

Equivariant Tensor Property Prediction with Graph Neural Networks

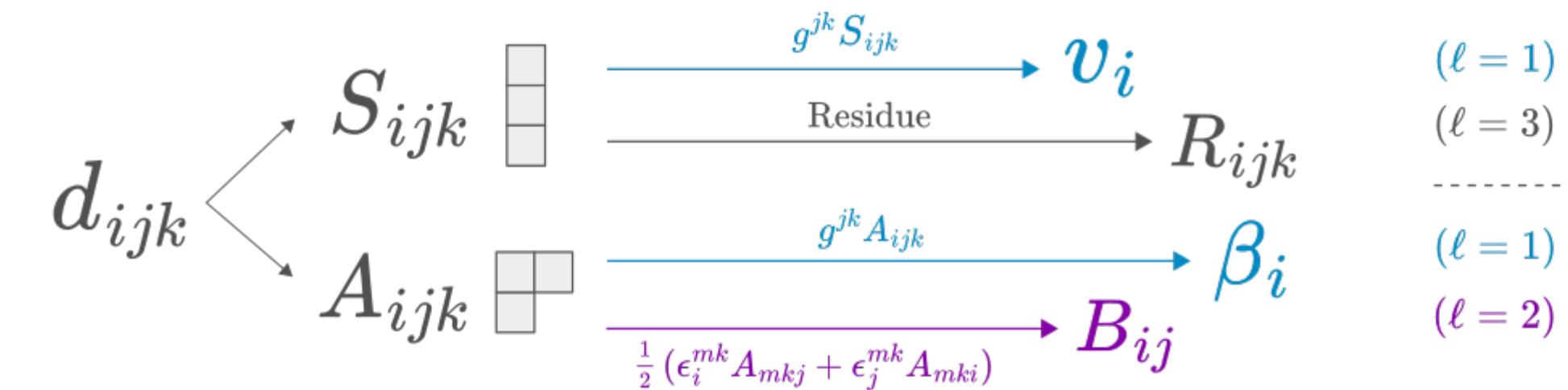
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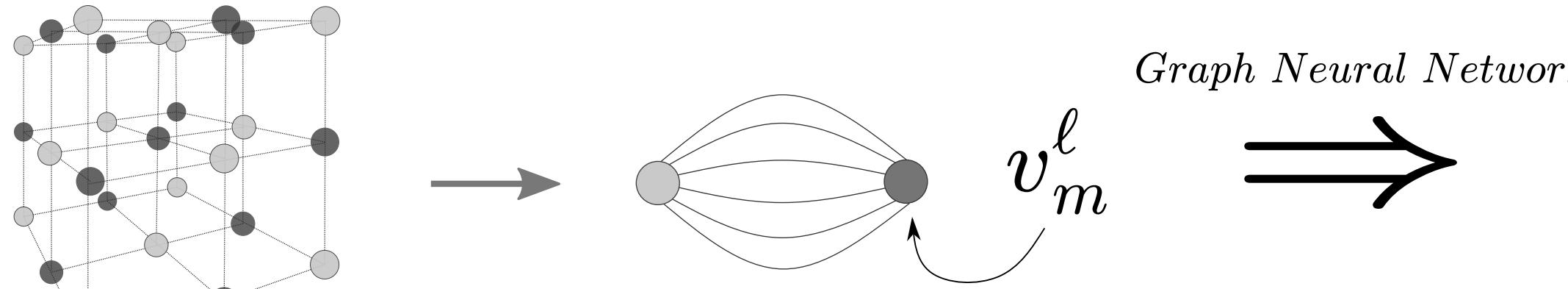
Equivariance

$$\begin{array}{ccc} x & \xrightarrow{f} & y \\ D^x(R) \downarrow & & \downarrow D^y(R) \\ Rx & \xrightarrow{f} & Ry \end{array}$$

Harmonic Tensor Decompositions



Equivariant Networks



Tensor Prediction

- Dielectric ϵ_{ij}
- Piezoelectric d_{ijk}
- Elasticity C_{ijkl}