Supplementary information: An SO(3)-equivariant reciprocal space neural potential for long-range interactions

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1 Comparison with existing long-range methods

Existing approaches to long-range modeling in machine-learned interatomic potentials can be understood as a progression from local corrections to global, symmetry-aware architectures. Early empirical correction schemes simply appended predefined electrostatic or dispersion baselines to short-range MLIPs. Although such schemes are simple and computationally efficient, these post hoc corrections separate the long-range contribution from the learned energy surface, may weaken the consistency between energy and force predictions, and cannot account for environment-dependent effects such as charge transfer or polarization. An important advance was the prediction of physically meaningful quantities from local atomic environments, followed by the use of these quantities to construct long-range interactions. PhysNet (Unke and Meuwly, 2019) jointly learned atomic energies and partial charges in a multitask framework, allowing the predicted charges to be used for both electrostatic energy prediction and observables such as dipole moments. 4G-HDNNP (Ko et al., 2021) extended this idea by introducing charge equilibration, which enabled self-consistent charge distributions and long-range charge transfer globally. DPLR (Zhang et al., 2022) followed a different strategy by predicting maximally localized Wannier function centers, thereby avoiding the ambiguity of partial-charge definitions, but at the cost of additional labels, increased model complexity, and applicability that is largely limited to insulating systems. Despite their physical interpretability, these early real-space methods share several limitations: they generally follow a two-step strategy, assume that the relevant long-range variables are largely determined by local environments, and mainly rely on scalar quantities such as charges, thereby neglecting the directional and tensorial structure of long-range interactions.

Message-passing neural networks such as SchNet (Schütt et al., 2018), NequIP (Batzner et al., 2022), and MACE (Batatia et al., 2022) address the locality problem from a different angle by enlarging the receptive field through multiple layers of graph-based communication. This improves the modeling of short- and intermediate-range interactions, and equivariant variants further improve sensitivity to directional information. However, MPNNs still have a basic limitation in connectivity: when two subsystems are separated by more than the cutoff radius, they are disconnected in the graph and cannot exchange information, regardless of network depth. As a result, even equivariant message passing is not sufficient for truly long-range electrostatics beyond the effective graph radius.

Fourier space methods offer a more natural way to incorporate global communication. LODE (Huguenin-Dumittan et al., 2023) encodes physically motivated long-range fields, such as $1/r^p$ potentials, into equivariant descriptors by first constructing a global potential field and then projecting it onto spherical harmonics in a local form. This gives LODE clear physical interpretability and rotational equivariance, and also allows different choices of p to capture Coulombic, dipolar, or dispersive interactions. However, LODE remains sensitive to the choice of p, can become high-dimensional, and tends to work best on chemically homogeneous datasets. Ewald message-passing (Kosmala et al., 2023) methods made Fourier space modeling more data-driven by replacing predefined interaction forms with learnable frequency filters applied to structure factors

computed from atomic descriptors rather than charges. Still, these early Ewald message-passing schemes relied mainly on scalar structure factors. This made them efficient, but also limited their ability to represent anisotropy and multipolar correlations. LES (Cheng, 2025) further simplified Fourier space long-range modeling. Instead of predicting physically constrained charges, it learned latent variables q_i directly from invariant atomic features and applied Ewald summation to these learned quantities. This made LES simple, flexible, and trainable directly from energies and forces without explicit charge labels. When restricted to one dimension, the latent variable could even be interpreted as an effective charge and used to recover dipoles, quadrupoles, and Born effective charges. Even so, LES still represented long-range communication through scalar structure factors. Therefore, although it avoided the ambiguity of charge definitions and performed well on molecular dimers, molten salts, and aqueous systems, it did not explicitly preserve the full tensorial structure of long-range interactions.

Against this background, EquiEwald represents a qualitatively distinct stage in the development of long-range modeling. As emphasized in our review, the central limitation of most earlier Fourier space methods is not the lack of global information, but rather their reliance on scalar representations. Scalar structure factors and scalar descriptors lose essential directional and tensorial information through angular averaging, even though such information is critical for dipole–dipole interactions, quadrupolar effects, and anisotropic polarization, particularly in systems with strong directional dependence. EquiEwald addresses this limitation by embedding Ewald summation directly into the irreducible representation space of an $SO(3)$-equivariant model. For each spherical-harmonic degree and magnetic index, it constructs degree-resolved structure factors, applies learnable Fourier space filters shared across all m-components within the same degree to preserve equivariance, and maps the filtered signals back to atomic features via an inverse transform. It also combines degree-specific nonlinearities with scalar gating to modulate higher-order features. In this way, EquiEwald preserves the full set of angular-momentum components throughout the Fourier space communication pathway, explicitly captures anisotropy and multipolar correlations, and treats long-range physics not as an external correction, but as an architectural component of the representation itself. For this reason, it marks the final stage in the development summarized in this review, from local to global modeling, from scalar to tensor representations, and from post hoc correction to deep architectural integration.

2 Equivariance of the EquiEwald Module

We distinguish between the equivariance of the continuous Fourier space operator, the periodic discrete implementation, and the finite-grid implementation used for aperiodic structures. The periodic implementation is equivariant under a rigid co-rotation of the atomic coordinates and the simulation cell, subject to the conditions stated below. By contrast, the fixed Cartesian frequency grid used for aperiodic structures provides an approximate, resolution-dependent discretization of the corresponding continuous equivariant operator.

2.1 Degree-resolved Fourier space operator

At a given interaction layer, the atom-wise feature of degree ℓ is written as

$$\mathbf{x}_j^{(\ell)} = \left[\mathbf{x}_{j,m}^{(\ell)}\right]_{m=-\ell}^{\ell}, \qquad \mathbf{x}_{j,m}^{(\ell)} \in \mathbb{R}^C, \tag{1}$$

where $m = -\ell, \ldots, \ell$ indexes the m-components and C denotes the number of channels associated with degree ℓ. Under a rotation $R \in SO(3)$, these features transform as

$$\mathbf{x}_{j,m}^{(\ell)\prime} = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(\ell)}(R)\mathbf{x}_{j,m'}^{(\ell)}, \tag{2}$$

where $D^{(\ell)}(R)$ is the Wigner matrix for the degree-ℓ irreducible representation. The Wigner matrix acts on the magnetic index, whereas the channel index is unchanged.

For a discrete set of reciprocal vectors $\mathcal{K} = \{\mathbf{k}_\alpha\}_{\alpha=1}^{N_k}$, the degree-resolved forward accumulation is

$$\mathbf{s}_{\alpha,m}^{(\ell)} = \sum_{j\in\mathcal{S}} \omega_\Delta\left(\mathbf{k}_\alpha, \mathbf{r}_j\right) \exp\left(-\mathrm{i}\mathbf{k}_\alpha^\top \mathbf{r}_j\right) \mathbf{x}_{j,m}^{(\ell)} \in \mathbb{C}^C. \tag{3}$$

Here $\omega_\Delta(\mathbf{k}, \mathbf{r})$ is the scalar sampling factor associated with the selected Fourier space discretization. For the periodic reciprocal-lattice implementation, $\omega_\Delta = 1$.

2.2 Sufficient conditions for equivariance

Consider a rotated structure $X' = RX$, with

$$\mathbf{r}_j' = R\mathbf{r}_j. \tag{4}$$

A discrete equivariance result requires the reciprocal sampling set to co-rotate with the structure,

$$\mathcal{K}(X') = R\mathcal{K}(X) = \{R\mathbf{k}_\alpha : \mathbf{k}_\alpha \in \mathcal{K}(X)\}. \tag{5}$$

In addition, the sampling factor and spectral filter satisfy

$$\omega_\Delta\left(R\mathbf{k}, R\mathbf{r}\right) = \omega_\Delta\left(\mathbf{k}, \mathbf{r}\right), \tag{6}$$

$$\mathbf{W}_\ell(R\mathbf{k}) = \mathbf{W}_\ell(\mathbf{k}). \tag{7}$$

For a frequency-dependent channel filter, rotational equivariance additionally requires Eq. (7). Sharing the channel operation across all components guarantees commutation with the Wigner-$D^{(\ell)}$ action at fixed $\mathbf{k}$, but does not by itself ensure rotational consistency of the filter's dependence on $\mathbf{k}$.

For a reciprocal vector $\mathbf{k}_\alpha$ and its rotated counterpart

$$\mathbf{k}'_\alpha = R\mathbf{k}_\alpha, \tag{8}$$

the Fourier phase is invariant under the simultaneous rotation of positions and reciprocal vectors:

$$(\mathbf{k}'_\alpha)^\top \mathbf{r}'_j = (R\mathbf{k}_\alpha)^\top (R\mathbf{r}_j) = \mathbf{k}_\alpha^\top \mathbf{r}_j. \tag{9}$$

Using Eqs. (2), (6), and (9), the transformed structure factor satisfies

$$\begin{aligned}
\mathbf{s}^{(\ell)\prime}_{R\mathbf{k}_\alpha,m} &= \sum_{j\in\mathcal{S}} \omega_\Delta\left(R\mathbf{k}_\alpha, R\mathbf{r}_j\right) \exp\left[-\mathrm{i}(R\mathbf{k}_\alpha)^\top (R\mathbf{r}_j)\right] \mathbf{x}^{(\ell)\prime}_{j,m} \\
&= \sum_{m'=-\ell}^{\ell} D^{(\ell)}_{mm'}(R) \sum_{j\in\mathcal{S}} \omega_\Delta\left(\mathbf{k}_\alpha, \mathbf{r}_j\right) \exp\left(-\mathrm{i}\mathbf{k}_\alpha^\top \mathbf{r}_j\right) \mathbf{x}^{(\ell)}_{j,m'} \\
&= \sum_{m'=-\ell}^{\ell} D^{(\ell)}_{mm'}(R) \mathbf{s}^{(\ell)}_{\alpha,m'}.
\end{aligned} \tag{10}$$

Thus, paired structure factors evaluated at $\mathbf{k}_\alpha$ and $R\mathbf{k}_\alpha$ transform according to the same degree-ℓ irreducible representation as the input features.

2.3 Frequency filtering and inverse accumulation

The Fourier filter acts on the channel dimension:

$$\widetilde{\mathbf{s}}^{(\ell)}_{\alpha,m} = \mathbf{W}_\ell(\mathbf{k}_\alpha)\mathbf{s}^{(\ell)}_{\alpha,m}, \qquad \mathbf{W}_\ell(\mathbf{k}_\alpha) \in \mathbb{R}^{C\times C}. \tag{11}$$

For each fixed ℓ, the same channel matrix is applied to all $m = -\ell, \ldots, \ell$. Because $\mathbf{W}_\ell$ acts on the channel index and $D^{(\ell)}(R)$ acts on the magnetic index, these two operations commute. Together with Eq. (7), this gives

$$\widetilde{\mathbf{s}}^{(\ell)\prime}_{R\mathbf{k}_\alpha,m} = \sum_{m'=-\ell}^{\ell} D^{(\ell)}_{mm'}(R) \widetilde{\mathbf{s}}^{(\ell)}_{\alpha,m'}. \tag{12}$$

The atom-wise Fourier space message is obtained by inverse accumulation:

$$\mathbf{M}^{(\ell)}_{i,m} = \mathrm{Re} \sum_{\alpha=1}^{N_k} \omega_\Delta\left(\mathbf{k}_\alpha, \mathbf{r}_i\right) \exp\left(\mathrm{i}\mathbf{k}_\alpha^\top \mathbf{r}_i\right) \widetilde{\mathbf{s}}^{(\ell)}_{\alpha,m} \in \mathbb{R}^C. \tag{13}$$

For the rotated structure, the inverse accumulation is evaluated over $R\mathcal{K}$. Applying Eqs. (6), (9), and (12) yields

$$\begin{aligned}\mathbf{M}_{i,m}^{(\ell)\prime} &= \mathrm{Re}\sum_{\alpha=1}^{N_k}\omega_\Delta\left(R\mathbf{k}_\alpha, R\mathbf{r}_i\right)\exp\left[\mathrm{i}(R\mathbf{k}_\alpha)^\top(R\mathbf{r}_i)\right]\widetilde{\mathbf{s}}_{R\mathbf{k}_\alpha,m}^{(\ell)\prime} \\ &= \sum_{m'=-\ell}^{\ell} D_{mm'}^{(\ell)}(R)\mathbf{M}_{i,m'}^{(\ell)}. \end{aligned} \tag{14}$$

The inverse-accumulated message therefore transforms as a degree-ℓ feature whenever the frequency-set, sampling-factor, and filter conditions in Eqs. (5)–(7) are satisfied.

2.4 Equivariant atom-wise update

After inverse accumulation, EquiEwald applies a degree-specific linear channel map

$$\mathbf{U}_{i,m}^{(\ell)} = \eta\,\mathbf{A}_\ell\mathbf{M}_{i,m}^{(\ell)}, \qquad \mathbf{A}_\ell \in \mathbb{R}^{C\times C}, \tag{15}$$

where η is the normalization factor used in the implementation. The same matrix $\mathbf{A}_\ell$ is applied to every m-components within degree ℓ. Consequently,

$$\mathbf{U}_{i,m}^{(\ell)\prime} = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(\ell)}(R)\mathbf{U}_{i,m'}^{(\ell)}. \tag{16}$$

For $\ell > 0$, the projected message is modulated by a channel-wise gate computed from the invariant scalar block:

$$\mathbf{g}_i^{(\ell)} = \sigma\left(\mathbf{W}_g^{(\ell)}\mathbf{x}_i^{(0)}\right) \in \mathbb{R}^C. \tag{17}$$

Because $\mathbf{x}_i^{(0)}$ is invariant under rotations,

$$\mathbf{g}_i^{(\ell)\prime} = \mathbf{g}_i^{(\ell)}. \tag{18}$$

The atom-wise long-range update is

$$\mathbf{x}_{i,m}^{\mathrm{Ewald},(\ell)} = \begin{cases}\mathbf{U}_i^{(0)}, & \ell = 0,\\ \mathbf{g}_i^{(\ell)} \odot \mathbf{U}_{i,m}^{(\ell)}, & \ell > 0,\end{cases} \tag{19}$$

where the same invariant gate is applied to all m-components. It follows that

$$\mathbf{x}_{i,m}^{\mathrm{Ewald},(\ell)\prime} = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(\ell)}(R)\mathbf{x}_{i,m'}^{\mathrm{Ewald},(\ell)}. \tag{20}$$

Importantly, no ordinary element-wise nonlinear activation is applied independently to the m components of a non-scalar feature. Applying the same ReLU, SiLU, or general nonlinear MLP independently to every m component would not commute with $D^{(\ell)}(R)$. In the implemented update, nonlinearity enters through the invariant scalar gate in Eq. (17), while $\mathbf{A}_\ell$ remains linear on the non-scalar feature blocks.

The complete long-range representation is the direct sum

$$\mathbf{x}_i^{\mathrm{Ewald}} = \bigoplus_{\ell=0}^{\ell_{\max}} \mathbf{x}_i^{\mathrm{Ewald},(\ell)}. \tag{21}$$

Under the conditions above, it transforms according to the block-diagonal direct-sum representation

$$\mathbf{x}_i^{\mathrm{Ewald}\prime} = \left[\bigoplus_{\ell=0}^{\ell_{\max}} D^{(\ell)}(R)\right] \mathbf{x}_i^{\mathrm{Ewald}}. \tag{22}$$

2.5 Periodic system and aperiodic system implementation

For a periodic simulation cell with lattice vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, the sampled reciprocal vectors are

$$\mathbf{k}_{n_x,n_y,n_z} = n_x\mathbf{b}_1 + n_y\mathbf{b}_2 + n_z\mathbf{b}_3, \tag{23}$$

where $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are the corresponding reciprocal-lattice vectors. When the complete periodic structure is rotated, the cell and reciprocal basis co-rotate:

$$\mathbf{a}'_p = R\mathbf{a}_p, \qquad \mathbf{b}'_p = R\mathbf{b}_p. \tag{24}$$

The same reciprocal indices (n_x, n_y, n_z) therefore generate

$$\mathbf{k}'_{n_x,n_y,n_z} = R\mathbf{k}_{n_x,n_y,n_z}. \tag{25}$$

Thus Eq. (5) holds. In the periodic implementation, $\omega_\Delta = 1$ and the filter $\mathbf{W}^{\mathrm{pbc}}$ is independent of $\mathbf{k}$ and shared across the m-components. Equations (6) and (7) therefore also hold. Consequently, the periodic EquiEwald implementation is $SO(3)$-equivariant under a rigid co-rotation of the atomic coordinates and the periodic simulation cell.

For aperiodic structures, the implementation uses the fixed Cartesian frequency set

$$\mathcal{K}_\Delta = \left\{\Delta k\,\mathbf{n} : \mathbf{n} \in \mathbb{Z}^3,\ \|\Delta k\,\mathbf{n}\| \le k_{\max}\right\}. \tag{26}$$

Although the continuous domain $\{\mathbf{k} : \|\mathbf{k}\| \le k_{\max}\}$ is rotationally invariant, its finite Cartesian sampling is not closed under an arbitrary rotation:

$$R\mathcal{K}_\Delta \neq \mathcal{K}_\Delta \qquad \text{for a general } R \in SO(3). \tag{27}$$

The discrete condition in Eq. (5) therefore does not hold when the atomic structure is rotated while the Cartesian grid remains fixed.

The aperiodic Frequency filter depends only on the rotational invariant $\|\mathbf{k}\|$ and hence satisfies $\mathbf{W}_\ell(R\mathbf{k}) = \mathbf{W}_\ell(\mathbf{k})$. Nevertheless, the lack of closure of the finite frequency grid introduces a resolution-dependent equivariance error. If a Cartesian voxel window is included in ω_Δ, its rotational compatibility must also be assessed through Eq. (6); a Cartesian product window is not, in general, invariant under arbitrary rotations.

Accordingly, the degree-wise channel operations remain consistent with the corresponding irreducible transformation laws, but the complete finite-grid aperiodic implementation is only approximately $SO(3)$-equivariant. It should not be identified with the equivariance of the continuous Fourier space operator.

3 eSCN and EquiformerV2 Model structures

Atomic numbers are embedded to initialize per-atom features, which are then refined by an equivariant encoder, eSCN (Passaro and Zitnick, 2023) or EquiformerV2 (Liao et al., 2023). In eSCN, atom-level features are represented as spherical-harmonic coefficients and are updated through stacked equivariant message-passing layers over local neighborhoods. This representation allows the model to maintain explicit angular information throughout the encoding process while preserving the symmetry constraints required for three-dimensional molecular systems. For each edge, invariant embeddings that depend on interatomic distance and atom types are first constructed to characterize the local geometric and chemical context of the interaction. The node features are then rotated into an edge-aligned local frame, so that the subsequent equivariant transformation can be performed in a coordinate system adapted to the pairwise geometry. This alignment leverages the fact that, once the principal axis is determined by the edge direction, the interaction can be formulated through a significantly less expensive $SO(2)$ operation rather than a dense $SO(3)$ tensor product. As a result, eSCN reduces the computational burden of equivariant message passing while retaining the ability to model rich angular dependencies. The resulting order-wise linear transformations, together with spherical point-wise nonlinearities and neighborhood aggregation, enable eSCN to encode fine-grained angular structure with substantially improved efficiency, thereby making higher-degree directional representations practically feasible. Through repeated layer-wise updates, the encoder progressively integrates geometric signals from neighboring atoms and produces local features that capture short-range anisotropic interactions with high directional sensitivity.

EquiformerV2 extends this idea by incorporating eSCN-style equivariant convolution into a Transformer architecture. Each block consists of equivariant graph attention followed by an equivariant feed-forward network, which together enable iterative refinement of atom representations under equivariance constraints. Within the attention block, pairwise node features are rotated into edge-aligned coordinates, modulated by radial distance embeddings, processed by $SO(2)$ linear operators, and rotated back before aggregation. In this way, the attention mechanism inherits the efficiency advantages of edge-aligned equivariant computation while preserving the expressive power of Transformer-style contextual interaction. Compared with the original Equiformer (Liao and Smidt, 2022), EquiformerV2 is designed to more effectively exploit higher-degree equivariant features and to improve optimization stability in deep equivariant architectures. Specifically, attention re-normalization improves the stability of attention-score computation, Separable S^2 Activation enhances the nonlinear expressivity of non-scalar channels, and Separable Layer Normalization preserves informative magnitude relationships across non-scalar degrees. These architectural refinements improve both numerical stability and representational capacity, allowing the model to better capture complex local geometric patterns and anisotropic atomic interactions within the cutoff radius. The output of this encoder is used as the local representation $\mathbf{x}_i^{\text{Local}}$, which summarizes high-frequency local structural information before it is combined with other representation pathways.

4 Hyperparameter Settings

Supplementary Table S1: Hyperparameter settings on charged molecular dimer dataset.

Hyperparameter	**eSCN + EquiEwald Configuration**
Model	
Sphere channels	128
Hidden channels	128
Edge channels	128
$l_{\max}$	3
$m_{\max}$	2
Number of layers	3
Cutoff distance	5.0
EquiEwald Block	
k_{cutoff}	0.6
Δk	0.2
k-space RBFs	128
Downprojection	8
hidden layers	1
Training	
Epochs	500
Batch size	1
Learning rate	0.001
Weight decay	0.0
LR warmup steps	100
LR step size	15
LR decay factor	0.9
Energy loss weight	1.0
Force loss weight	100.0

Supplementary Table S2: Hyperparameter settings for the **eSCN + EquiEwald** configuration on the AIMD-Chig dataset.

Hyperparameter	**eSCN + EquiEwald Configuration**
Model	
Sphere channels	128
Hidden channels	128
Edge channels	128
$l_{\max}$	2
$m_{\max}$	2
Number of layers	3
Cutoff distance	5.0
EquiEwald Block	
k_{cutoff}	1.0
Δk	0.2
k-space RBFs	128
Downprojection	8
hidden layers	1
Training	
Epochs	100
Eval batch size	2
Learning rate	0.0001
Energy loss weight	1
Force loss weight	100
Gradient clipping	10.0

Supplementary Table S3: Hyperparameter settings for the **eSCN + EquiEwald** configuration on the Molten NaCl dataset.

Hyperparameter	**eSCN + EquiEwald Configuration**
Model	
Sphere channels	128
Hidden channels	128
Edge channels	128
$l_{\max}$	3
$m_{\max}$	2
Number of layers	3
Cutoff distance	5.29
Max neighbors	80
EquiEwald Block	
n_{k_x}	1
n_{k_y}	1
n_{k_z}	3
Downprojection	8
Number of hidden layers	0
Training	
Max epochs	500
Batch size	4
Learning rate	0.0005
LR factor	0.9
LR step size	15
Gradient clipping	10.0
Energy loss weight	1
Force loss weight	100
Early stopping patience	20

Supplementary Table S4: Hyperparameter settings for the **eSCN + EquiEwald** configuration on the OC20 dataset.

Hyperparameter	**eSCN + EquiEwald Configuration**
Model	
Sphere channels	128
Hidden channels	256
Edge channels	128
$l_{\max}$	4
$m_{\max}$	2
Number of layers	6
Cutoff distance	6.0
EquiEwald Block	
n_{k_x}	1
n_{k_y}	1
n_{k_z}	3
Downprojection	8
Training	
Max epochs	10
Batch size	16
Learning rate	0.0008
LR factor	0.8
LR patience	10
Gradient clipping	10.0
Energy loss weight	1
Force loss weight	100

Supplementary Table S5: Hyperparameter settings for the **EquiformerV2 + EquiEwald** configuration on the OC20 dataset.

Hyperparameter	**EquiformerV2+EquiEwald Configuration**
Model	
Sphere channels	64
Atom hidden channels	512
Attention hidden channels	64
FFN hidden channels	512
Edge channels	128
Number of attention heads	4
Attention alpha channels	32
Attention value channels	16
$l_{\max}$	6
$m_{\max}$	2
Number of layers	4
Cutoff distance	6.0
Maximum number of neighbors	50
EquiEwald Block	
n_{k_x}	1
n_{k_y}	1
n_{k_z}	3
Downprojection	8
Training	
Max epochs	25
Batch size	4
Learning rate	0.0001
LR factor	0.8
LR patience	3
Gradient clipping	10.0
Energy loss weight	1
Force loss weight	100

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