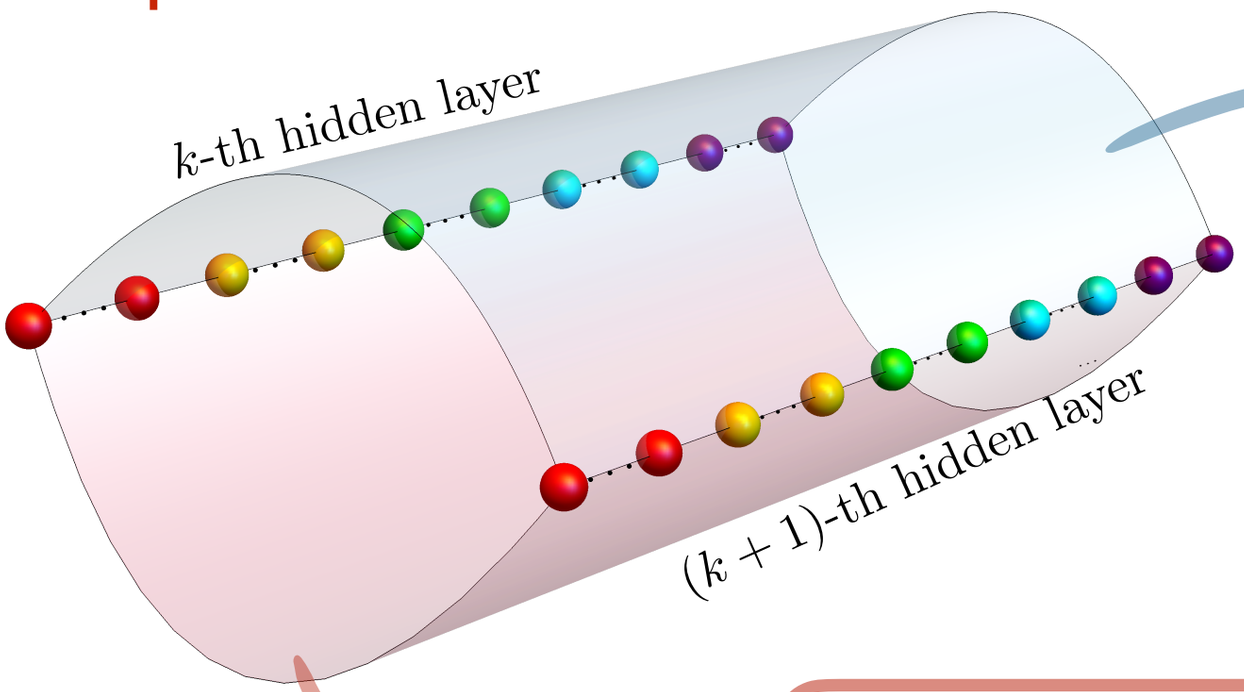


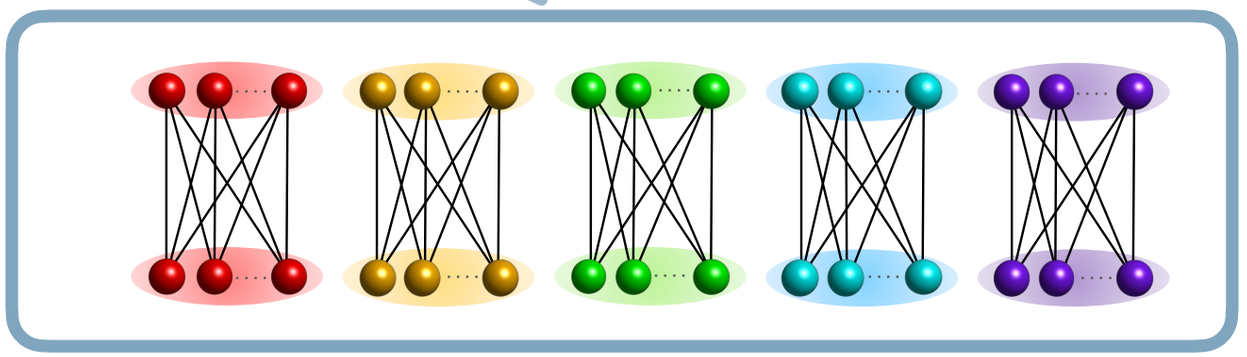
# Equivariant Neural Networks

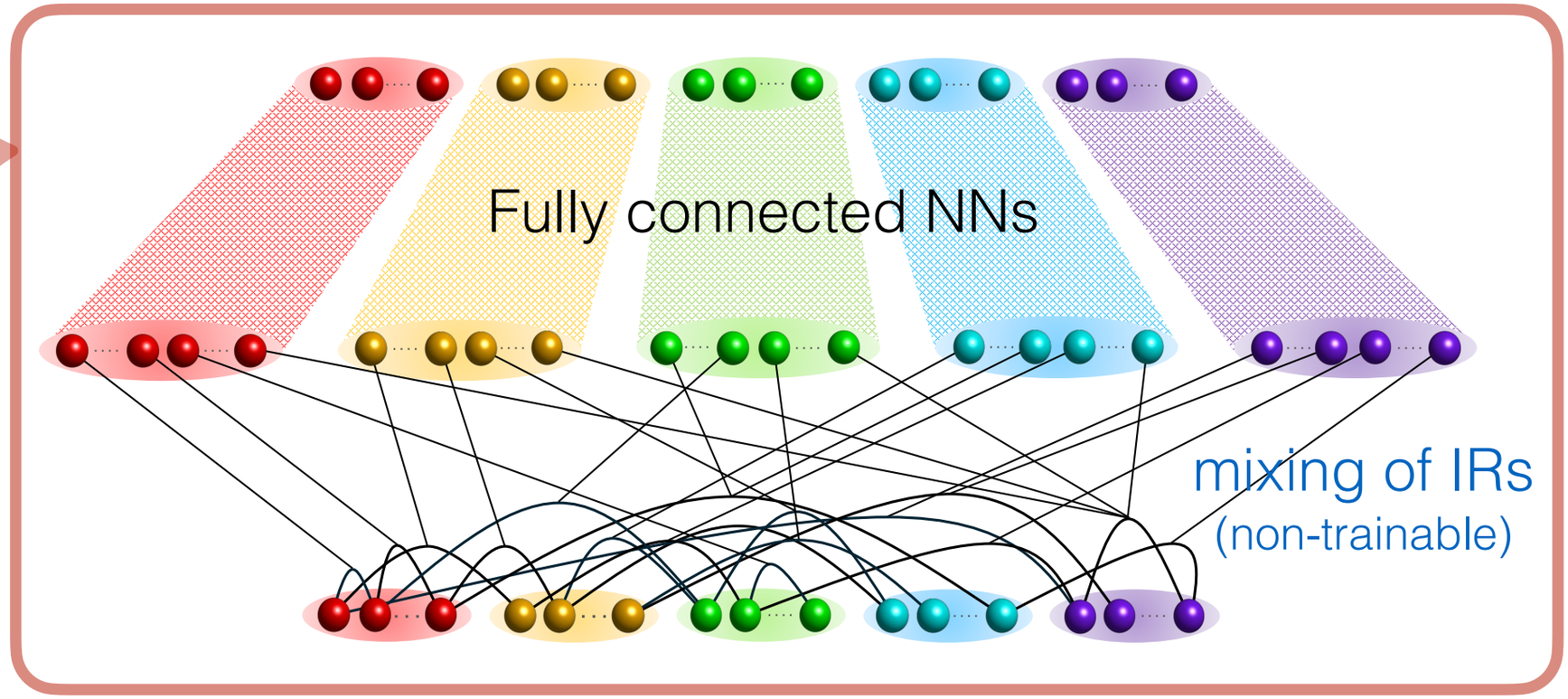
## Implementations




multiplication table of IRs

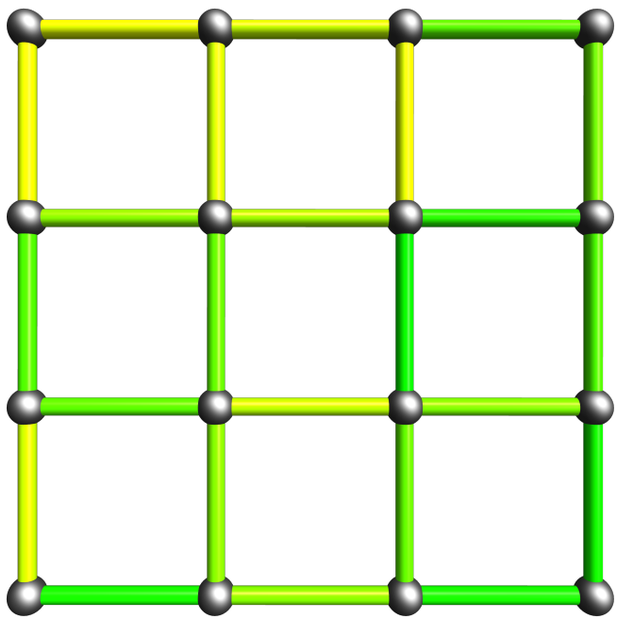




# Gauge (local) symmetry in ML surrogate models

$U_1$

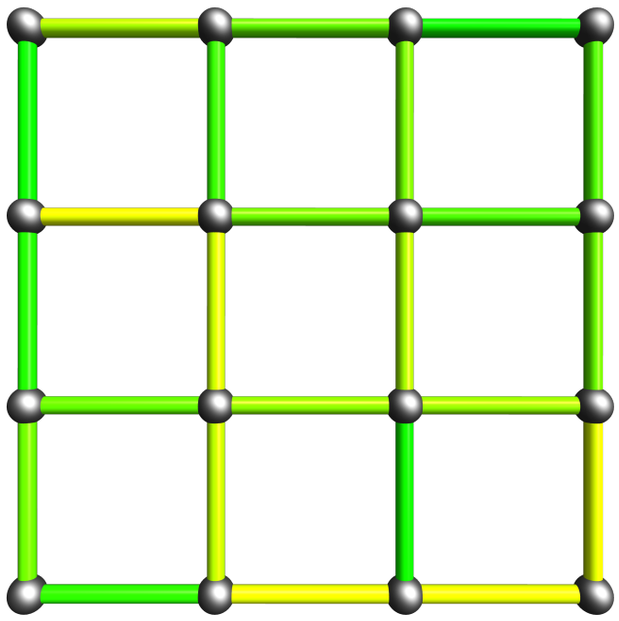


$U_{ij}$

$$\mathcal{F}_{\boldsymbol{\theta}}: \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$

Gauge transformation

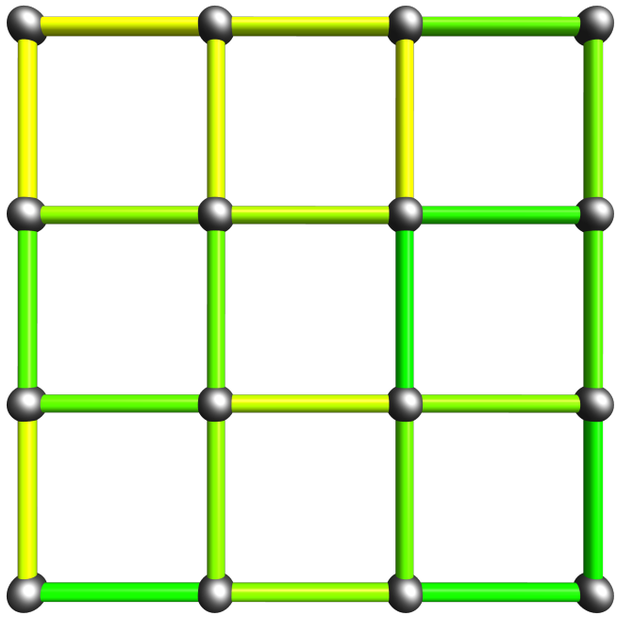
$U_2$



$$U'_{ij} = g_i U_{ij} g_j^\dagger$$

# Gauge (local) symmetry in ML surrogate models

$U_1$



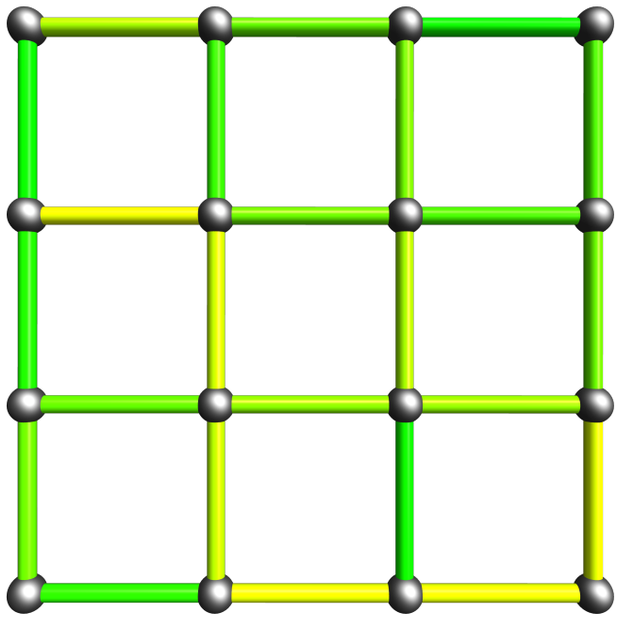
$U_{ij}$

$$\mathcal{F}_{\boldsymbol{\theta}}: \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$

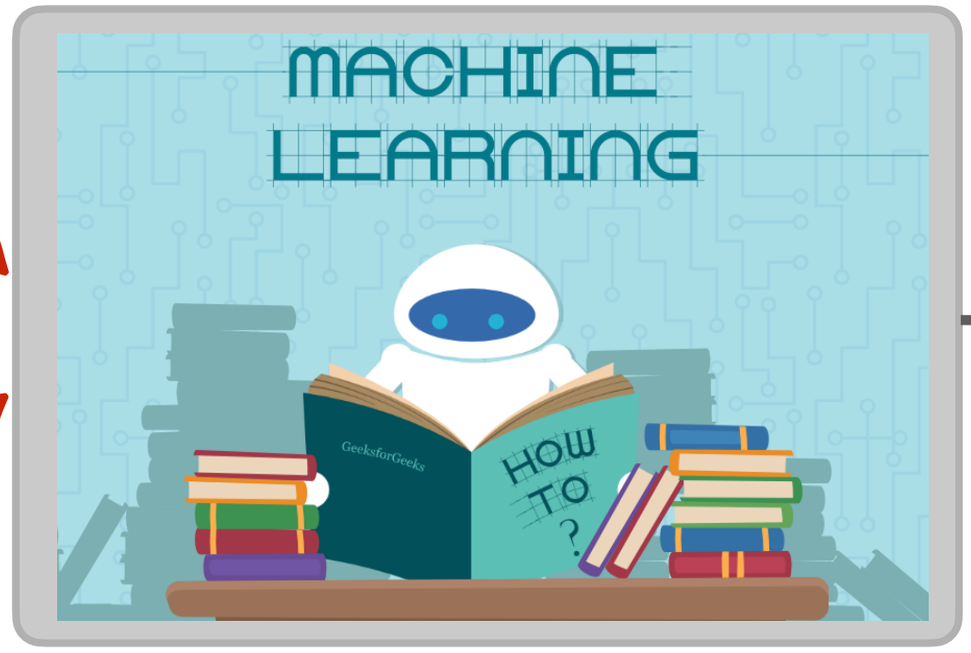
$$\overset{?}{\mathcal{O}_1 = \mathcal{O}_2}$$

Gauge transformation

$U_2$



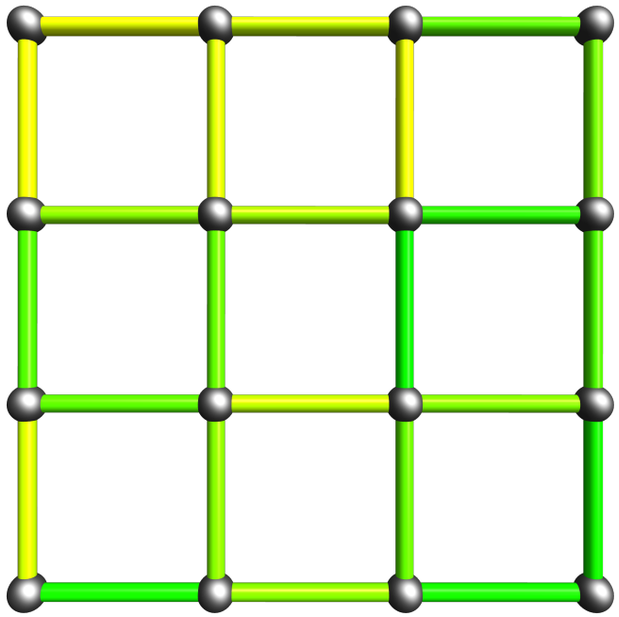
$$U'_{ij} = g_i U_{ij} g_j^\dagger$$




$\mathcal{O}$

# Gauge (local) symmetry in ML surrogate models

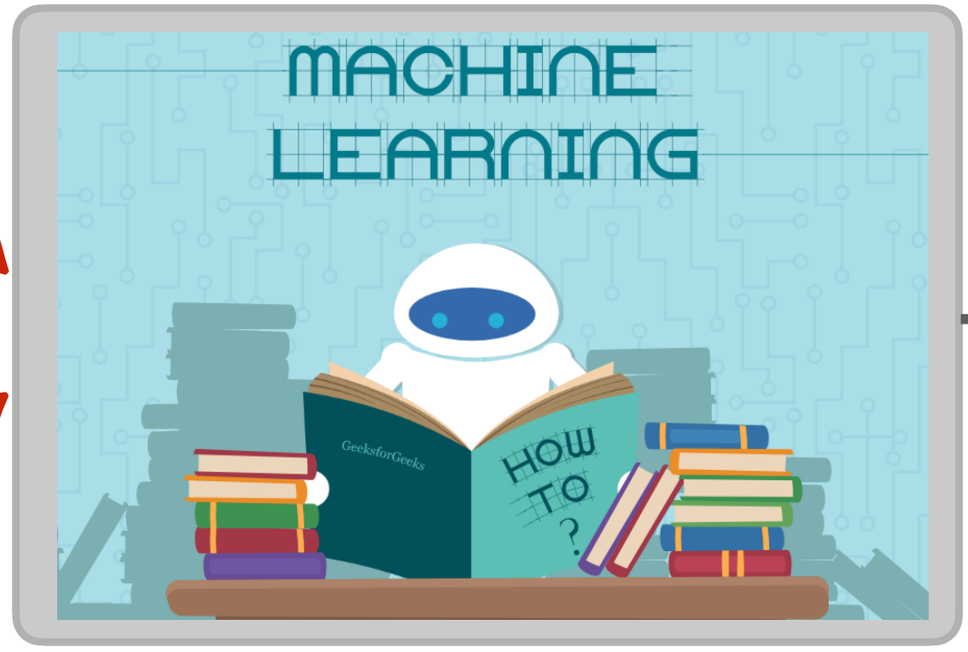
$U_1$



$U_{ij}$

$$\mathcal{F}_{\boldsymbol{\theta}}: \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$

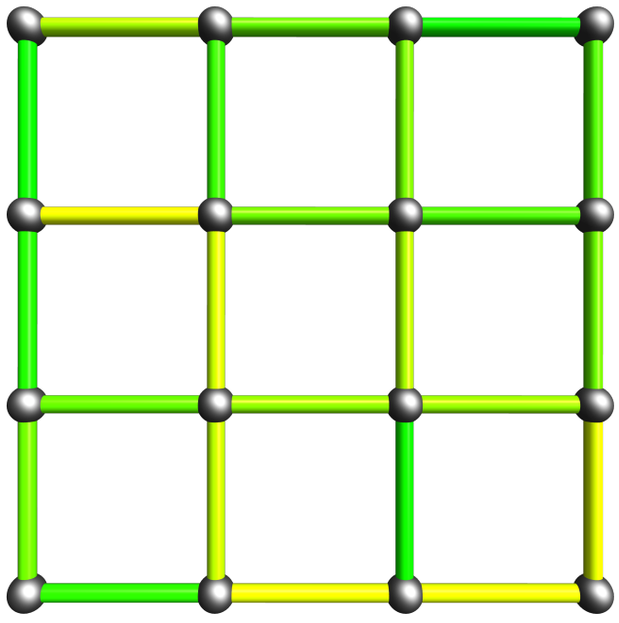
$$\overset{?}{\mathcal{O}_1 = \mathcal{O}_2}$$




$\mathcal{O}$

Gauge transformation

$U_2$



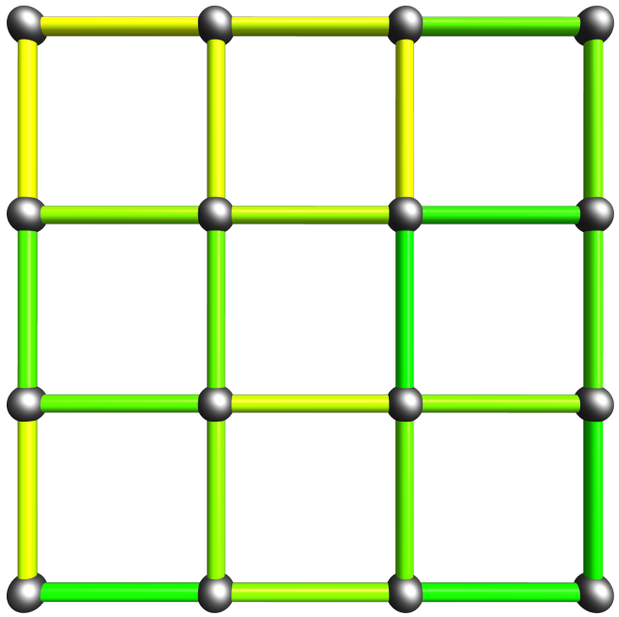
$$U'_{ij} = g_i U_{ij} g_j^\dagger$$

- Group theory?

$$SU(N)_1 \otimes SU(N)_2 \otimes \cdots$$

# Gauge (local) symmetry in ML surrogate models

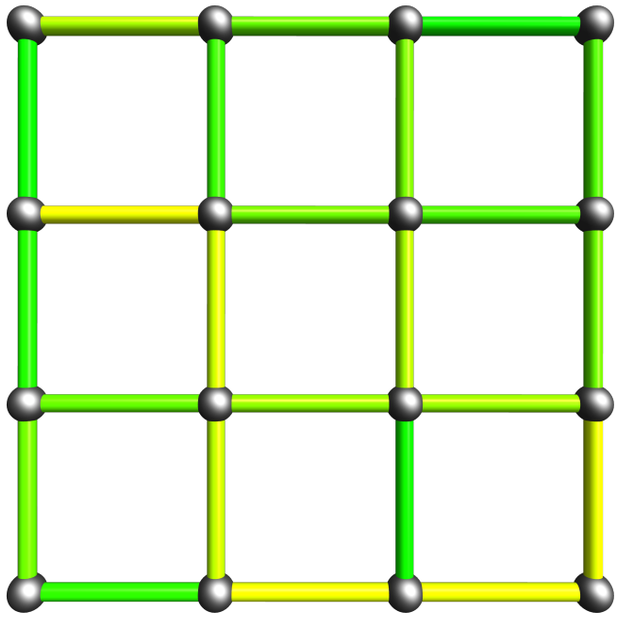
$U_1$



$U_{ij}$

Gauge transformation

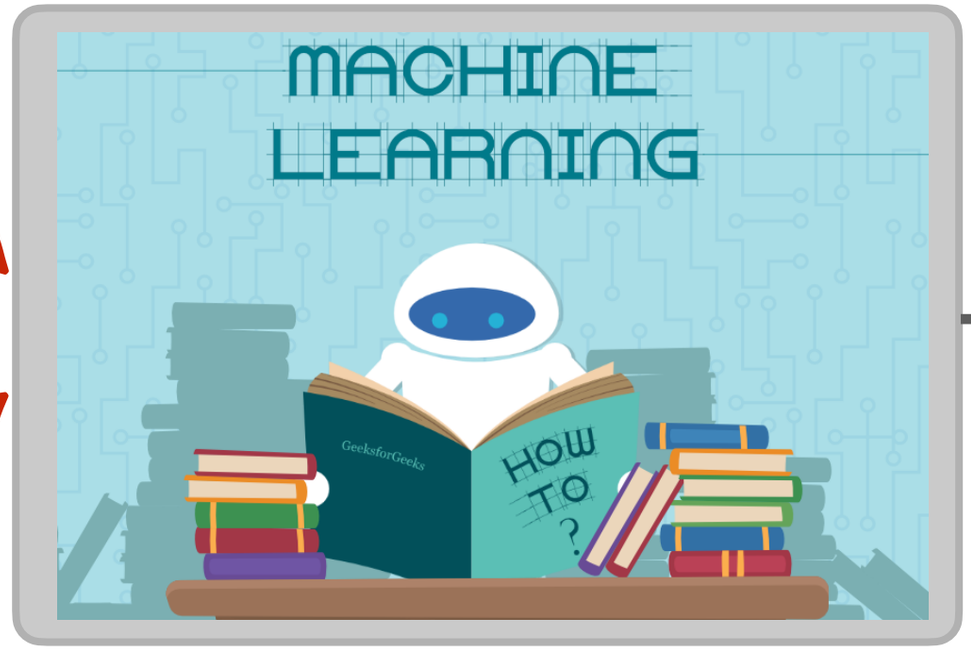
$U_2$



$$U'_{ij} = g_i U_{ij} g_j^\dagger$$

$$\mathcal{F}_{\boldsymbol{\theta}} : \{U_{ij}\} \Longrightarrow \mathcal{O}_i$$

$$\overset{?}{\mathcal{O}_1 = \mathcal{O}_2}$$




$\mathcal{O}$

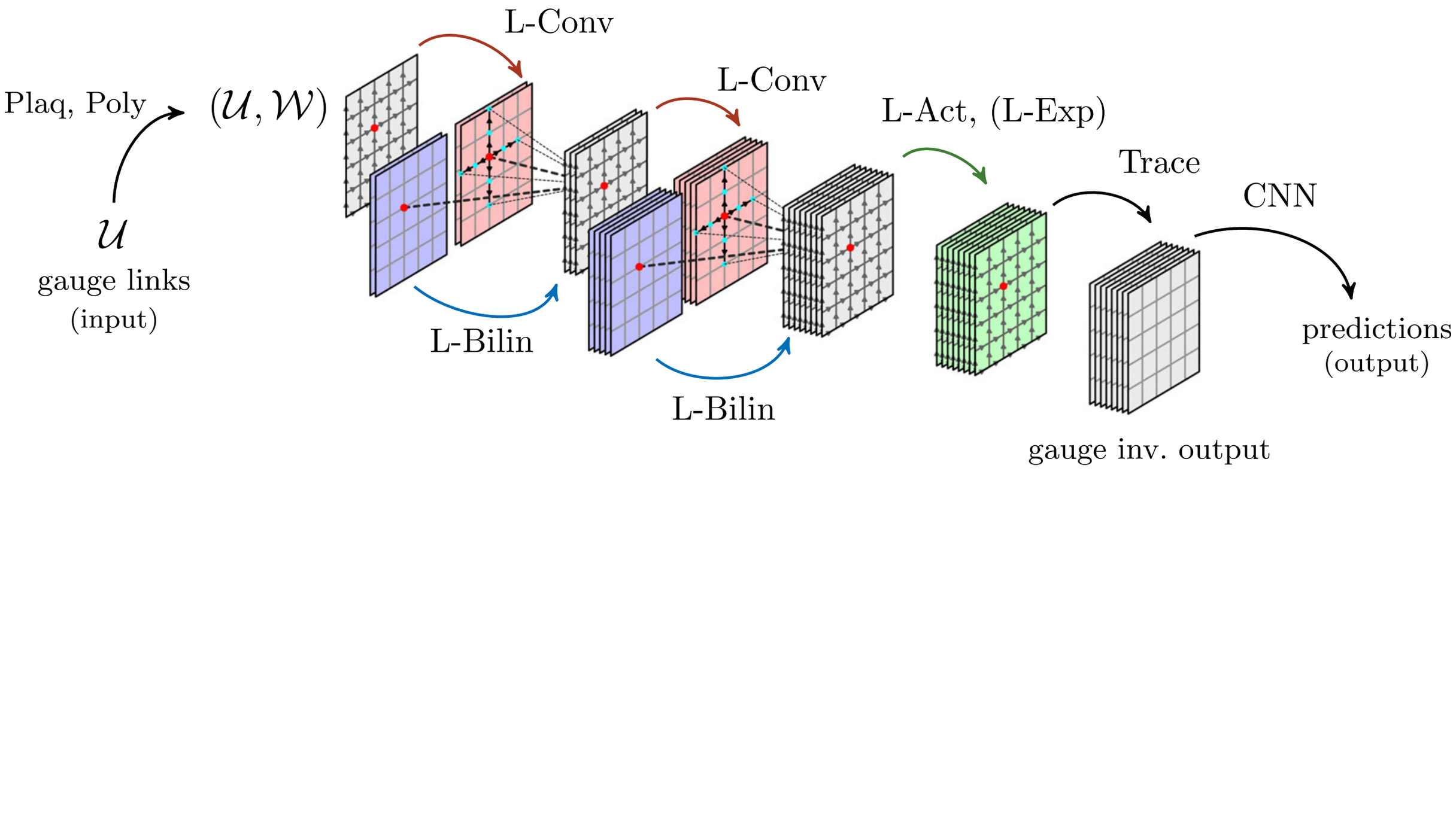
- Group theory?

$$SU(N)_1 \otimes SU(N)_2 \otimes \cdots$$

- Gauge-equivariant GNN

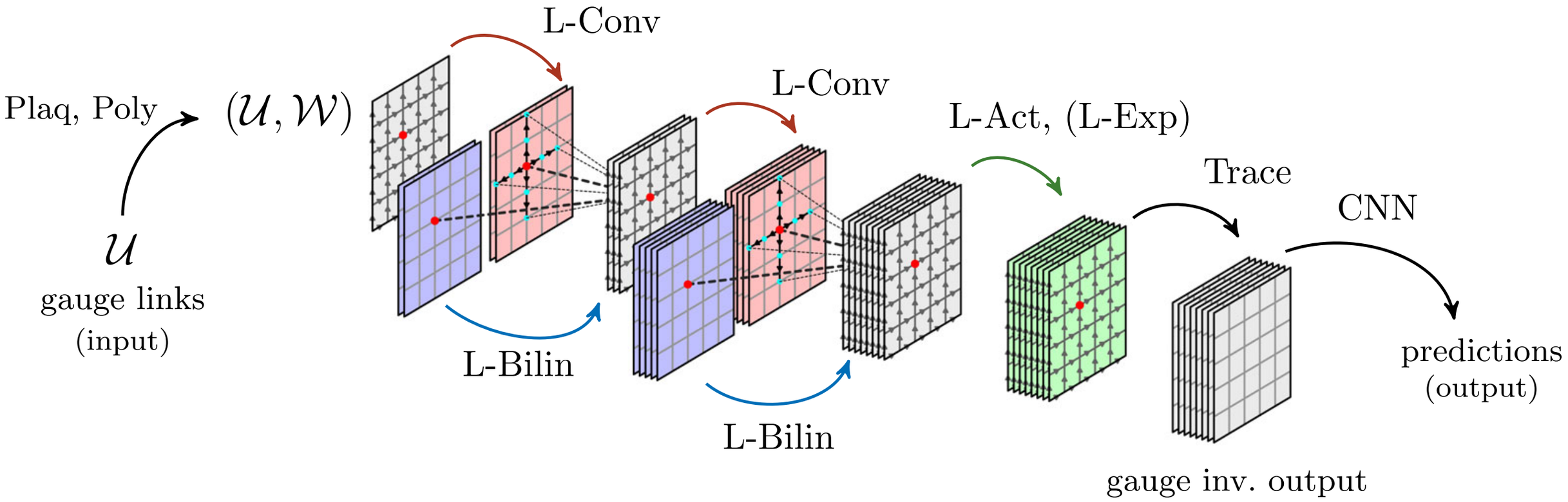
# Lattice Gauge Equivariant Convolutional Neural Networks

Matteo Favoni,[†] Andreas Ipp,[‡] David I. Müller,[*] and Daniel Schuh[§]
*Institute for Theoretical Physics, TU Wien, A-1040 Wien, Austria*



# Lattice Gauge Equivariant Convolutional Neural Networks

Matteo Favoni,[†] Andreas Ipp,[‡] David I. Müller,[*] and Daniel Schuh[§]
*Institute for Theoretical Physics, TU Wien, A-1040 Wien, Austria*



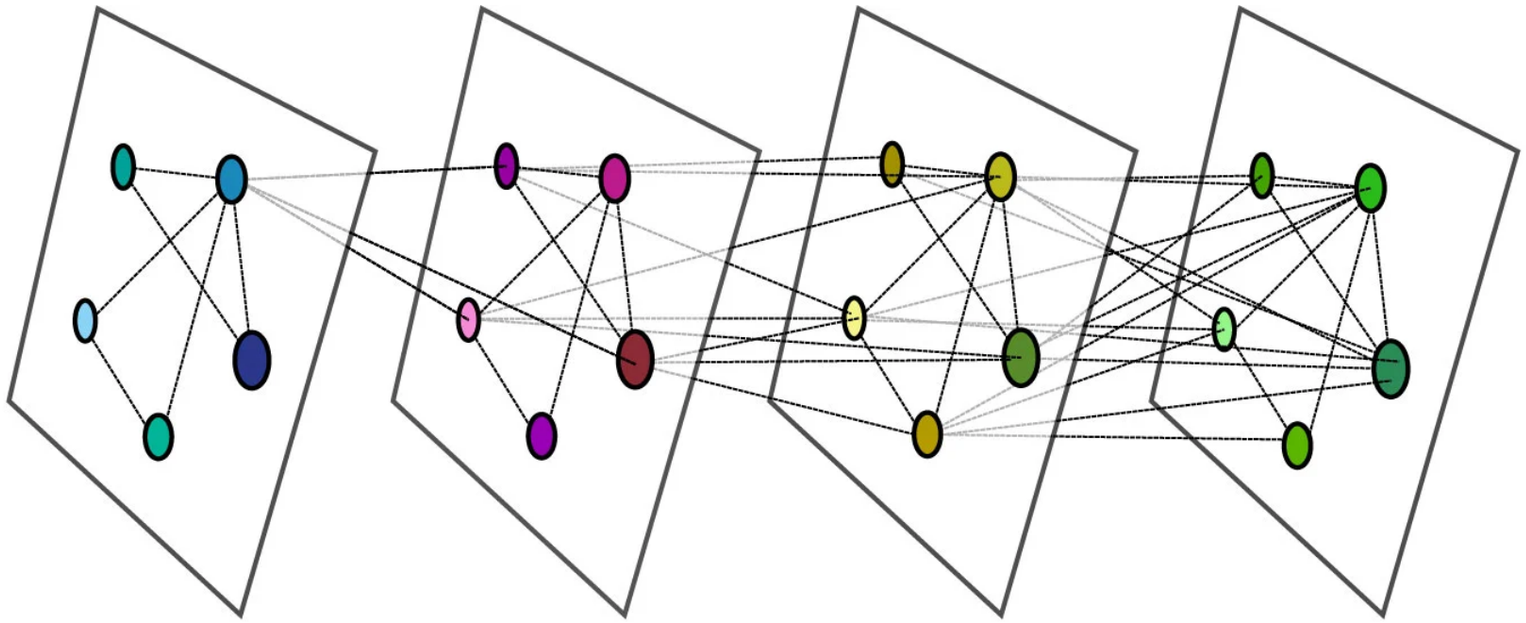

- Local CNN operation already very similar to message passing
- Matrix-valued embeddings

$$W_i \rightarrow g_i^\dagger W_i g_i^\dagger$$

- Updating rules a bit ad hoc but general enough

# Graph Neural Network (Message passing)

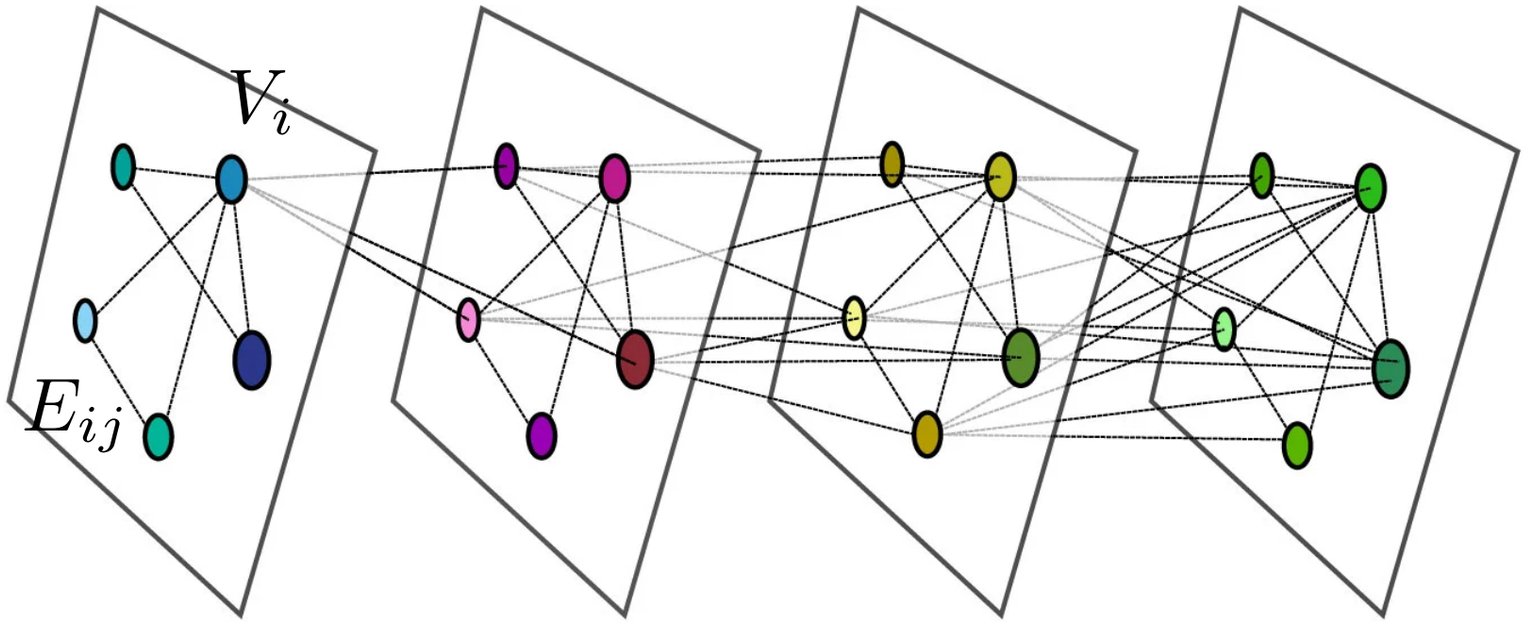
- Physical system as a graph (molecules, crystals, lattice, …)



# Graph Neural Network (Message passing)

- Physical system as a graph (molecules, crystals, lattice, …)

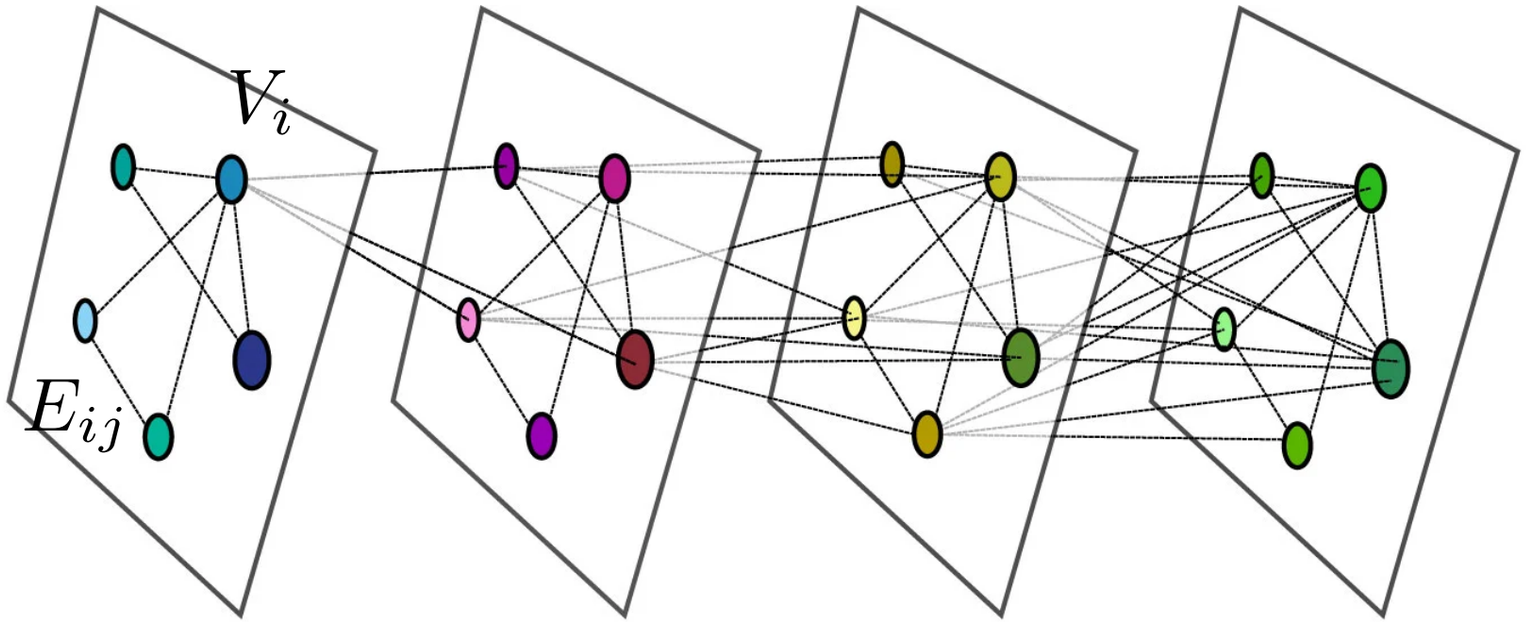
  - Node features $V_i$
  - Edge features $E_{ij}$
  - Global features



# Graph Neural Network (Message passing)

- Physical system as a graph (molecules, crystals, lattice, …)

  - Node features $V_i$
  - Edge features $E_{ij}$
  - Global features

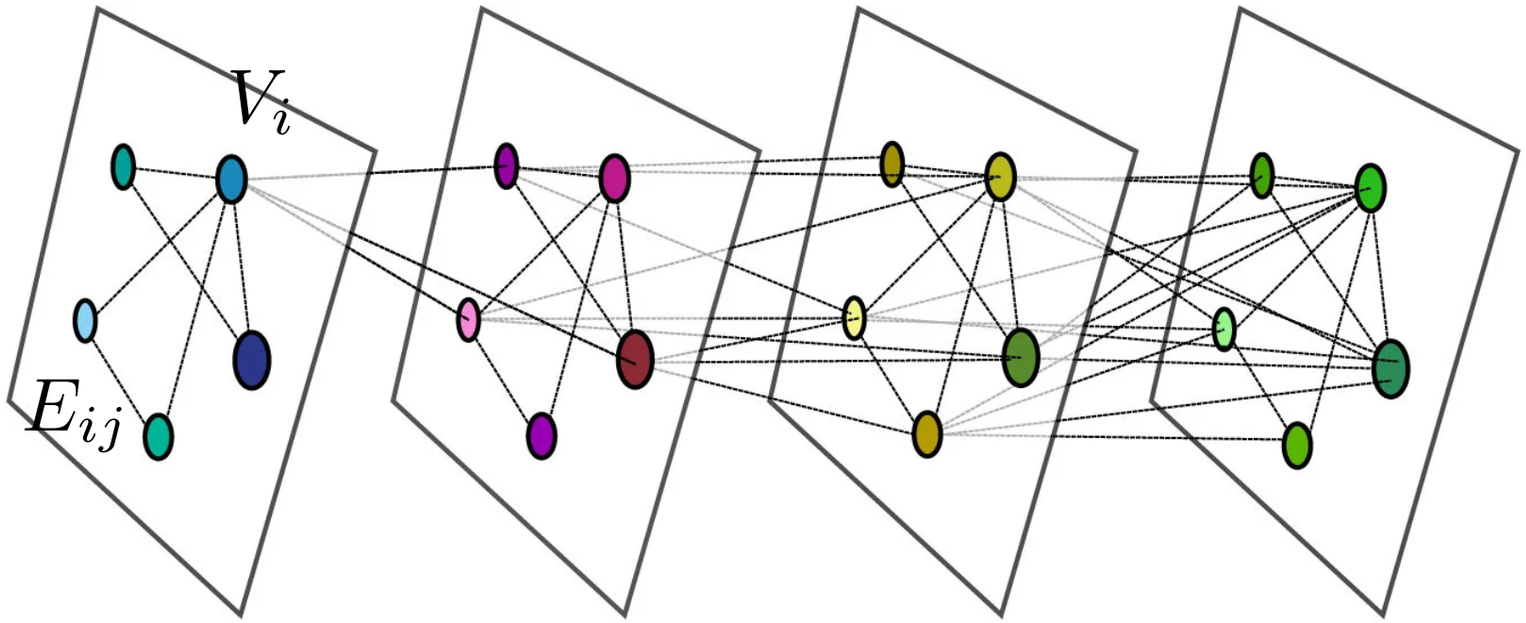



- Suited for incorporating locality, relational dependences, symmetry, …

# Graph Neural Network (Message passing)

- Physical system as a graph (molecules, crystals, lattice, …)

  - Node features $V_i$
  - Edge features $E_{ij}$
  - Global features




- Suited for incorporating locality, relational dependences, symmetry, …

- Message passing:

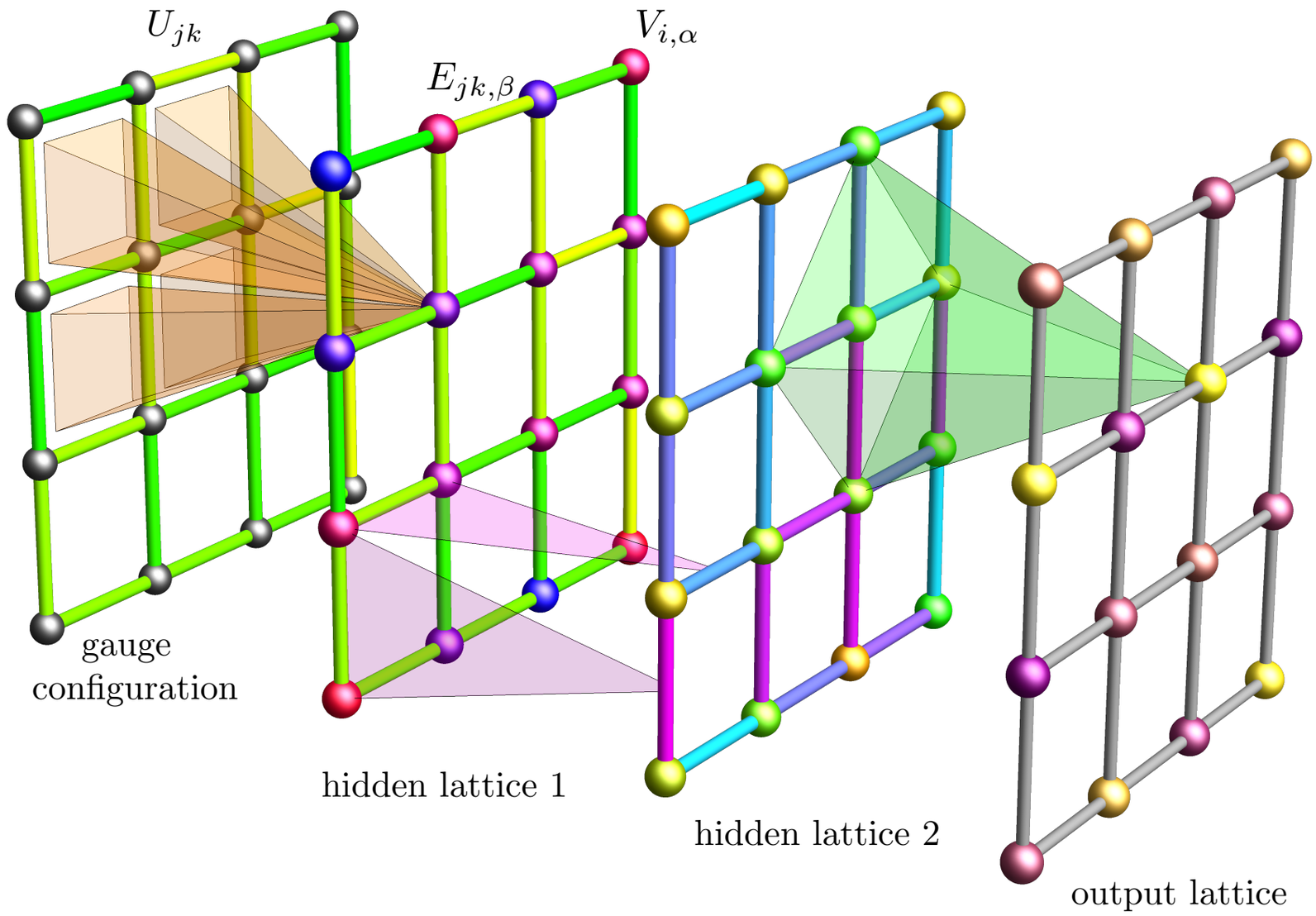
$$M_{ij} = \phi(V_i, V_j, E_{ij})$$

- Update

$$V_i^{(\text{next})} = \psi\left(V_i, \sum_{j \in \mathcal{N}_i} M_{ij}\right)$$

# Gauge-Equivariant GNN: Architecture

- SU(N)-matrix-valued node features $\mathbf{V}_i^{(\ell)} = [V_{i,1}^{(\ell)}, V_{i,2}^{(\ell)}, \cdots, V_{i,n}^{(\ell)}]$
- SU(N)-matrix-valued edge features $\mathbf{E}_{ij}^{(\ell)} = [E_{ij,1}^{(\ell)}, E_{ij,2}^{(\ell)}, \cdots, E_{ij,n'}^{(\ell)}]$

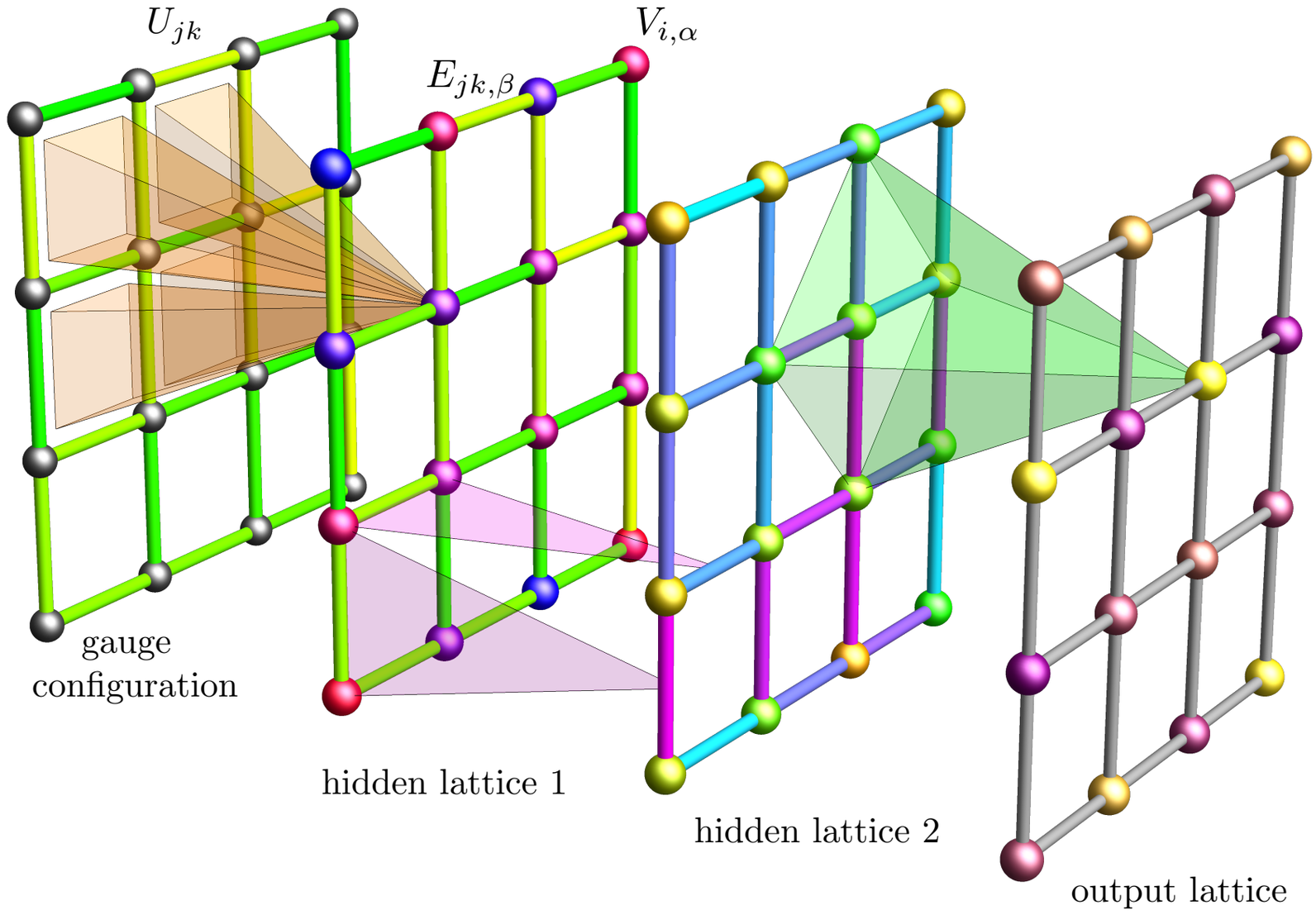


# Gauge-Equivariant GNN: Architecture

- SU(N)-matrix-valued node features $\mathbf{V}_i^{(\ell)} = [V_{i,1}^{(\ell)}, V_{i,2}^{(\ell)}, \cdots, V_{i,n}^{(\ell)}]$
- SU(N)-matrix-valued edge features $\mathbf{E}_{ij}^{(\ell)} = [E_{ij,1}^{(\ell)}, E_{ij,2}^{(\ell)}, \cdots, E_{ij,n'}^{(\ell)}]$
- Gauge transform

$$V_i \to g_i V_i g_i^\dagger$$

$$E_{ij} \to g_i E_{ij} g_j^\dagger$$



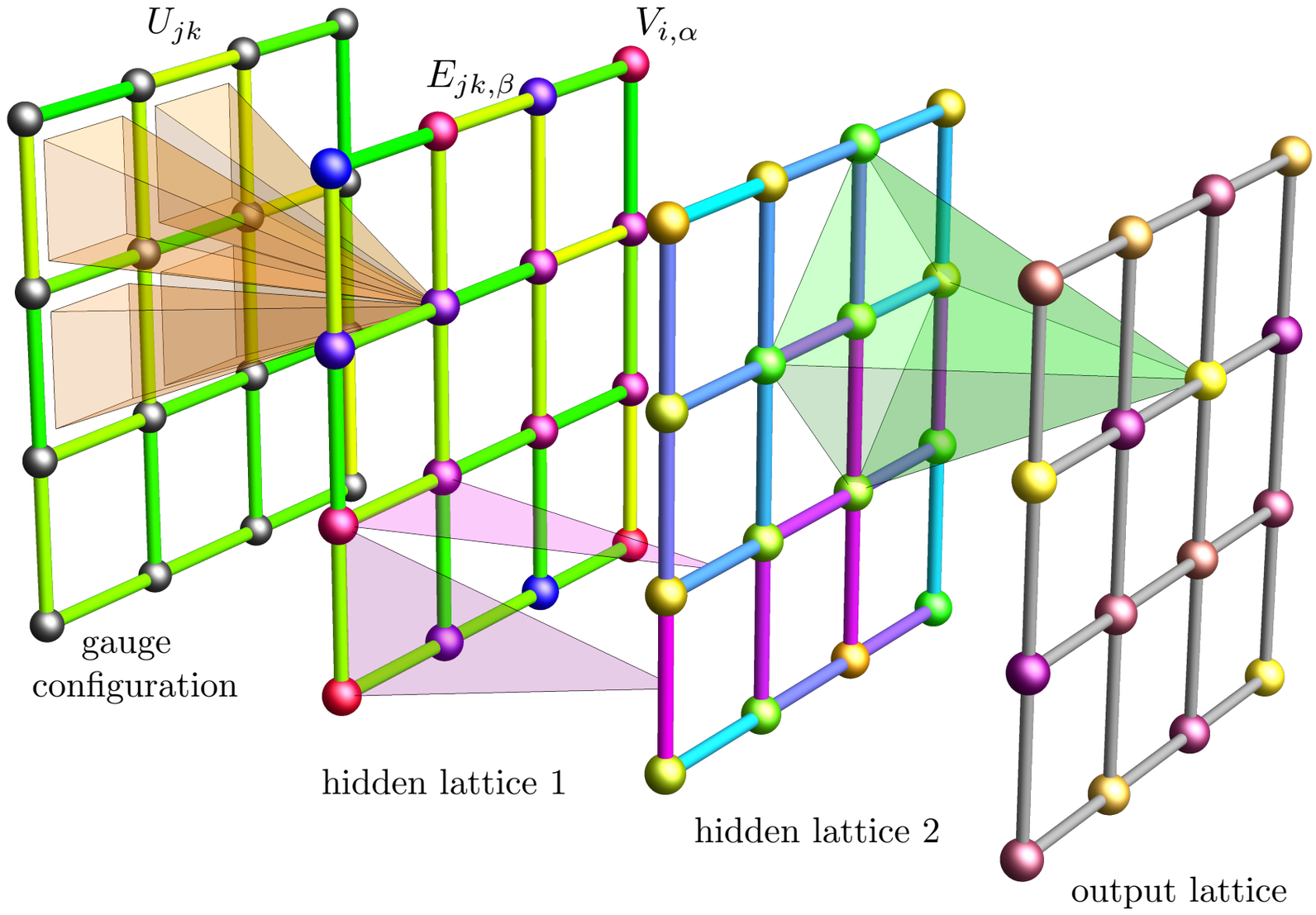
# Gauge-Equivariant GNN: Architecture

- SU(N)-matrix-valued node features $\mathbf{V}_i^{(\ell)} = [V_{i,1}^{(\ell)}, V_{i,2}^{(\ell)}, \cdots, V_{i,n}^{(\ell)}]$
- SU(N)-matrix-valued edge features $\mathbf{E}_{ij}^{(\ell)} = [E_{ij,1}^{(\ell)}, E_{ij,2}^{(\ell)}, \cdots, E_{ij,n'}^{(\ell)}]$
- Gauge transform

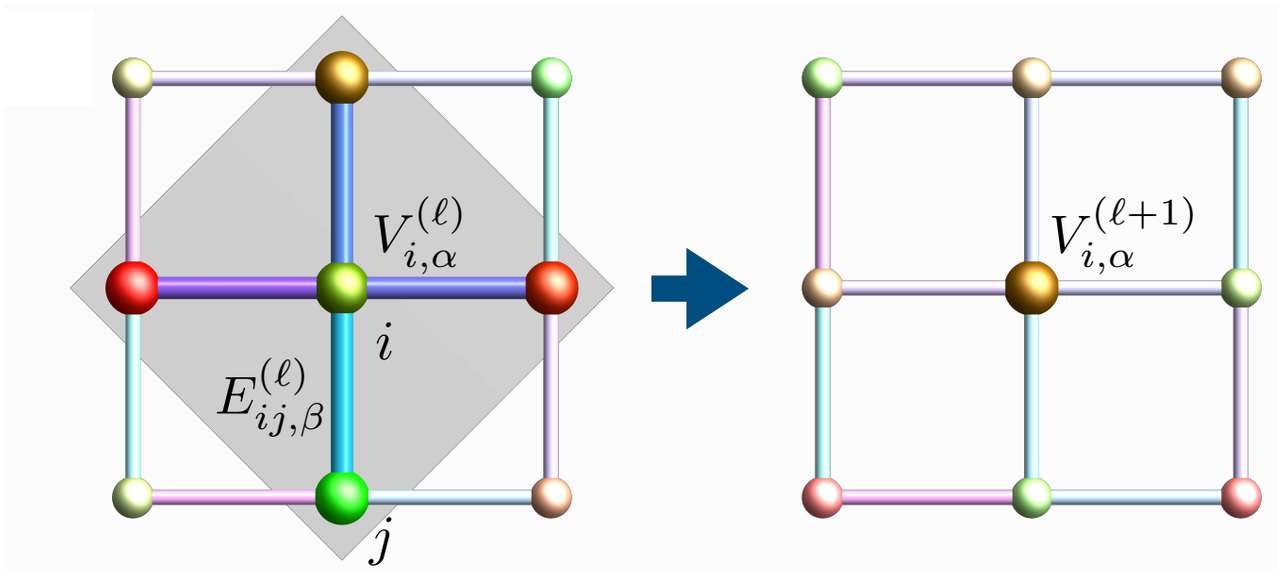
$$V_i \to g_i V_i g_i^\dagger$$

$$E_{ij} \to g_i E_{ij} g_j^\dagger$$

- Update Scheme?



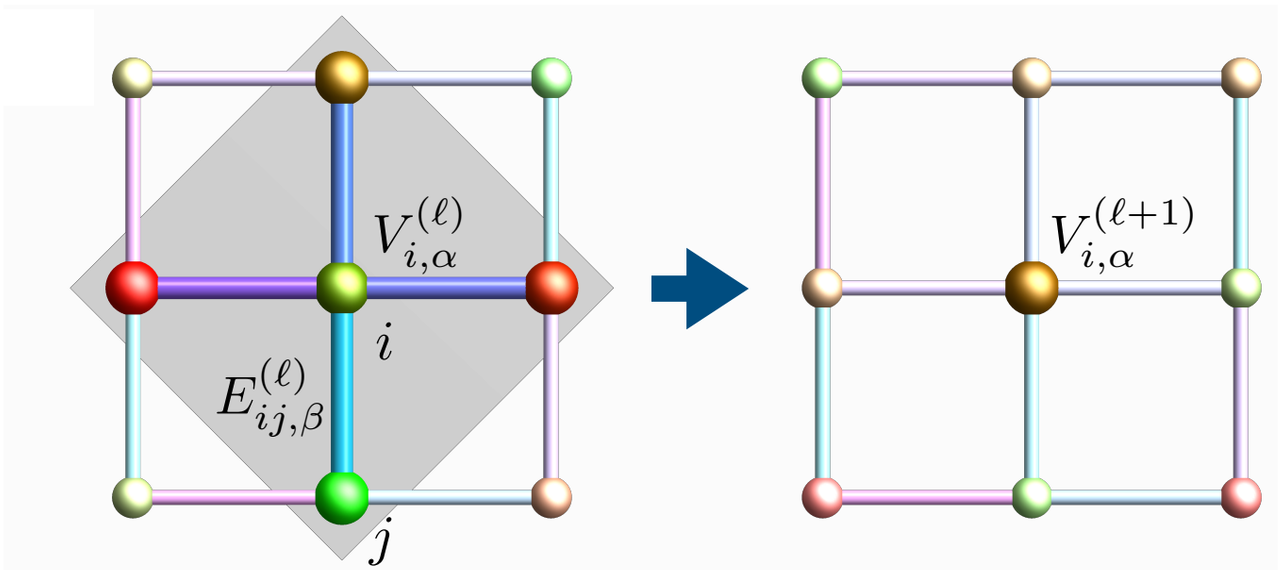
# Update of node features




- Gauge-equivariant Message gathering:

$$\mathbf{X}_i^{(\ell)} = \eta_1 \, \mathcal{W}_1 \big[\mathbf{V}_i^{(\ell)}\big] + \eta_2 \, \mathcal{W}_2 \big[\mathbf{V}_i^{(\ell)} \mathbf{V}_i^{(\ell)}\big] + \eta_3 \sum_{j \in \mathcal{N}(i)} \mathcal{W}_3 \big[\mathbf{E}_{ij}^{(\ell)} \mathbf{V}_j^{(\ell)} \mathbf{E}_{ji}^{(\ell)}\big].$$

# Update of node features




- Gauge-equivariant Message gathering:

$$\mathbf{X}_i^{(\ell)} = \eta_1 \, \mathcal{W}_1\big[\mathbf{V}_i^{(\ell)}\big] + \eta_2 \, \mathcal{W}_2\big[\mathbf{V}_i^{(\ell)}\mathbf{V}_i^{(\ell)}\big] + \eta_3 \sum_{j\in\mathcal{N}(i)} \mathcal{W}_3\big[\mathbf{E}_{ij}^{(\ell)}\mathbf{V}_j^{(\ell)}\mathbf{E}_{ji}^{(\ell)}\big].$$

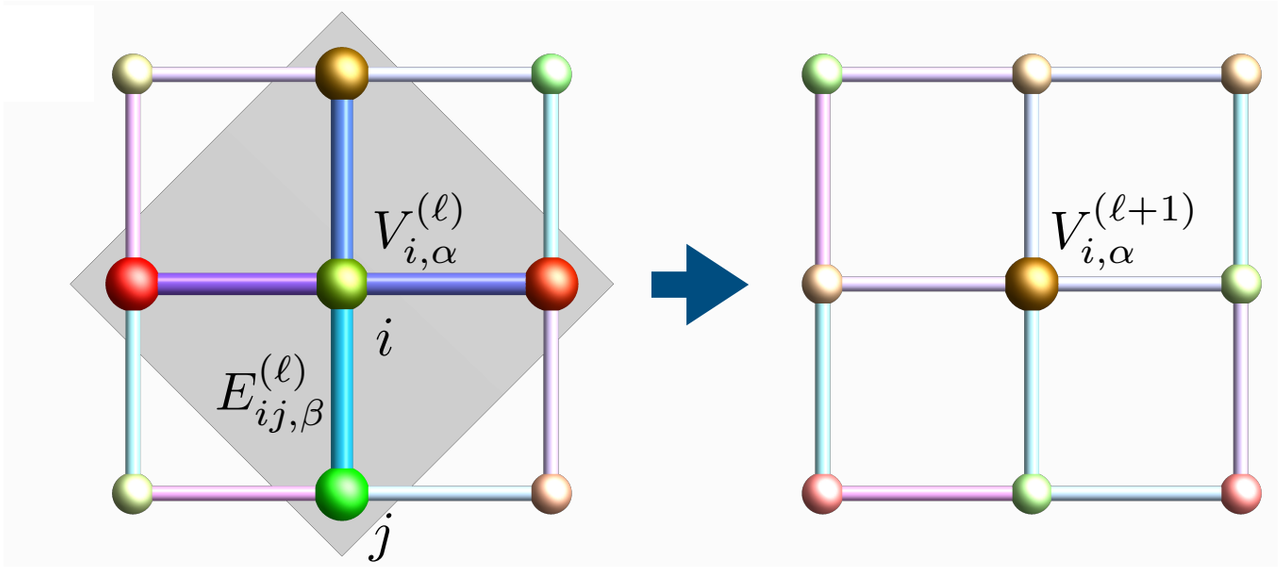
- Message passing & Nonlinearity $\quad \mathrm{Norm}(\mathbf{X}) = \{X_\alpha / \|X_\alpha\|\} \qquad \|A\| = \sqrt{\mathrm{Tr}(A^\dagger A)}$

Frobenius norm

$$\mathbf{V}_i^{(\ell+1)} = \sigma\Big(\mathrm{Re}\,\mathrm{Tr}\big[\mathrm{Norm}\big(\mathbf{X}_i^{(\ell)}\big)\big] + \mathbf{b}\Big) \odot \mathrm{Norm}\big(\mathbf{X}_i^{(\ell)}\big).$$

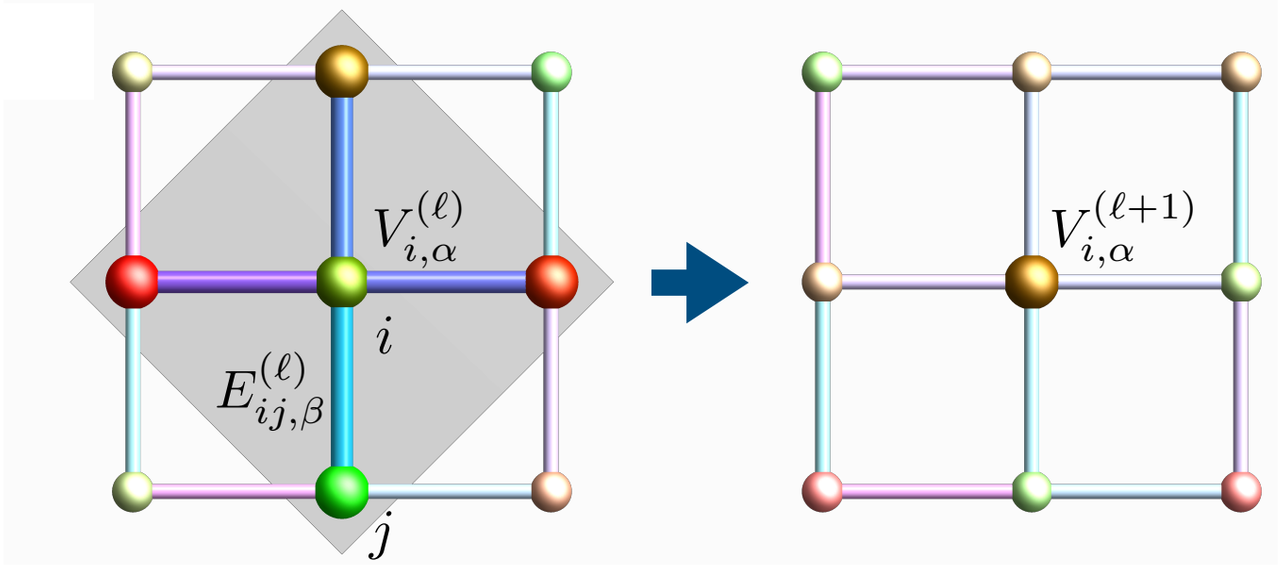
Activation function, e.g. ReLU

# Update of node features




$$\mathbf{X}_i^{(3)} = \sum_{j \in \mathcal{N}_i} \mathcal{W}[\mathbf{E}_{ij}\mathbf{V}_j\mathbf{E}_{ji}]$$

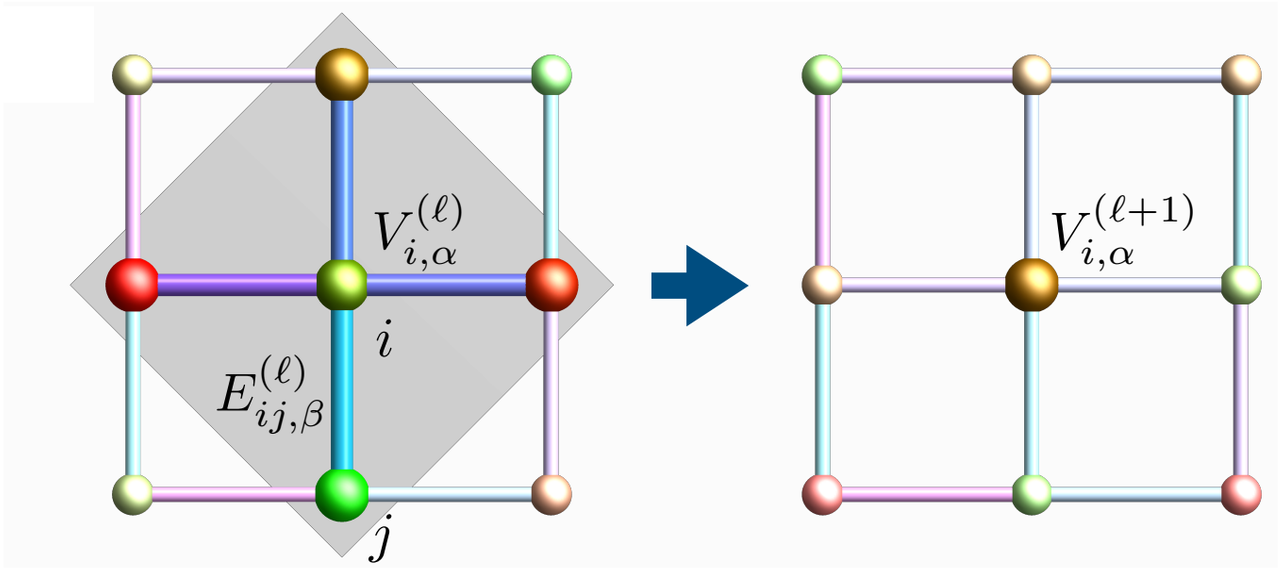
# Update of node features




$$\mathbf{X}_i^{(3)} = \sum_{j \in \mathcal{N}_i} \mathcal{W}[\mathbf{E}_{ij}\mathbf{V}_j\mathbf{E}_{ji}]$$

$$X_{i,\alpha}^{(3)} = \sum_{j \in \mathcal{N}(i)} \sum_{\beta,\gamma,\delta} W_{\alpha\beta\gamma\delta}\, E_{ij,\beta} V_{j,\gamma}\, E_{ji,\delta}$$

# Update of node features



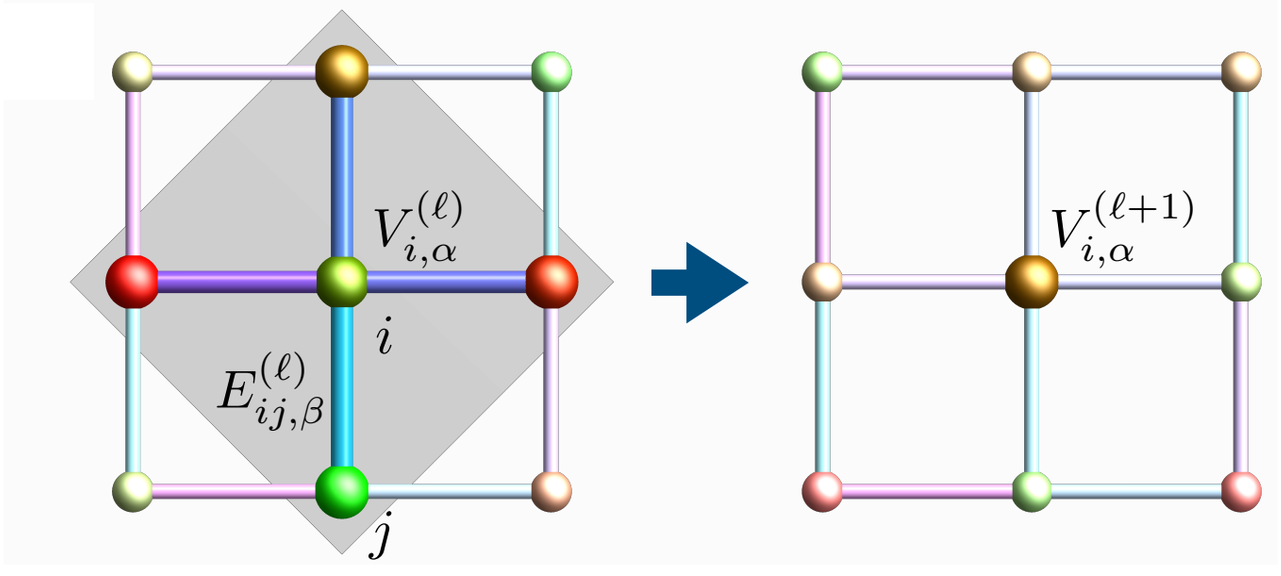

$$\mathbf{X}_i^{(3)} = \sum_{j \in \mathcal{N}_i} \mathcal{W}[\mathbf{E}_{ij}\mathbf{V}_j\mathbf{E}_{ji}]$$

$$X_{i,\alpha}^{(3)} = \sum_{j \in \mathcal{N}(i)} \sum_{\beta,\gamma,\delta} W_{\alpha\beta\gamma\delta}\, E_{ij,\beta} V_{j,\gamma}\, E_{ji,\delta}$$

Gauge transformation

$$\tilde{X}_{i,\alpha}^{(3)} = \sum_{j \in \mathcal{N}(i)} \sum_{\beta,\gamma,\delta} W_{\alpha\beta\gamma\delta}\, g_i E_{ij,\beta} g_j^\dagger\, g_j V_{j,\gamma} g_j^\dagger\, g_j E_{ji,\delta} g_i^\dagger$$

# Update of node features




$$\mathbf{X}_i^{(3)} = \sum_{j \in \mathcal{N}_i} \mathcal{W}[\mathbf{E}_{ij}\mathbf{V}_j\mathbf{E}_{ji}]$$

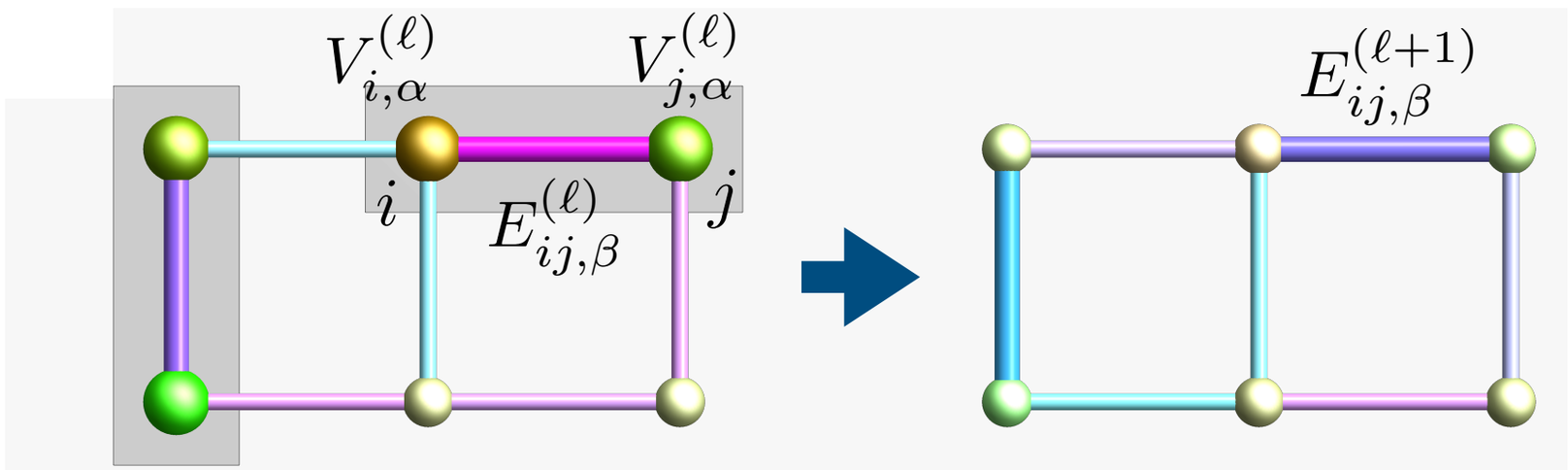
$$X_{i,\alpha}^{(3)} = \sum_{j\in\mathcal{N}(i)} \sum_{\beta,\gamma,\delta} W_{\alpha\beta\gamma\delta}\, E_{ij,\beta} V_{j,\gamma}\, E_{ji,\delta}$$

Gauge transformation

$$\tilde{X}_{i,\alpha}^{(3)} = \sum_{j\in\mathcal{N}(i)} \sum_{\beta,\gamma,\delta} W_{\alpha\beta\gamma\delta}\, g_i E_{ij,\beta} g_j^\dagger\, g_j V_{j,\gamma} g_j^\dagger\, g_j E_{ji,\delta} g_i^\dagger$$

$$\tilde{X}_{i,\alpha}^{(3)} = g_i \left( \sum_{j\in\mathcal{N}(i)} \sum_{\beta,\gamma,\delta} W_{\alpha\beta\gamma\delta}\, E_{ij,\beta} V_{j,\gamma}\, E_{ji,\delta} \right) g_i^\dagger = g_i^\dagger\, X_{i,\alpha}^{(3)}\, g_i^\dagger$$

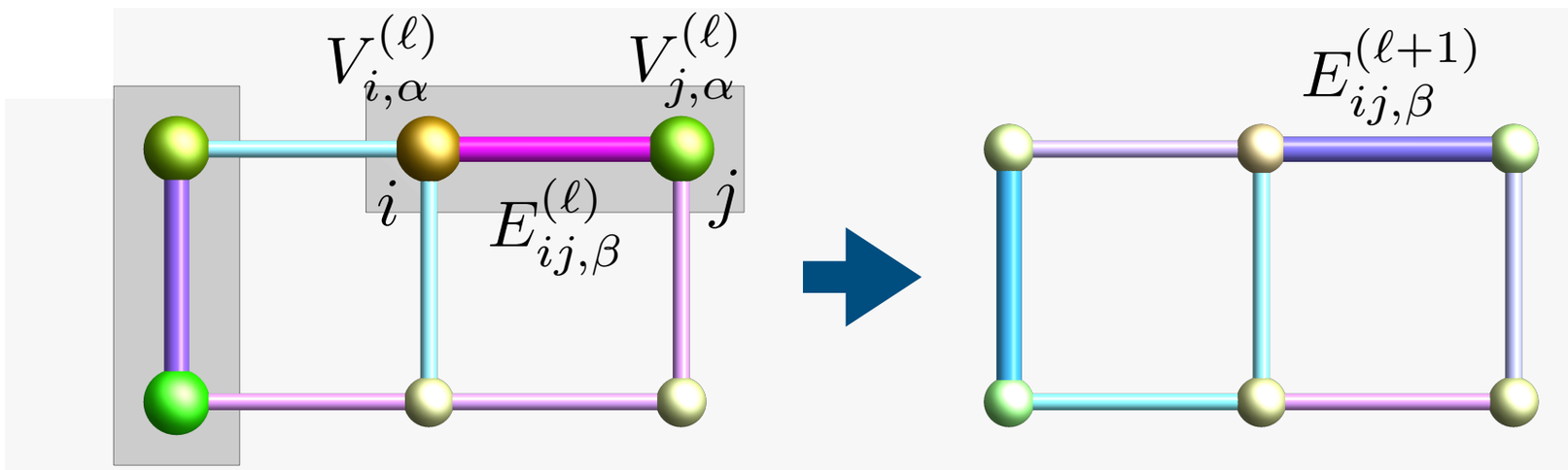
# Update of edge features




- Gauge-equivariant Message gathering:

$$\mathbf{Y}^{(\ell)}_{ij} = \tilde{\eta}_1 \tilde{\mathcal{W}}_1 \left[\mathbf{E}^{(\ell)}_{ij}\right] + \tilde{\eta}_2 \tilde{\mathcal{W}}_2 \left[\mathbf{E}^{(\ell)}_{ij}\mathbf{V}^{(\ell)}_{j} + \mathbf{V}^{(\ell)}_{i}\mathbf{E}^{(\ell)}_{ij}\right] + \tilde{\eta}_3 \tilde{\mathcal{W}}_3 \left[\mathbf{V}^{(\ell)}_{i}\mathbf{E}^{(\ell)}_{ij}\mathbf{V}^{(\ell)}_{j}\right]$$

# Update of edge features




- Gauge-equivariant Message gathering:

$$\mathbf{Y}_{ij}^{(\ell)} = \tilde{\eta}_1 \tilde{\mathcal{W}}_1 \left[\mathbf{E}_{ij}^{(\ell)}\right] + \tilde{\eta}_2 \tilde{\mathcal{W}}_2 \left[\mathbf{E}_{ij}^{(\ell)} \mathbf{V}_j^{(\ell)} + \mathbf{V}_i^{(\ell)} \mathbf{E}_{ij}^{(\ell)}\right] + \tilde{\eta}_3 \tilde{\mathcal{W}}_3 \left[\mathbf{V}_i^{(\ell)} \mathbf{E}_{ij}^{(\ell)} \mathbf{V}_j^{(\ell)}\right]$$

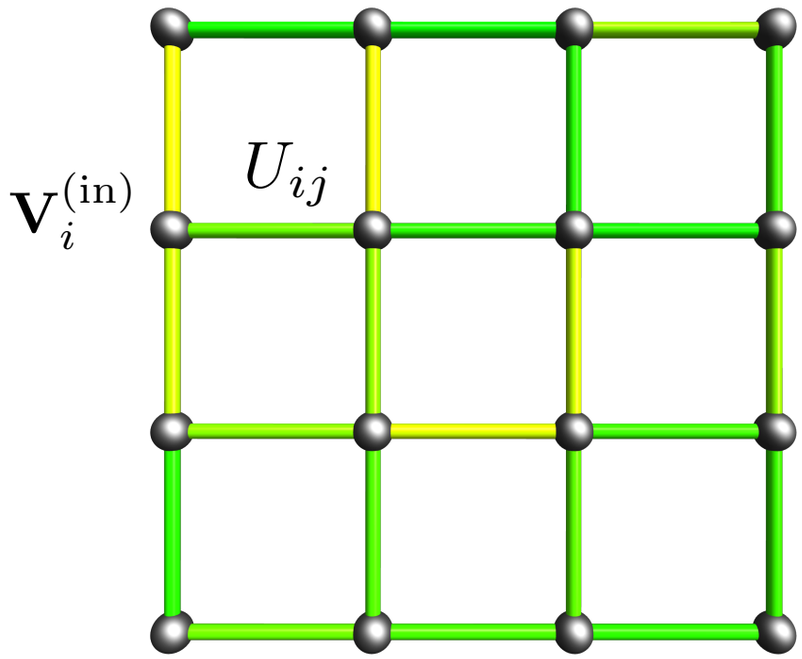
- Message passing & Nonlinearity

$$\mathbf{E}_{ij}^{(\ell+1)} = \sigma\left(\|\mathbf{Y}_{ij}^{(\ell)}\| + \tilde{\mathbf{b}}\right) \odot \mathrm{Norm}\left(\mathbf{Y}_{ij}^{(\ell)}\right)$$

# Initialization of node and edge features

- Initialization of edge features

$$\mathbf{E}_{ij}^{(\mathrm{in})} = \{U_{ij}\}$$



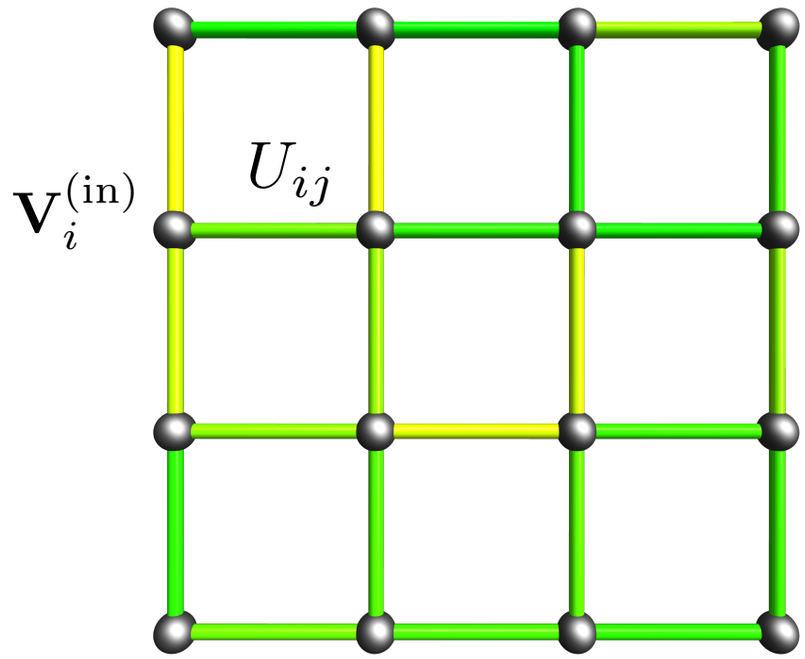
# Initialization of node and edge features

- Initialization of edge features

$$\mathbf{E}_{ij}^{(\mathrm{in})} = \{U_{ij}\}$$

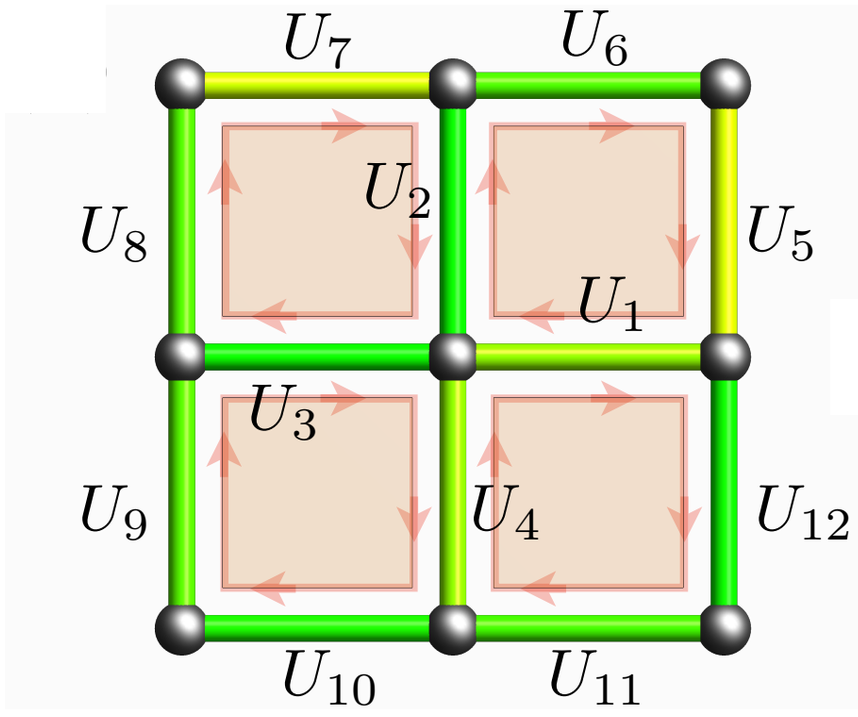
- Initialization of node features

$$\mathbf{V}_{i}^{(\mathrm{in})} = \{V_{i,1}^{(\mathrm{in})}, V_{i,2}^{(\mathrm{in})}, V_{i,3}^{(\mathrm{in})}, V_{i,4}^{(\mathrm{in})}\}$$




$$V_{i,1}^{(0)} = U_1\, U_{12}\, U_{11}\, U_4 \qquad V_{i,3}^{(0)} = U_3\, U_8\, U_7\, U_2$$

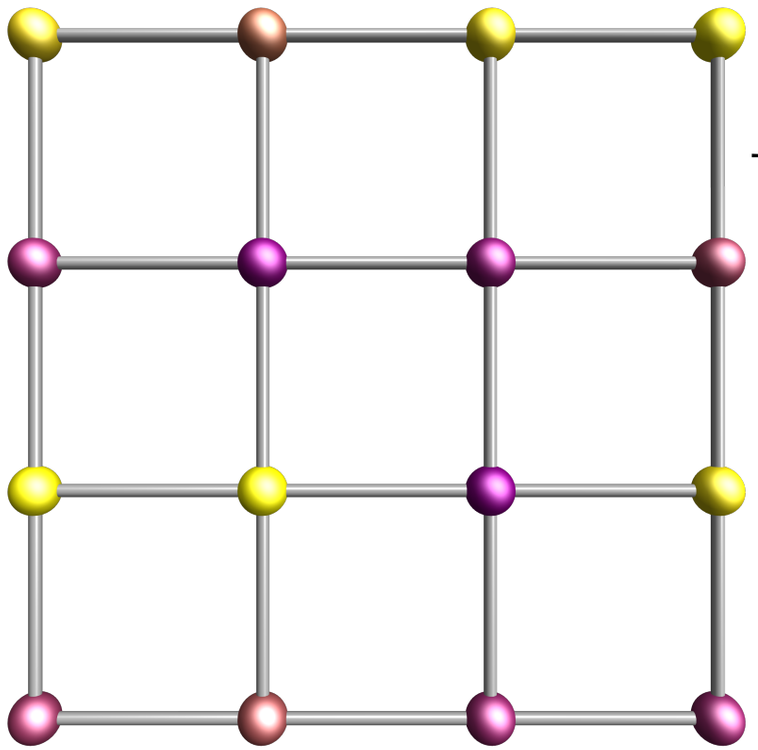
$$V_{i,2}^{(0)} = U_2\, U_6\, U_5\, U_1 \qquad V_{i,4}^{(0)} = U_4\, U_{10}\, U_9\, U_3$$



# Prediction of Gauge-invariant observables

- Non-local dependence —> depth (# of layers) of GNN

  - Output layer

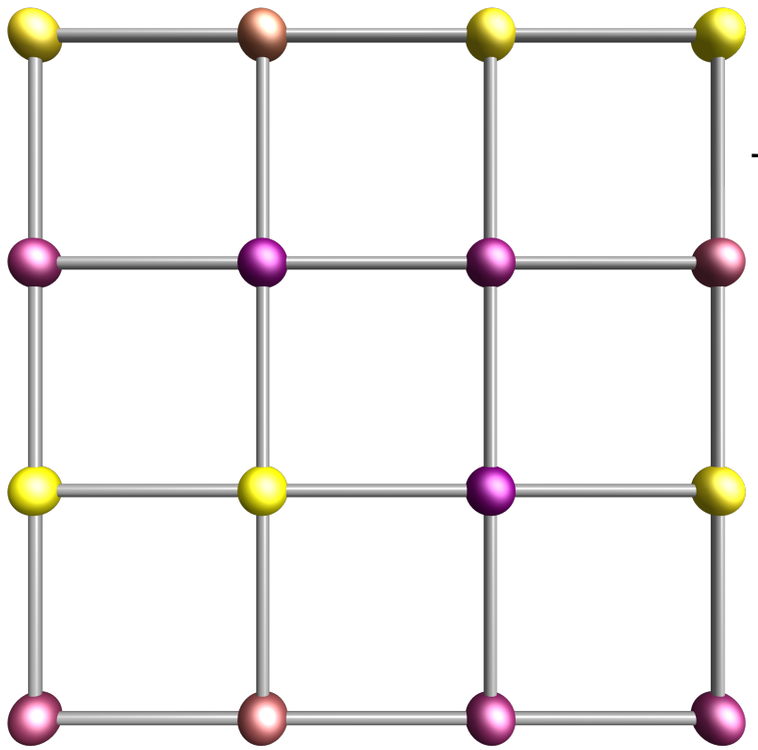


$\mathbf{V}_i^{(\mathrm{out})}$

# Prediction of Gauge-invariant observables

- Non-local dependence —> depth (# of layers) of GNN
- Increase model complexity without significantly increasing depth?

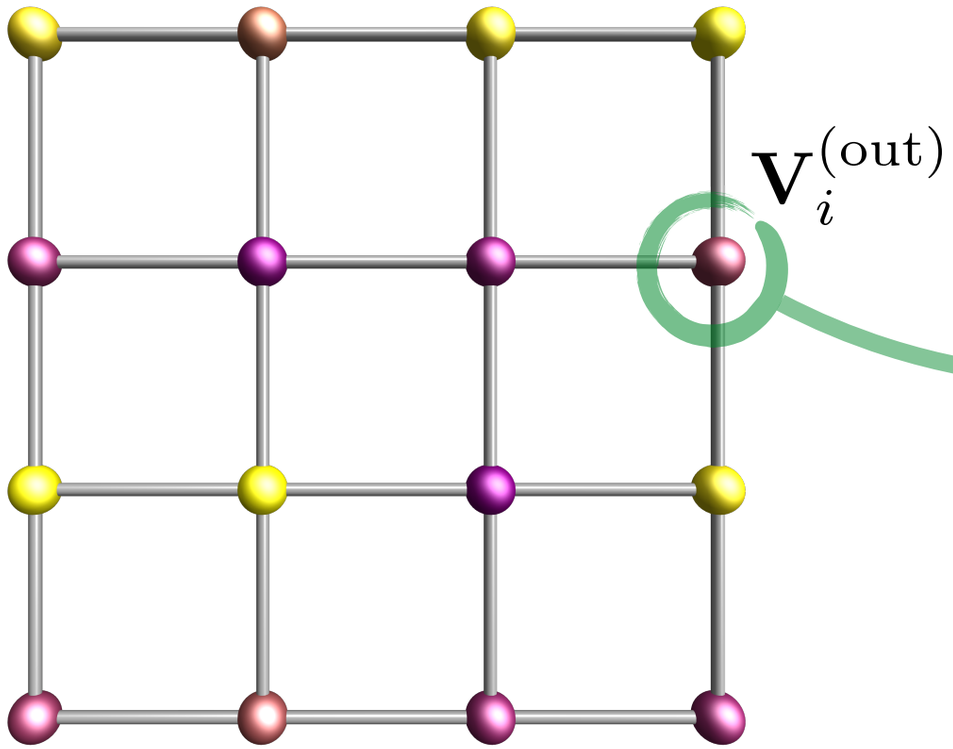
  - Output layer



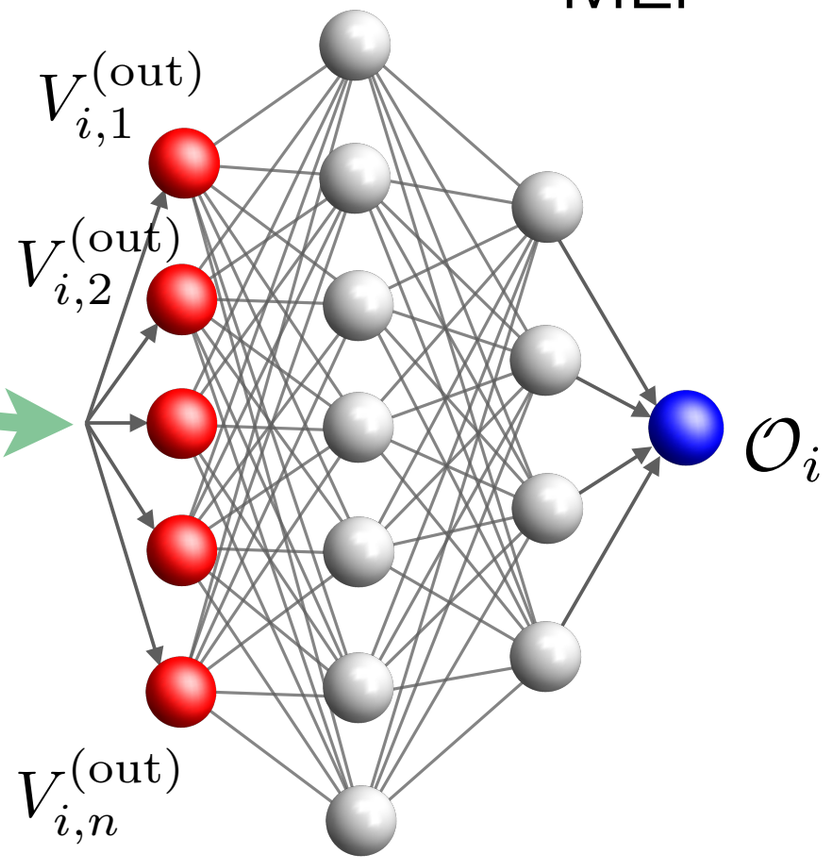
# Prediction of Gauge-invariant observables

- Non-local dependence —> depth (# of layers) of GNN
- Increase model complexity without significantly increasing depth?

- Output layer



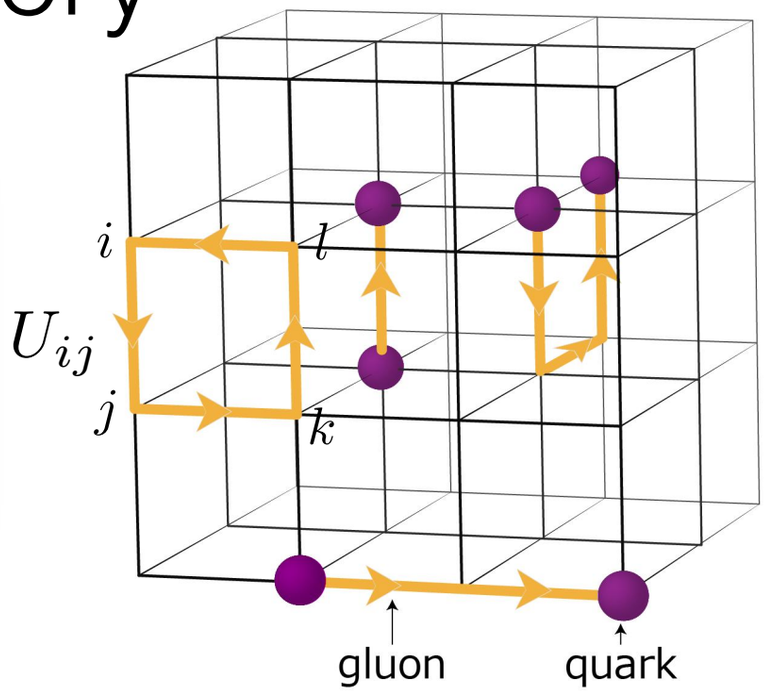

- MLP




$$\mathcal{O}_i = \mathrm{MLP}_{\boldsymbol{\theta}}\Big(\mathrm{Re\,Tr}[\mathbf{V}_i^{(\mathrm{out})}],\ \mathrm{Re\,Tr}[\mathbf{P}]\Big).$$

# Benchmark: 4D Wilson gauge theory

$$S[U] \;=\; -\frac{\beta}{2}\sum_{\square}\mathrm{Re}\,\mathrm{Tr}\left(U_{ij}U_{jk}U_{kl}U_{li}\right),$$

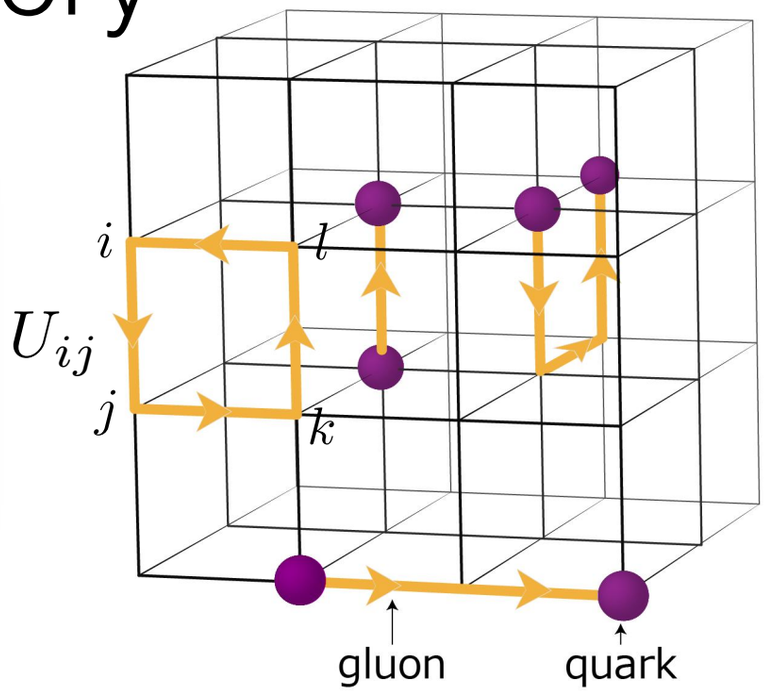



- Similar to the Behler-Parrinello scheme

$$S = \sum_i \epsilon_i$$

# Benchmark: 4D Wilson gauge theory

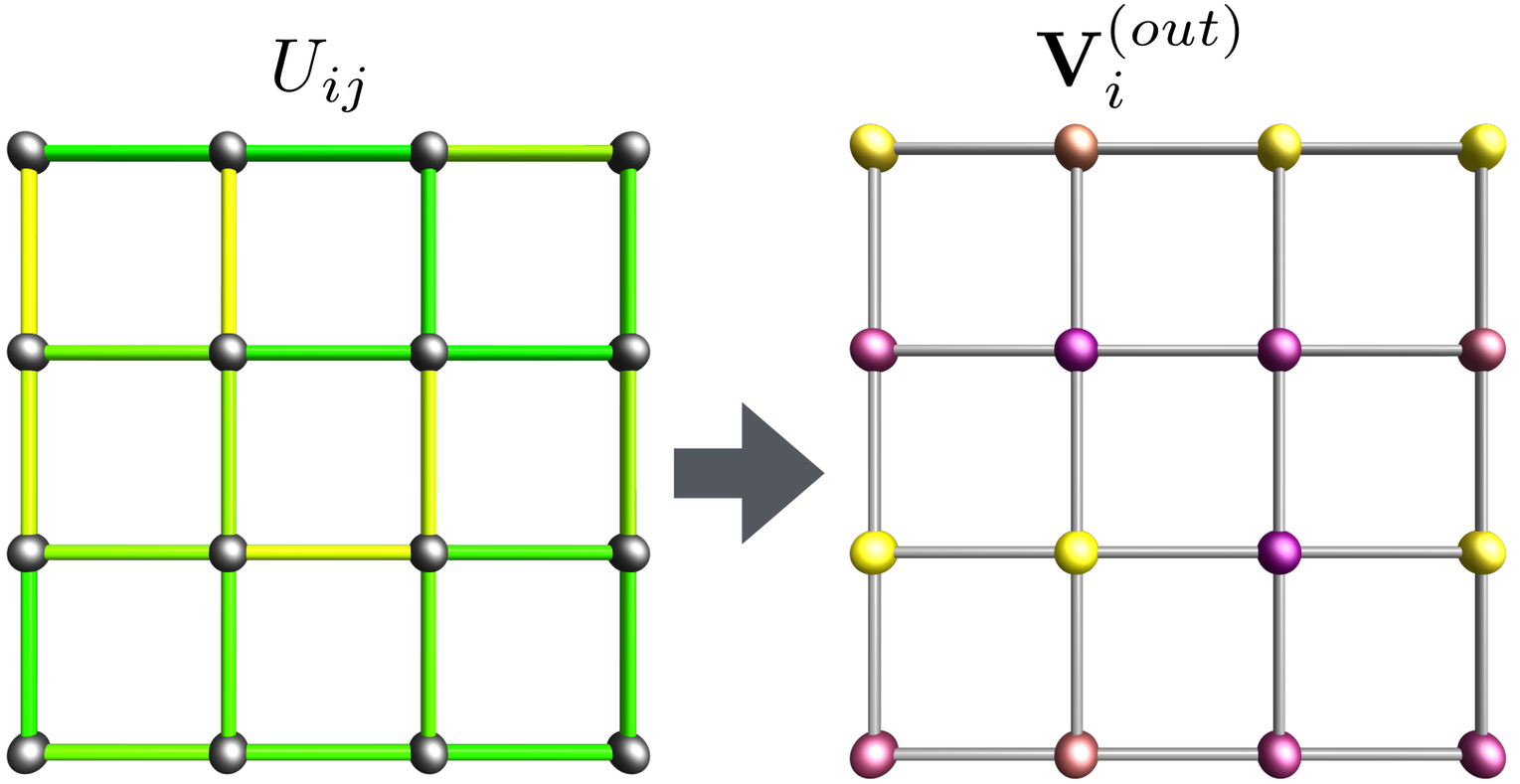
$$S[U] \;=\; -\frac{\beta}{2}\sum_{\square}\mathrm{Re}\,\mathrm{Tr}\left(U_{ij}U_{jk}U_{kl}U_{li}\right),$$




- Similar to the Behler-Parrinello scheme

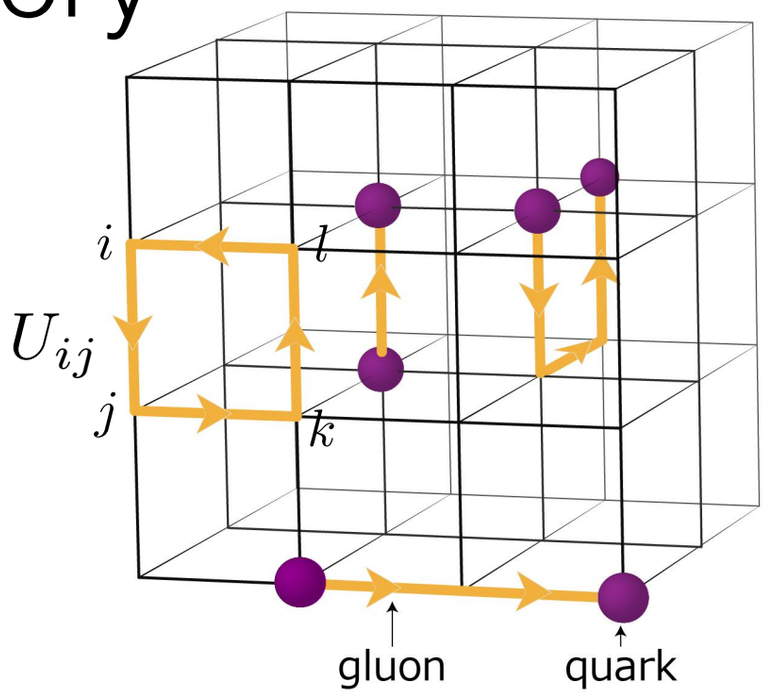
$$S = \sum_i \epsilon_i$$

$$\epsilon_i = \mathrm{MLP}_{\boldsymbol{\theta}}(\mathbf{V}_i^{(\mathrm{out})}) = \mathcal{E}(\{U_{jk}\})$$



# Benchmark: 4D Wilson gauge theory

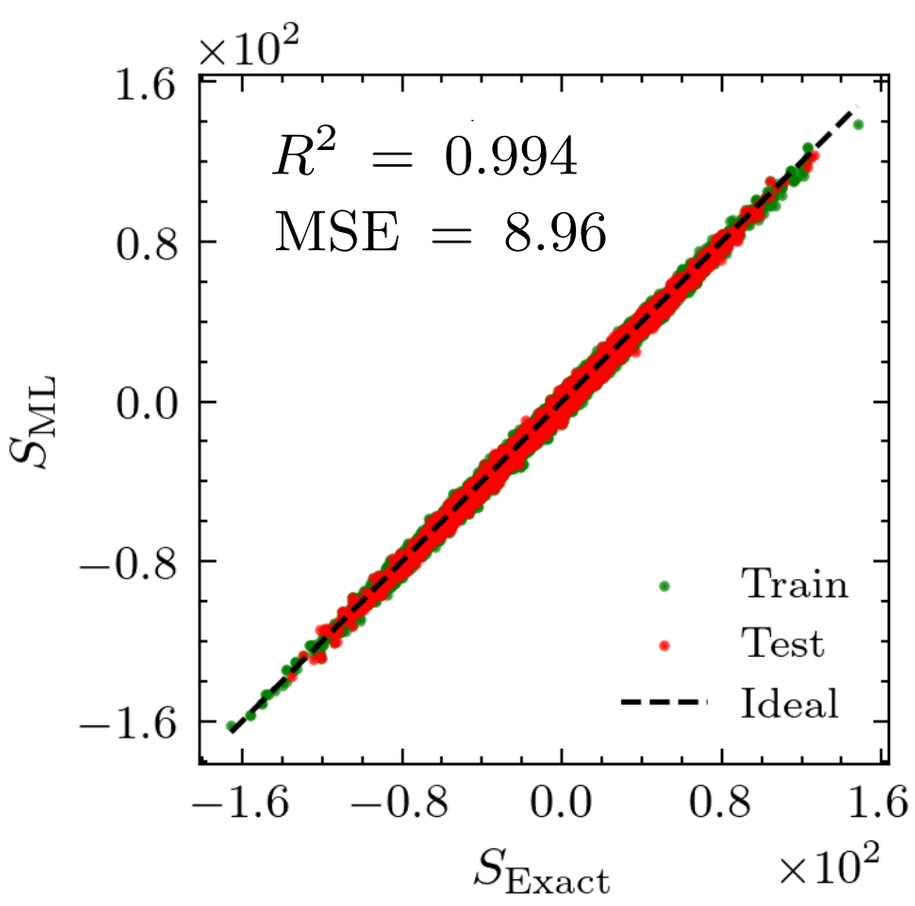
$$S[U] = -\frac{\beta}{2}\sum_{\square}\mathrm{Re}\,\mathrm{Tr}\left(U_{ij}U_{jk}U_{kl}U_{li}\right),$$

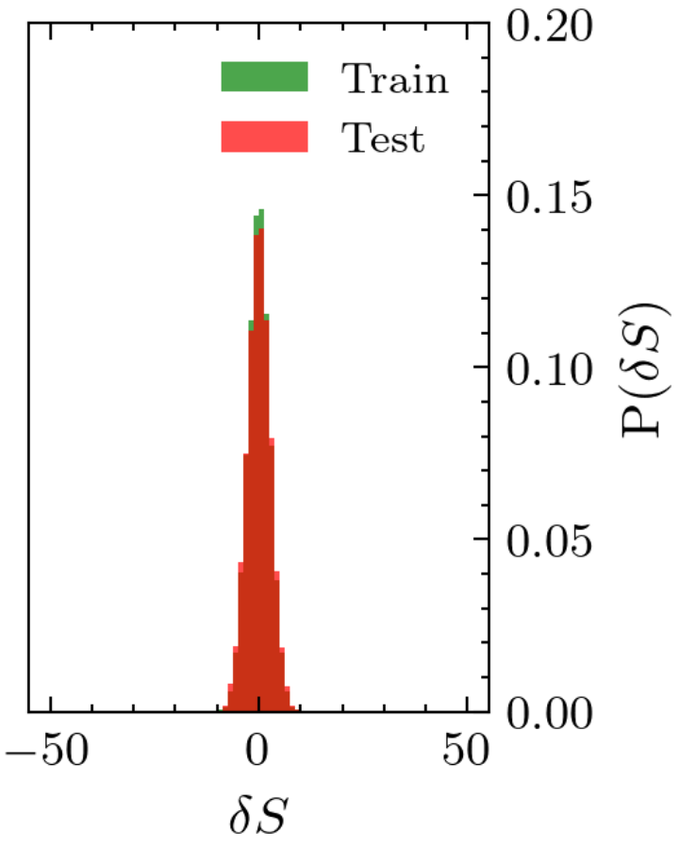



- Similar to the Behler-Parrinello scheme

$$S = \sum_i \epsilon_i$$

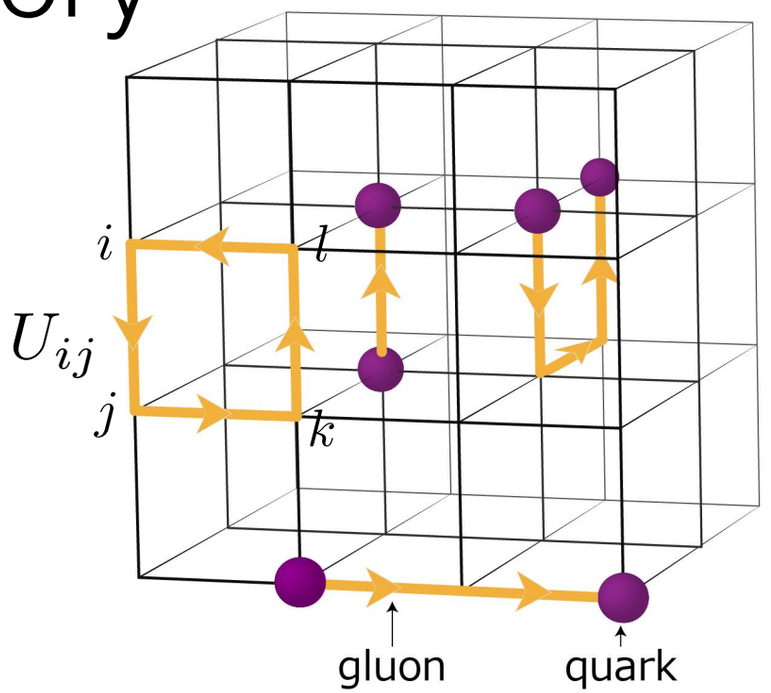
$$\epsilon_i = \mathrm{MLP}_{\boldsymbol{\theta}}(\mathbf{V}_i^{(\mathrm{out})}) = \mathcal{E}(\{U_{jk}\})$$



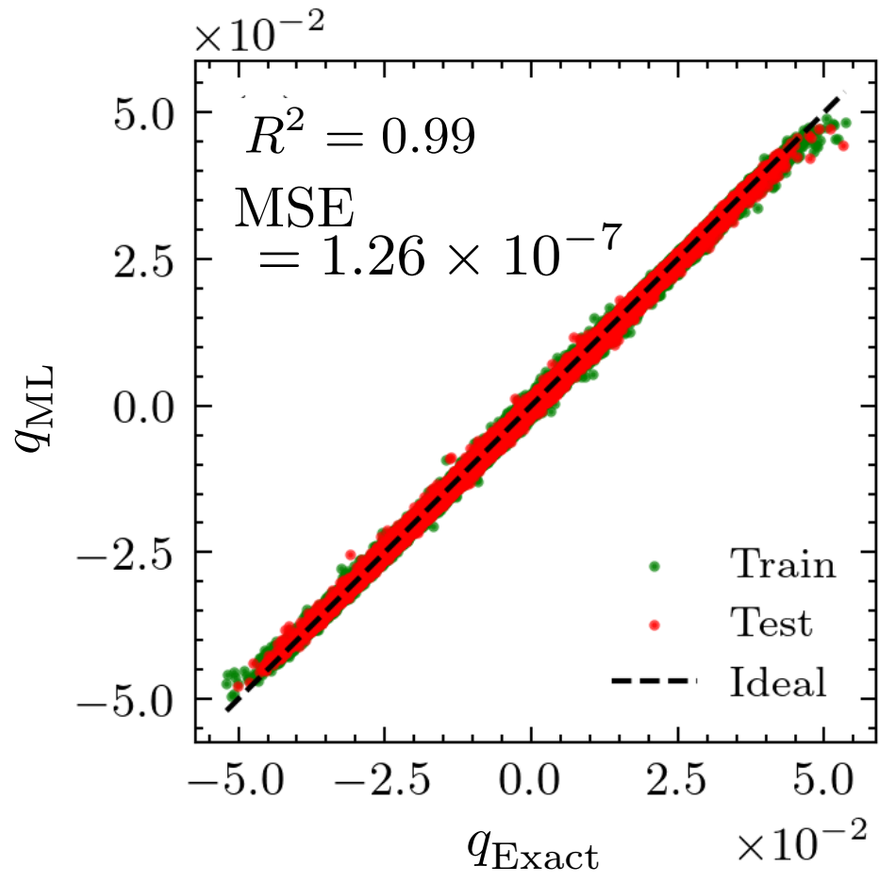
# Benchmark: 4D Wilson gauge theory

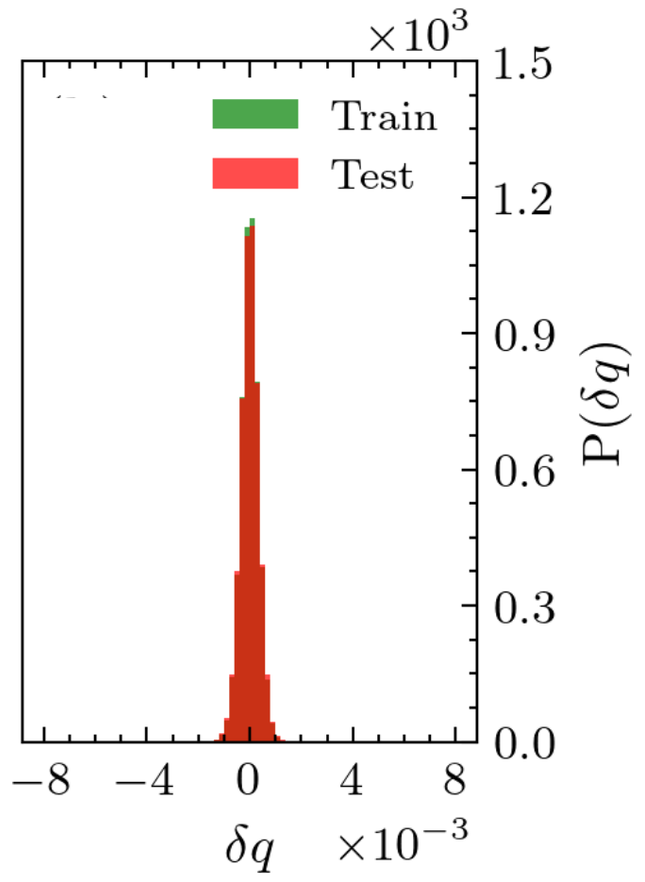
$$q_i = \frac{1}{32\pi^2}\,\epsilon_{\mu\nu\rho\sigma}\,\mathrm{Tr}\left[\frac{U_{i,\mu\nu}-U_{i,\mu\nu}^{\dagger}}{2i}\,\frac{U_{i,\rho\sigma}-U_{i,\rho\sigma}^{\dagger}}{2i}\right],$$




$$q_i = \mathrm{MLP}_{\boldsymbol{\theta}}(\mathbf{V}_i^{(\mathrm{out})})$$

$$= \mathcal{Q}(\{U_{jk}\})$$



# Benchmark: minimal gauge-matter model

- Tight-binding model

$$\mathcal{H} = \sum_{\langle ij \rangle} \psi_i^\dagger U_{ij} \psi_j + \text{h.c.},$$

$$\psi = (\psi_1, \psi_2, \cdots, \psi_N)^\dagger$$

$$U_{ij} \in \mathrm{SU(N)}$$

# Benchmark: minimal gauge-matter model

- Tight-binding model

$$\mathcal{H} = \sum_{\langle ij \rangle} \psi_i^\dagger U_{ij} \psi_j + \text{h.c.},$$

$$\psi = (\psi_1, \psi_2, \cdots, \psi_N)^\dagger$$

$$U_{ij} \in \text{SU(N)}$$

- Gauge symmetry $\quad U_{ij} \to g_i U_{ij} g_j^\dagger \qquad \psi_j \to g_j \psi_j$

# Benchmark: minimal gauge-matter model

- Tight-binding model

$$\mathcal{H} = \sum_{\langle ij \rangle} \psi_i^\dagger U_{ij} \psi_j + \text{h.c.},$$

$$\psi = (\psi_1, \psi_2, \cdots, \psi_N)^\dagger$$

$$U_{ij} \in \text{SU(N)}$$

- Gauge symmetry $\quad U_{ij} \to g_i U_{ij} g_j^\dagger \qquad \psi_j \to g_j \psi_j$

- Total energy: $\quad E(\{U_{ij}\}) = \langle \mathcal{H} \rangle = \sum_m f_{\text{FD}}(\varepsilon_m - \varepsilon_F)\epsilon_m$

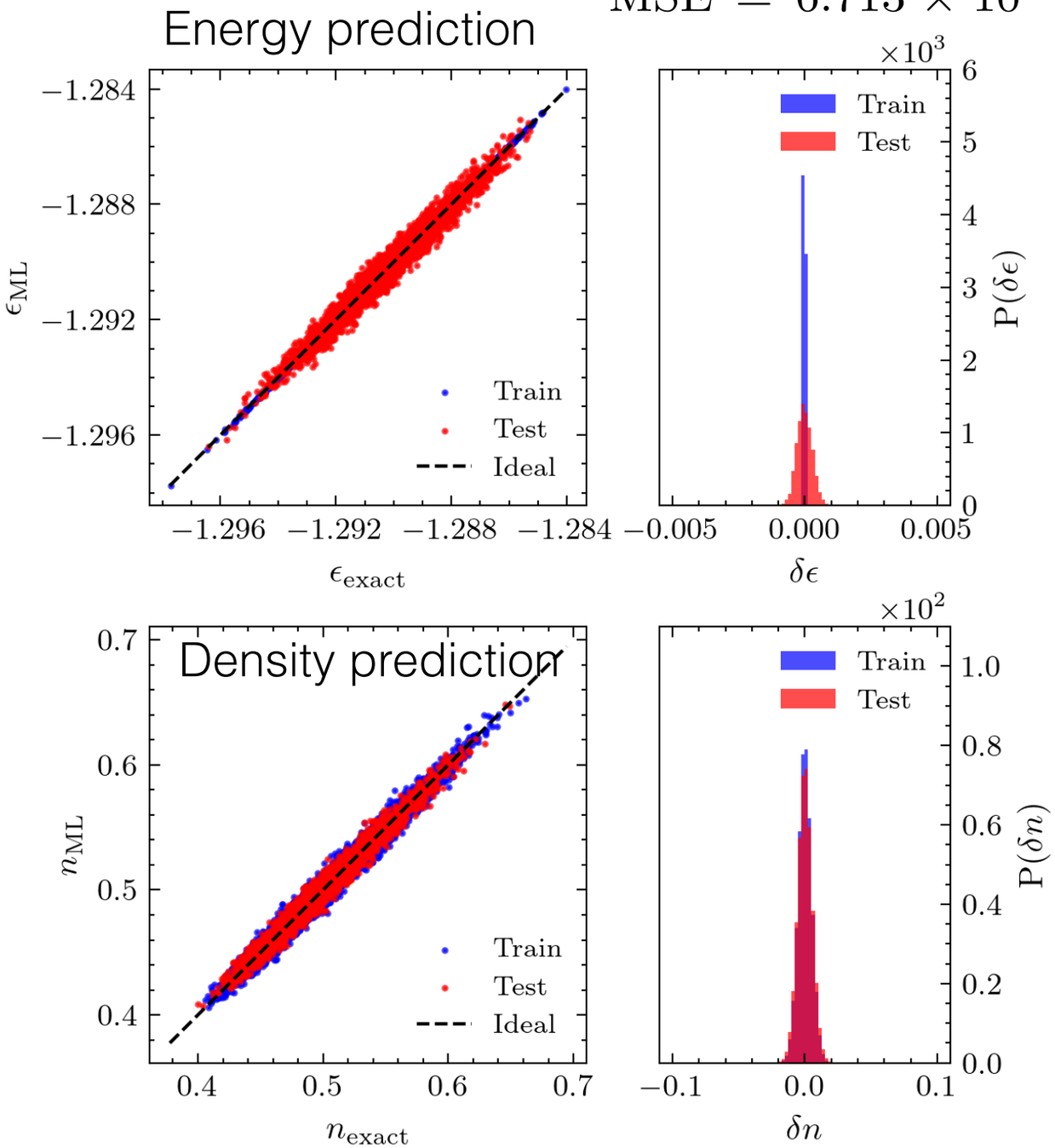
- Local fermion density:

$$n_i(\{U_{ij}\}) = \langle \psi_i^\dagger \psi_i \rangle = \sum_m f_{\text{FD}}(\varepsilon_m - \epsilon_F)|\phi_i^{(m)}|^2$$

Computed by exact diagonalization

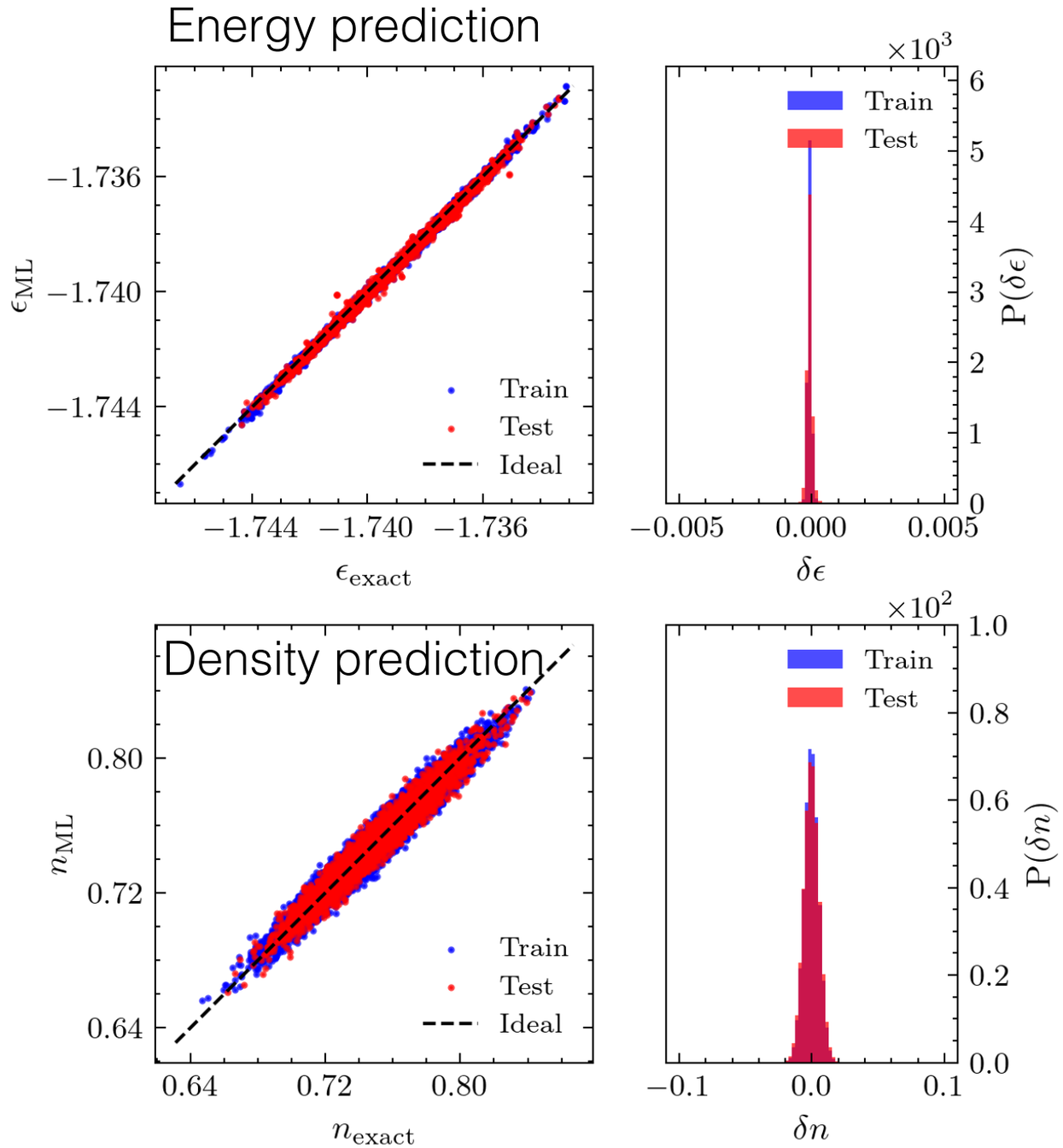
# Benchmark: minimal gauge-matter model

- SU(2) model: $R^2 = 0.9732$
  $\mathrm{MSE} = 6.713 \times 10^{-8}$




$R^2 = 0.9759 \quad \mathrm{MSE} = 2.8878 \times 10^{-5}$

- SU(3) model: $R^2 = 0.9941$
  $\mathrm{MSE} = 1.615 \times 10^{-8}$




$R^2 = 0.9525 \quad \mathrm{MSE} = 3.2615 \times 10^{-5}$

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

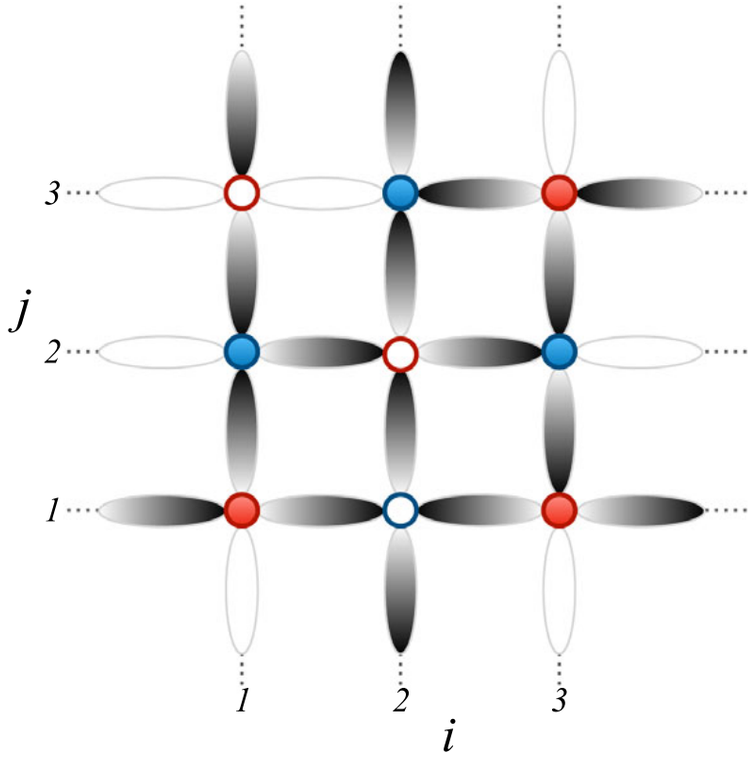
Chandrasekharan & Wiese, Nucl. Phys. B 492, 455 (1997)

- Finite-dimensional reformulation of lattice gauge theories
- Gauge fields represented by quantum spin/link operators

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

Chandrasekharan & Wiese, Nucl. Phys. B 492, 455 (1997)

- Finite-dimensional reformulation of lattice gauge theories
- Gauge fields represented by quantum spin/link operators
- Realizable in AMO experiments




Matter field

$$(-1)^{i+j} = +1 : \begin{cases} = \varnothing \\ = q \end{cases}$$

$$(-1)^{i+j} = -1 : \begin{cases} = \varnothing \\ = -q \end{cases}$$

Gauge field

$$E_{x,\mu_x} = \begin{cases} = |\rightarrow\rangle \\ = |\varnothing\rangle \\ = |\leftarrow\rangle \end{cases}$$

$$\hat{H} = -t\sum_{x,\mu}(\hat{\psi}^{\dagger}_{x}\hat{U}_{x,\mu}\hat{\psi}_{x+\mu} + \text{H.c.})$$

$$+ m\sum_{x}(-1)^{x}\hat{\psi}^{\dagger}_{x}\hat{\psi}_{x} + \frac{g_e^2}{2}\sum_{x,\mu}\hat{E}^2_{x,\mu}$$

$$- \frac{g_m^2}{2}\sum_{x}(\hat{U}_{x,\mu_x}\hat{U}_{x+\mu_x,\mu_y}\hat{U}^{\dagger}_{x+\mu_y,\mu_x}\hat{U}^{\dagger}_{x,\mu_y} + \text{H.c.}),$$

$$U_{ij} \sim \hat{S}^{\pm}_{ij} \qquad E_{ij} \sim \hat{S}^{z}_{ij}$$

PHYSICAL REVIEW X **10,** 041040 (2020)

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

- Minimal SU(2) QLM model

$$H = \sum_{\langle ij \rangle} \frac{g^2}{2} \mathbf{L}_{ij}^2 + \sum_{\langle ij \rangle} \psi_i^\dagger U_{ij} \psi_j,$$

$$U_{ij} \in \mathrm{SU}(2)$$

$$\mathbf{L}_{ij} = (L_{ij}^x, L_{ij}^y, L_{ij}^z) \in \mathfrak{su}(2)$$

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

- Minimal SU(2) QLM model

$$H = \sum_{\langle ij \rangle} \frac{g^2}{2} \mathbf{L}_{ij}^2 + \sum_{\langle ij \rangle} \psi_i^\dagger U_{ij} \psi_j,$$

$$U_{ij} \in \mathrm{SU}(2)$$

$$\mathbf{L}_{ij} = (L_{ij}^x, L_{ij}^y, L_{ij}^z) \in \mathfrak{su}(2)$$

- Commutators (Poisson brackets)

$$[\mathbf{L}_{ij}, U_{kl}] = -\frac{1}{2} \delta_{ik} \delta_{jl} \boldsymbol{\sigma} U_{ij} \qquad [L_{ij}^a, L_{kl}^b] = i \epsilon_{abc} \delta_{ik} \delta_{jl} L_{ij}^c$$

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

- Minimal SU(2) QLM model

$$H = \sum_{\langle ij \rangle} \frac{g^2}{2} \mathbf{L}_{ij}^2 + \sum_{\langle ij \rangle} \psi_i^\dagger U_{ij} \psi_j,$$

$$U_{ij} \in \mathrm{SU}(2)$$

$$\mathbf{L}_{ij} = (L_{ij}^x, L_{ij}^y, L_{ij}^z) \in \mathfrak{su}(2)$$

- Commutators (Poisson brackets)

$$[\mathbf{L}_{ij}, U_{kl}] = -\frac{1}{2} \delta_{ik} \delta_{jl} \boldsymbol{\sigma} U_{ij} \qquad [L_{ij}^a, L_{kl}^b] = i \epsilon_{abc} \delta_{ik} \delta_{jl} L_{ij}^c$$

- Equation of motion:

$$\frac{d}{dt} \mathbf{L}_{ij} = \mathbf{F}_{ij}[\{U\}] \qquad \frac{d}{dt} U_{ij} = -i \frac{g^2}{2} \left( \mathbf{L}_{ij} \cdot \boldsymbol{\sigma} \right) U_{ij} + \cdots$$

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

- "Force": $\frac{d}{dt}\mathbf{L}_{ij} = \mathbf{F}_{ij}[\{U\}] = -\mathrm{Im}\,\mathrm{Tr}[\boldsymbol{\sigma}\, U_{ij}\, \rho_{ij}]$

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

- "Force": $\frac{d}{dt}\mathbf{L}_{ij} = \mathbf{F}_{ij}[\{U\}] = -\mathrm{Im}\,\mathrm{Tr}[\boldsymbol{\sigma}\, U_{ij}\, \rho_{ij}]$

- Fermion density matrix

$$\rho_{ij} = \sum_m f_{\mathrm{FD}}(\varepsilon_m - \varepsilon_F)\phi_i^{(m)*}\phi_j^{(m)}$$

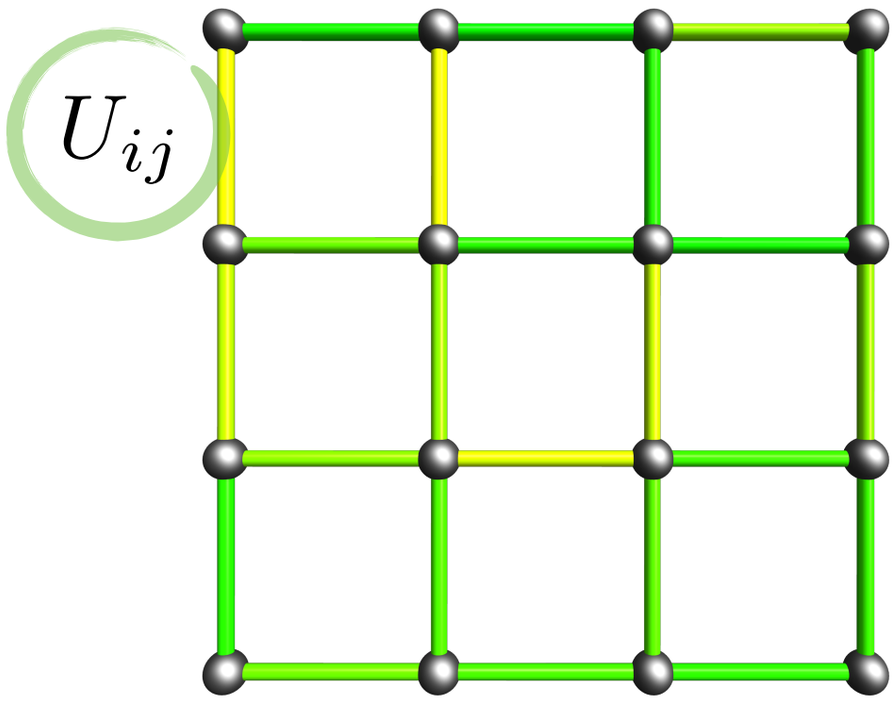
exact diagonalization

# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

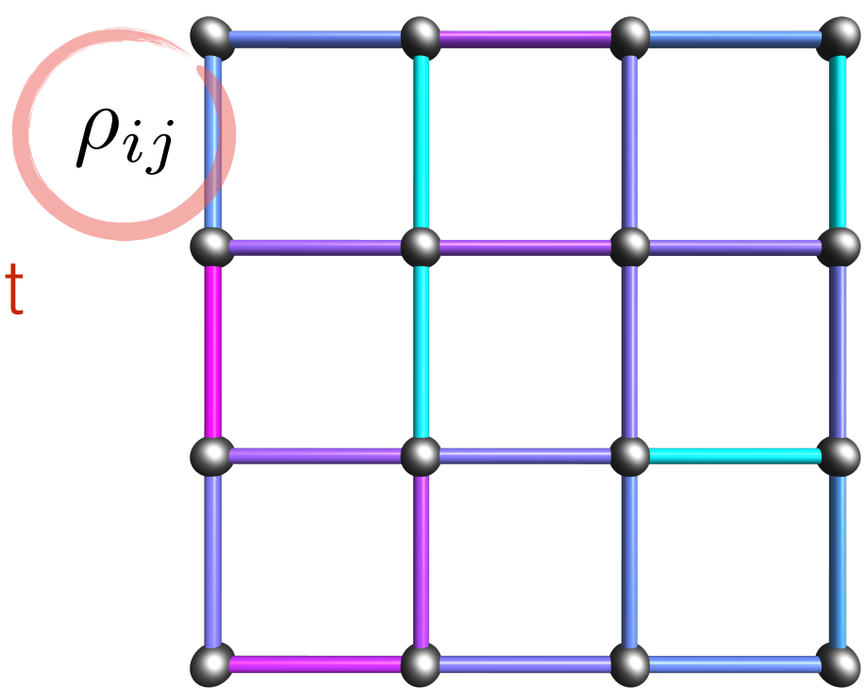
- "Force": $\frac{d}{dt}\mathbf{L}_{ij} = \mathbf{F}_{ij}[\{U\}] = -\mathrm{Im}\,\mathrm{Tr}[\boldsymbol{\sigma}\, U_{ij}\, \rho_{ij}]$

- Fermion density matrix exact diagonalization

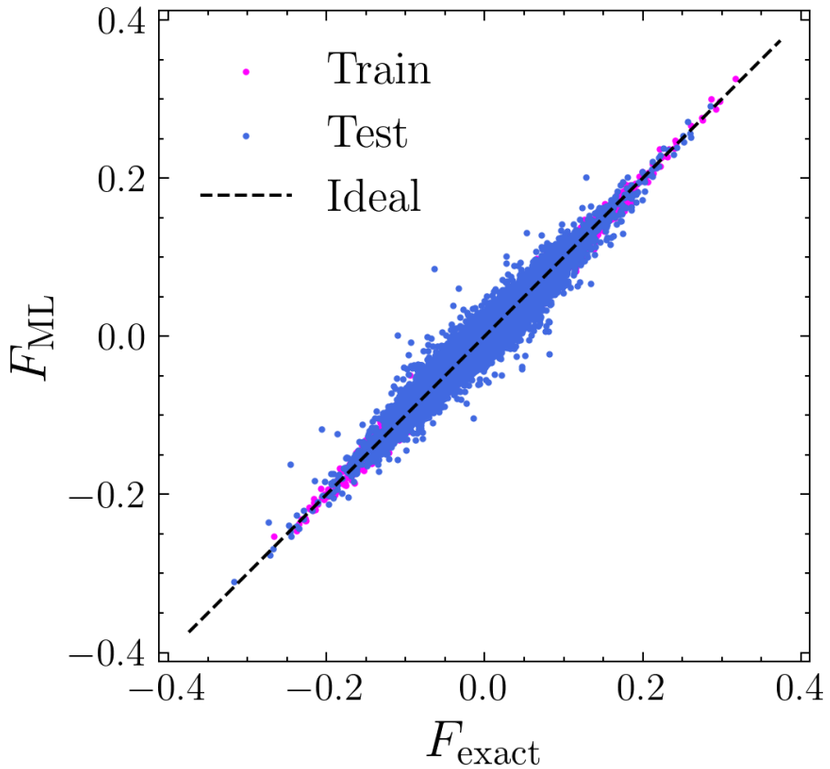
$$\rho_{ij} = \sum_m f_{\mathrm{FD}}(\varepsilon_m - \varepsilon_F)\phi_i^{(m)*}\phi_j^{(m)}$$

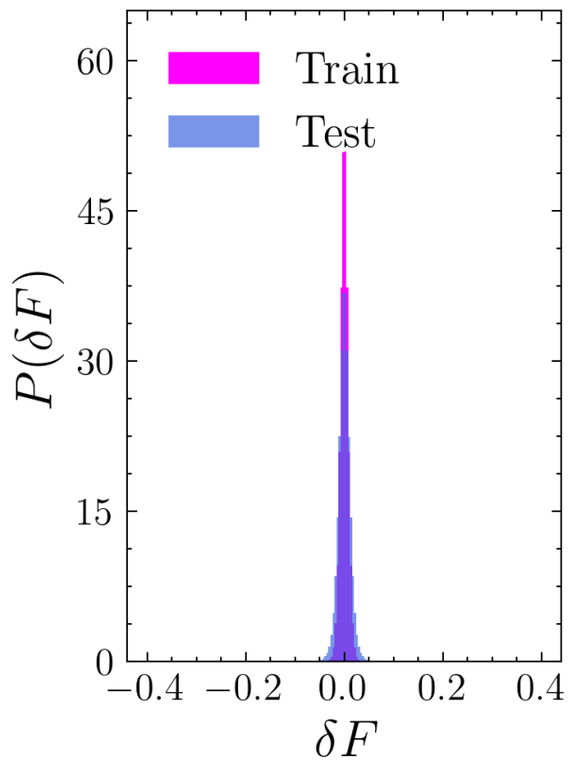



Gauge-Equivariant GNN



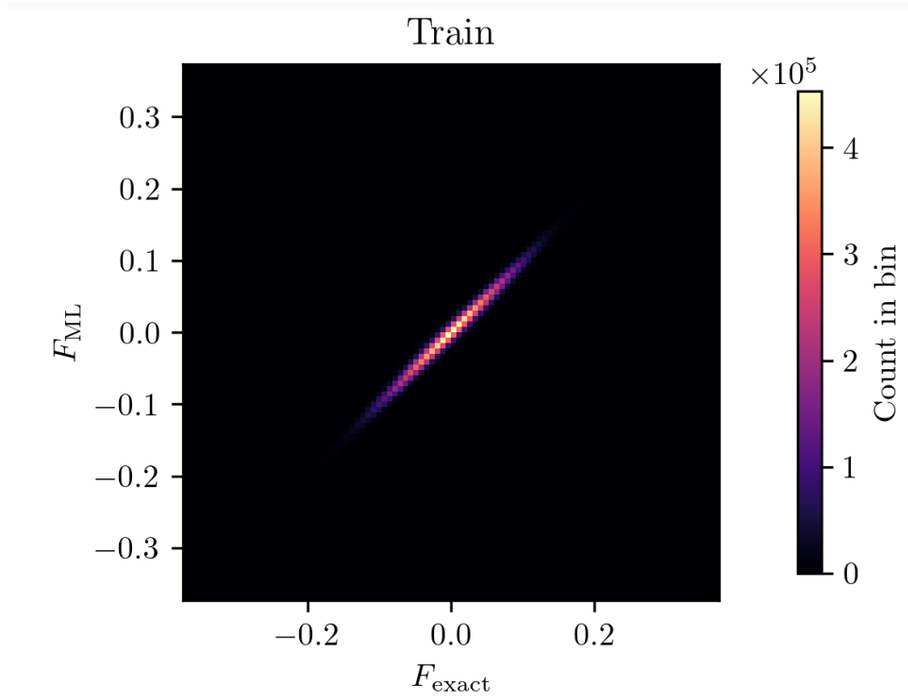
# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)



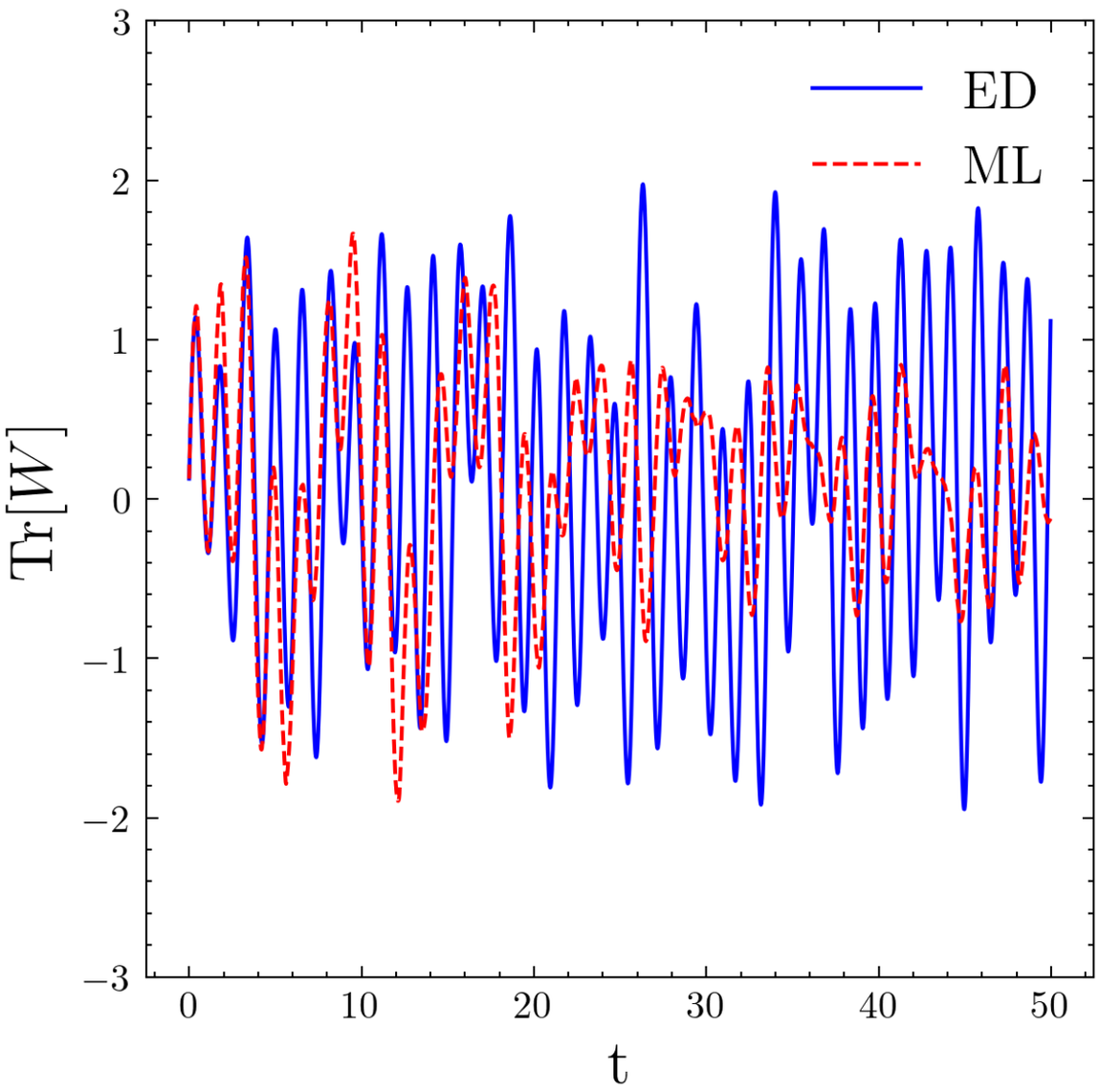



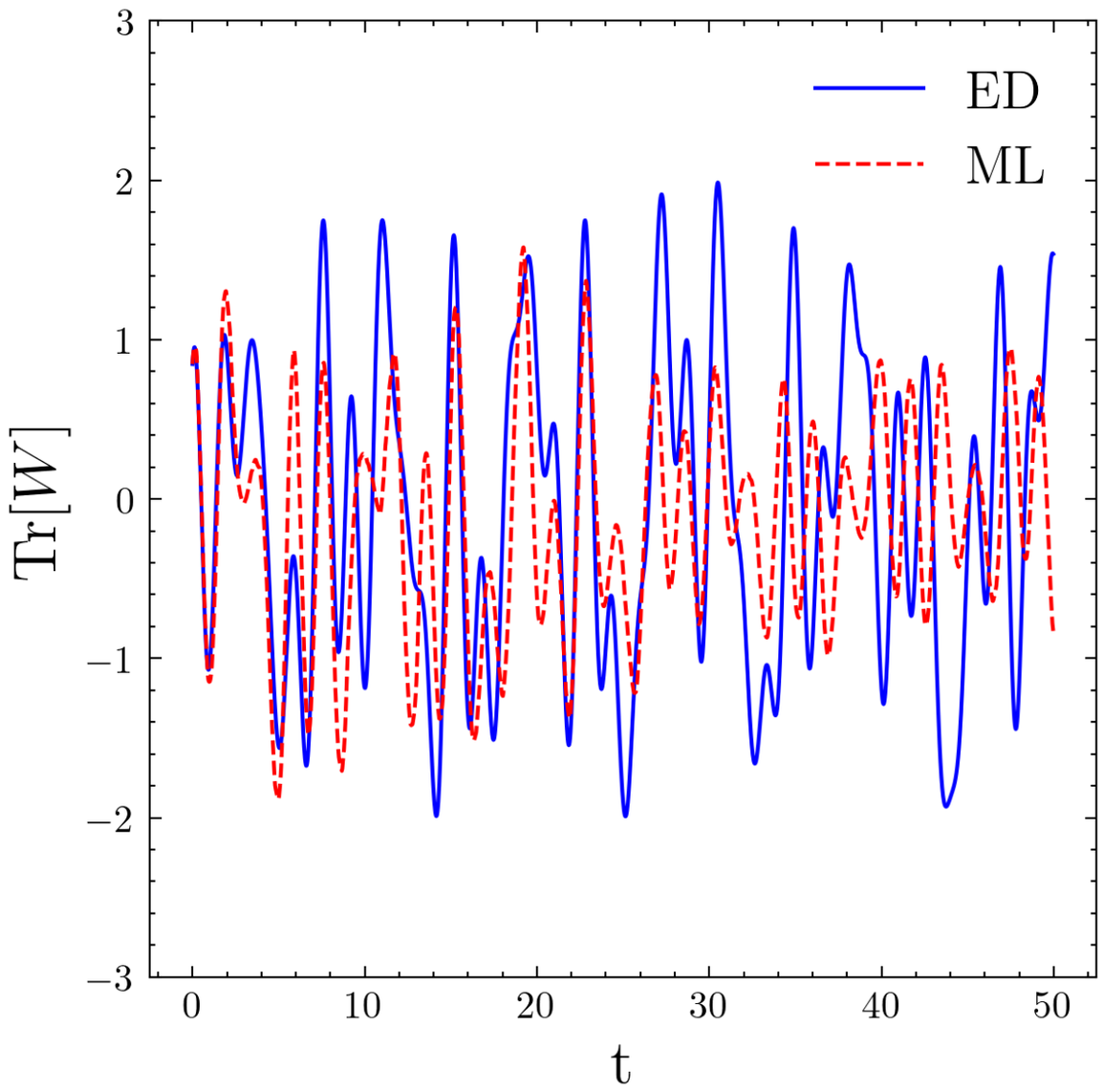

| Metric | Value |
|---|---|
| Train $R^2$ | 0.9813 |
| Test $R^2$ | 0.9541 |

$$\mathrm{MSE} = 1.57 \times 10^{-4}$$



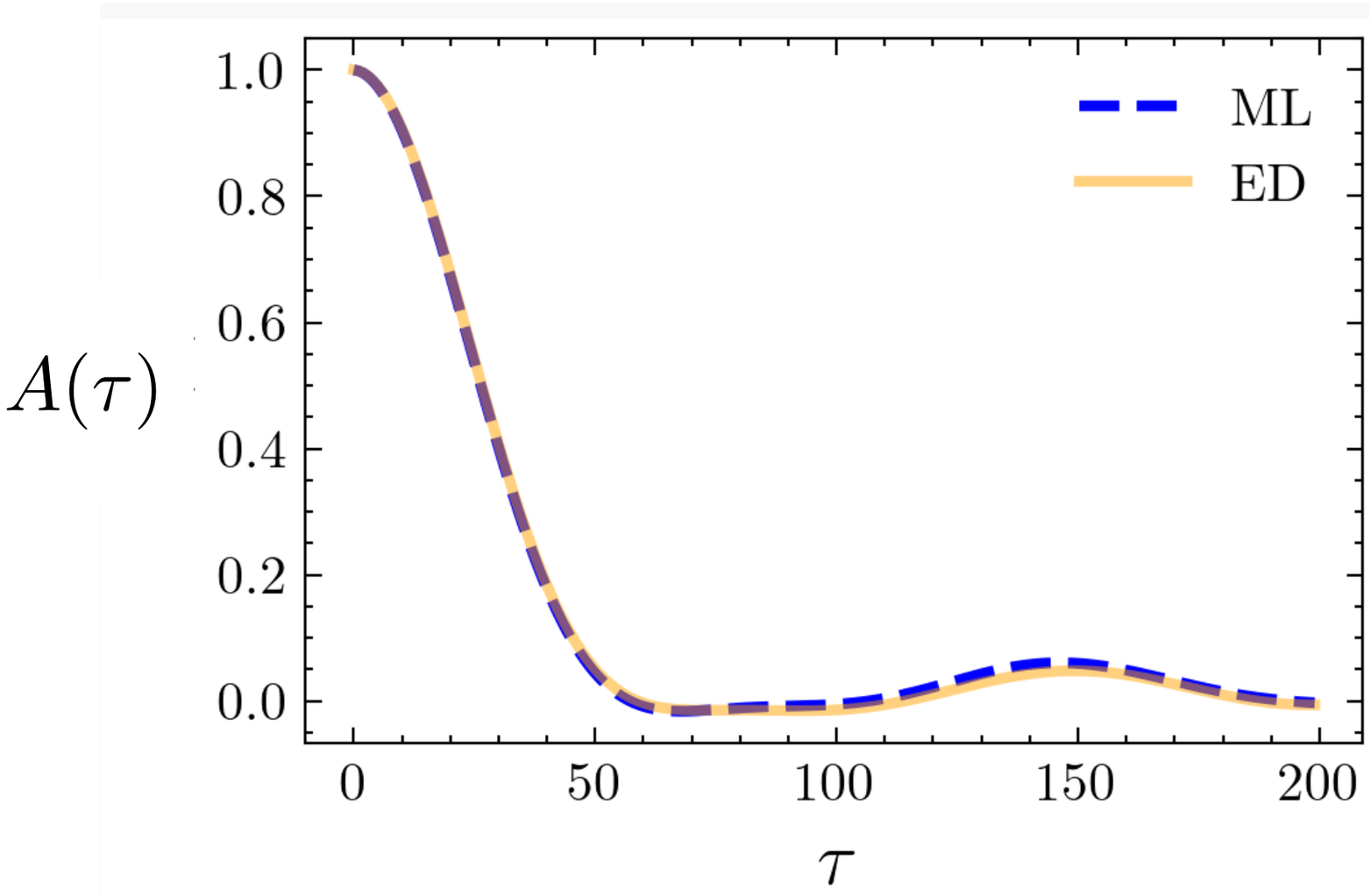
# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)



# Benchmark: semiclassical dynamics of Quantum Link Model (QLM)

- Autocorrelation function: $A(\tau) = \langle \mathrm{Re}[W_{\square}(t)]\, \mathrm{Re}[W_{\square}(t+\tau)] \rangle,$



# Summary and Outlook

- Gauge-equivariant message-passing framework with exact local symmetry built directly into the architecture.

  Benchmarks on 4D SU(3) Wilson gauge theory,
  gauge–matter systems, and dynamics of 2D SU(2) QLM

- Accurate and scalable surrogate modeling for lattice gauge systems.

- Gauge-equivariant ML approaches for preconditioning and accelerating fermionic inversions in full lattice QCD simulations.

- Symmetry-aware surrogate models for disconnected-diagram and all-to-all propagator calculations. (With M. Engelhardt, H.-W. Lin, S. Liuti)

Thank You !