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Why Equivariant Networks Fail for Magnetic Ordering: Broken Symmetries and Hidden Degeneracies

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Abstract

E(3)-equivariant networks have become central to materials machine learning because they encode spatial symmetries and achieve high accuracy for non-magnetic systems. Their underlying assumptions, however, break down for magnetic ordering, where spin degrees of freedom, time-reversal symmetry breaking, and near-degenerate magnetic states are essential to the physics but absent from coordinate-only representations. This paper argues that the mismatch between E(3) symmetry and the magnetic space-group structure of real materials makes standard equivariant architectures fundamentally unreliable for magnetic ordering tasks. We show that this mismatch produces systematic failures, including the collapse of distinct magnetic states, the erasure of hidden degeneracies, and the inability to capture finite-temperature ordering phenomena. By framing these limitations in symmetry-theoretic terms, the analysis clarifies why architectural modifications that incorporate spin, time reversal, and multi-valued outputs are necessary for physically faithful prediction in magnetic materials discovery.

Keywords Equivariant neural networks, Magnetic ordering, Broken symmetries, Hidden degeneracies, Magnetic space groups, Time-reversal symmetry

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Introduction

Equivariant graph neural networks (GNNs) have transformed computational materials engineering by embedding fundamental physical symmetries directly into the model architecture [1, 2]. Architectures such as NequIP and MACE enforce E(3) equivariance—invariance under rotations, translations, and reflections—allowing them to learn accurate interatomic potentials from far smaller datasets than their non-equivariant predecessors. These networks have delivered state-of-the-art performance for structural relaxation, phonon spectra, and defect energetics in non-magnetic inorganic solids [1–3]. Their built-in symmetry constraints reduce the effective dimensionality of the learning problem and guarantee that predictions remain physically consistent under rigid transformations of the input coordinates.

Yet the very strength that makes E(3)-equivariant networks so effective for non-magnetic systems becomes a critical weakness when the target property is magnetic ordering. Magnetic phenomena arise from the spontaneous breaking of time-reversal symmetry and the emergence of long-range spin order. Ferromagnetic, antiferromagnetic, and ferrimagnetic ground states are not uniquely determined by atomic positions; identical nuclear frameworks can support multiple, energetically competitive magnetic configurations whose macroscopic properties (magnetization, magnetocrystalline anisotropy, spin-wave spectra) differ by orders of magnitude [4–6]. Standard E(3) networks, which receive only Cartesian coordinates and nuclear charges as input, possess no mechanism to encode or differentiate these spin configurations.

Early high-throughput studies of magnetic materials relied on density-functional theory (DFT) combined with exhaustive enumeration of possible spin arrangements [4, 5]. More recent machine-learning approaches have attempted to accelerate this process by predicting magnetic moments or ordering types directly from crystal structure [7-17]. However, these efforts either operate in a post-processing regime—using an E(3) network for structure followed by a separate classifier—or implicitly assume that atomic geometry alone suffices to determine the magnetic ground state. Neither strategy confronts the fundamental symmetry mismatch.

This paper performs a rigorous failure-mode analysis of E(3)-equivariant networks applied to magnetic ordering prediction. We demonstrate that the networks’ core assumptions—atomic positions determine the physics, time-reversal invariance holds, and the magnetic ground state is unique—collapse precisely when these assumptions are violated by real magnetic materials. The analysis is conceptual and symmetry-based; no new simulations, datasets, or performance benchmarks are introduced. Instead, we synthesize insights from the literature on equivariant potentials [1, 2, 18, 19], magnetic space-group theory [20, 21], and degeneracy in magnetic ground states [6, 22, 23] to expose systematic blind spots.

Figure 1 summarizes the paper’s central claim: once magnetic ordering introduces broken time-reversal symmetry and hidden spin degeneracy, the standard E(3)-equivariant structure-to-property pipeline becomes systematically non-identifiable.

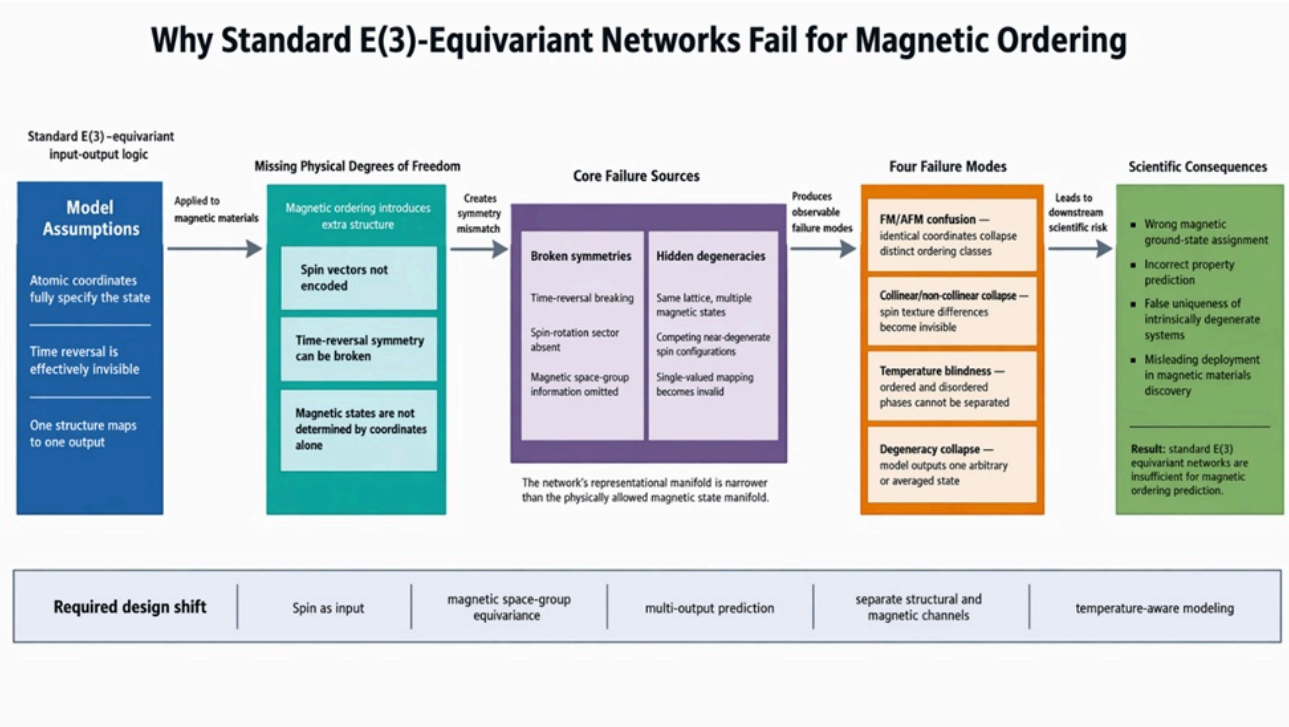


Figure 1. Conceptual pathway by which standard E(3)-equivariant networks fail for magnetic ordering prediction

What Equivariant Networks Assume

Equivariant neural networks are defined by their transformation properties under the Euclidean group E(3). Formally, a function f is E(3)-equivariant if, for any rotation R , translation t , and reflection P belonging to E(3), the output transforms identically to the input: $f(Rx + t) = Rf(x)$ and $f(Px) = Pf(x)$ [1]. In graph-neural-network implementations, this is achieved by constructing message-passing layers that operate on irreducible representations of the rotation group SO(3) and by using

only relative interatomic vectors as features [2]. The resulting architecture is guaranteed to respect all spatial symmetries of the underlying atomic configuration.

Three additional implicit assumptions are routinely embedded in these models when applied to materials. First, the network treats atomic positions as the sole determinant of the target property. Nuclear charges and coordinates fully specify the input graph; no auxiliary channels carry electronic or spin information. Second, the system is assumed to be invariant under time reversal. Because time reversal does not alter nuclear positions, the network’s output remains unchanged when all magnetic moments are reversed. Third, the mapping from structure to property is single-valued: a given atomic framework possesses exactly one physically relevant output (energy, forces, or magnetic moment) [1, 2].

These assumptions hold robustly for non-magnetic materials. In insulators and metals without spontaneous magnetism, the electronic ground state is uniquely determined (up to trivial degeneracies) by the nuclear framework, and time-reversal symmetry is preserved. Consequently, E(3)-equivariant networks have achieved remarkable accuracy for force-field prediction, phonon calculations, and defect formation energies [1-3].

The situation changes qualitatively once magnetism is present. Magnetic ordering arises from exchange interactions between localized or itinerant spins. The magnetic moment configuration constitutes an additional degree of freedom that is not encoded in the atomic coordinates alone. Moreover, magnetic order spontaneously breaks time-reversal symmetry: the ground state is no longer invariant under reversal of all spins. Finally, multiple distinct spin arrangements—related by symmetry operations outside E(3)—can possess identical or near-identical energies, violating the single-valued-output assumption [6, 22].

Literature that applies standard E(3) networks to magnetic systems either omits spin information entirely or treats magnetism as a post-hoc scalar property predicted from geometry [8, 9]. In both cases the network inherits the same three assumptions. Even architectures that claim “spin-aware” features often do so only through magnitude, not direction, thereby preserving time-reversal invariance and E(3) symmetry while discarding the vectorial nature of spin [18, 24]. The result is a model that is formally equivariant under spatial transformations yet fundamentally misaligned with the symmetry group of the magnetic Hamiltonian.

Table 1 clarifies that the failure is not merely a data limitation but a structural mismatch between the symmetry content of standard equivariant networks and the symmetry content required by magnetic order.

Table 1. Group-theoretic mismatch between standard E(3)-equivariant networks and the physics of magnetic ordering

Analytical dimension	Standard E(3)-equivariant network assumption	Magnetic-ordering requirement	Why the mismatch matters analytically	Resulting identifiability consequence
State description	Atomic coordinates and species are treated as sufficient descriptors of the material state	Magnetic order requires explicit spin degrees of freedom in addition to nuclear positions	The same crystal scaffold can realize multiple distinct magnetic states without any coordinate change	Structure alone is non-identifying for magnetic order
Symmetry group represented by the model	Spatial Euclidean symmetry only: rotations, translations, reflections	Magnetic systems require operations involving time reversal and spin-sector transformations	The network respects only a subset of the physically relevant symmetry algebra	Valid magnetic distinctions are projected out before prediction

Time-reversal treatment	Time reversal is effectively invisible because coordinates are unchanged	Magnetically ordered states arise through spontaneous breaking of time-reversal symmetry	States related by spin reversal are distinct in magnetic meaning even if structurally identical	The model collapses time-reversed magnetic states
Spin-rotation sector	No explicit SU(2) or spin-vector representation	Ordered magnetic phases depend on spin orientation, texture, and rotational symmetry breaking	Directional spin structure cannot be inferred from scalar geometry alone	Collinear and non-collinear states become underdetermined or indistinguishable
Space-group resolution	At best captures ordinary crystallographic space-group information	Magnetic crystals are classified by magnetic space groups, not ordinary space groups alone	Structural symmetry is an incomplete proxy for magnetic symmetry class	Multiple magnetic symmetry classes map to one structural representation
Output structure	One input structure should map to one stable output	Magnetic systems can have multiple degenerate or near-degenerate admissible states	Multi-branch physical landscapes are forced into a deterministic mapping	Degenerate manifolds collapse into arbitrary or averaged predictions
Thermodynamic framing	Implicitly aligned with static, often zero-temperature structural learning	Magnetic ordering depends on thermal transitions and phase stability	Order/disorder changes cannot be inferred if temperature is absent from the state description	Curie/Néel behavior remains outside the predictive domain
Failure implication	More data or deeper layers should improve approximation	Missing symmetry content cannot be recovered by scale alone	The limitation is architectural, not merely empirical	Systematic failure persists even with strong training performance on non-magnetic benchmarks

In short, E(3)-equivariant networks assume a symmetry-enriched version of classical mechanics in which nuclear positions dictate everything and time reversal is a good symmetry. Magnetic ordering violates all three assumptions simultaneously. The remainder of this analysis traces the precise mechanisms by which this mismatch produces failure.

Why Magnetic Ordering Is Different

Magnetic ordering is qualitatively distinct from structural or vibrational properties because it decouples the nuclear framework from the electronic spin degrees of freedom. The same set of atomic coordinates can support qualitatively different magnetic ground states whose macroscopic responses differ by orders of magnitude. Body-centered cubic iron is ferromagnetic with a Curie temperature of 1043 K, while body-centered cubic manganese is antiferromagnetic with a Néel temperature of approximately 95 K; the atomic positions in the two cases are crystallographically indistinguishable [4, 5]. An E(3)-equivariant network that receives only these positions cannot distinguish the two materials.

This degeneracy is not an exotic exception but a generic feature of magnetic materials. Layered van-der-Waals magnets such as CrI₃ exhibit stacking-dependent interlayer coupling that can switch the system between ferromagnetic and antiferromagnetic order while leaving the in-plane atomic arrangement unchanged [25]. Collinear antiferromagnets can be

continuously deformed into non-collinear or spiral states by small perturbations in exchange parameters, again without altering nuclear coordinates [6, 26]. Spin spirals incommensurate with the lattice further illustrate the point: the magnetic periodicity is independent of the structural periodicity, rendering any coordinate-only descriptor incomplete [20].

Temperature introduces an additional layer of complexity. Magnetic order is a finite-temperature phenomenon governed by the competition between exchange energy and entropy. Below the Curie or Néel temperature a spontaneous magnetization appears; above it the system becomes paramagnetic. Standard E(3) networks are trained on zero-temperature DFT data and possess no explicit temperature input. Their predictions are therefore frozen at $T = 0$ K and cannot capture the order–disorder transition or the associated critical exponents [7, 10, 13, 27].

The physical consequences are immediate. Ferromagnetic materials are used in permanent magnets and data storage; antiferromagnetic materials enable ultrafast spintronics and are robust against external fields. Predicting the wrong ordering type on the same atomic scaffold therefore misidentifies the entire application domain. Yet because E(3) networks see only the scaffold, they inevitably conflate these domains. Recent machine-learning classifiers trained on structural descriptors have reported reasonable accuracy on curated datasets, but closer inspection reveals that the models succeed only when the training set contains no pairs of iso-structural materials with opposite ordering types [8, 11]. Once such pairs are introduced, performance collapses—direct evidence of the underlying symmetry failure.

Magnetic ordering therefore occupies a unique position in the materials property landscape: it is a collective electronic phenomenon that is (i) invisible to atomic coordinates, (ii) symmetry-breaking with respect to time reversal, and (iii) degenerate with respect to multiple spin configurations. Any network whose input and symmetry group ignore these three facts is, by construction, incapable of faithful prediction.

Broken Symmetries as Failure Source

The root of the failure lies in a mismatch between the symmetry group assumed by the network and the symmetry group respected (or broken) by the physical system. E(3)-equivariant networks are invariant under spatial transformations but remain fully invariant under time reversal. Magnetic ordering explicitly breaks time-reversal symmetry.

Time-reversal symmetry maps each spin vector to its negative while leaving nuclear coordinates unchanged. In non-magnetic systems, time reversal is a symmetry of the Hamiltonian, and the total energy remains invariant. In magnetically ordered systems, however, the ground state is not invariant under time reversal; instead, applying time reversal produces a distinct but degenerate state corresponding to the reversed spin configuration.

Because E(3)-equivariant neural networks do not include spin degrees of freedom as input, they cannot distinguish between these states. As a result, their predictions for a given atomic structure are identical to those for its time-reversed counterpart, even though the two may differ in observable properties such as net magnetization or anomalous Hall conductivity [20, 21, 28].

Spin rotation symmetry SU(2) is likewise absent from E(3). In the paramagnetic phase, rotating all spins leaves the energy invariant. Once magnetic order sets in, the system spontaneously selects a preferred direction, breaking SU(2). Standard E(3) networks possess no representation of spin vectors and therefore cannot encode this breaking. Even when magnetic moment magnitudes are supplied as scalar node features, the directional information required for proper SU(2) transformation is missing [18, 24].

The crystallographic manifestation of these broken symmetries is the magnetic space group. Whereas ordinary crystals are classified into 230 space groups, magnetic crystals require 1651 magnetic space groups that combine spatial operations with time-reversal or spin-flip operations [21]. An E(3)-equivariant network operating on atomic coordinates can at best encode one of the 230 ordinary space groups. It is blind to the additional 1421 magnetic extensions.

Consequently, two structures that are symmetry-equivalent under a magnetic space group but inequivalent under an ordinary space group will be treated as identical by the network, even though their magnetic properties differ [20].

The consequence is not merely reduced accuracy but a categorical failure: the network's output manifold is smaller than the physically allowed manifold of magnetic states. Any prediction it makes is forced to lie in the intersection of all time-reversed and spin-rotated copies, erasing precisely the information that defines magnetic order.

Hidden Degeneracies as Failure Source

Hidden degeneracy arises when multiple magnetic configurations share identical atomic coordinates and nearly indistinguishable energies while yielding distinct physical observables. As single-valued functions of atomic positions, $E(3)$ -equivariant networks are structurally incapable of encoding this multiplicity. This limitation becomes evident across representative cases: competing collinear and non-collinear orders may converge energetically under finely balanced exchange interactions [6, 26], while ferro- and antiferromagnetic alignments can coexist on the same lattice, as exemplified by bcc Fe/Mn. A related manifestation appears in incommensurate spin spirals, whose propagation vectors are decoupled from the reciprocal lattice [20], as well as in van der Waals magnets where interlayer stacking alone modulates magnetic coupling without altering in-plane geometry [25].

Because the model perceives only the nuclear framework, these distinct configurations collapse onto a single representation, forcing an artificial resolution. In practice, this results either in an averaged prediction that corresponds to no physically realizable state or in the arbitrary selection of a specific configuration contingent on training dynamics. Both outcomes violate the underlying degeneracy. Large-scale density functional theory studies indicate that such near-degenerate magnetic states are not exceptional; many candidate materials exhibit multiple ground states within 1 meV per atom [4, 5, 22].

The consequences are particularly severe in property prediction, where single-output mappings obscure physically meaningful alternatives. A predicted magnetization, for instance, cannot convey the coexistence of degenerate states with opposite orientations, nor can it reflect the susceptibility of the system to perturbations such as strain or doping that may induce transitions between qualitatively distinct phases. This loss of information is intrinsic to the input representation, which omits the spin degrees of freedom that differentiate these states.

Hidden degeneracy thus reveals a fundamental incompatibility between the single-valued structure of $E(3)$ -equivariant mappings and the inherently multi-valued character of magnetic ground-state manifolds. Together with the symmetry-breaking limitations discussed previously, it defines a core constraint on the applicability of equivariant architectures to magnetic ordering phenomena.

A Typology of Failure Modes

The conceptual limitations of $E(3)$ -equivariant networks in magnetic ordering tasks can be understood as distinct but interrelated failure modes arising directly from the symmetry mismatch between the $E(3)$ group and the magnetic space-group structure of real materials [20, 21]. When only atomic coordinates are provided, configurations that differ solely in spin orientation become indistinguishable, rendering the network unable to separate ferromagnetic from antiferromagnetic ground states on the same lattice. This ambiguity reflects the implicit enforcement of time-reversal symmetry: reversing all spins leaves the input unchanged and therefore preserves the output, leading to systematic misclassification across fundamentally different magnetic regimes [6, 10, 22, 29].

A related limitation emerges in the inability to resolve collinear from non-collinear order. Even when such configurations are energetically proximate due to competing exchange interactions [6, 26], their distinction hinges on spin geometry, which remains unrepresented. As a result, the model collapses these states onto a common output, obscuring symmetry-

breaking within the spin sector and undermining predictions of properties sensitive to spin texture. Beyond this, the absence of an explicit temperature variable confines the network to the zero-temperature limit. Magnetic ordering, governed by the interplay of exchange and thermal fluctuations, undergoes qualitative transitions at finite temperature, yet the model treats ordered and paramagnetic phases as equivalent whenever atomic positions coincide, effectively removing the thermodynamic dimension [7, 10].

This representational constraint extends to systems with multiple nearly degenerate magnetic states. Because the mapping is single-valued, the network must either select one configuration without physical justification or produce an averaged response that corresponds to none of the realizable states. In practice, this leads to discontinuities under small structural perturbations that would otherwise lift degeneracy smoothly, thereby distorting downstream property predictions tied to specific magnetic configurations [4-6, 22]. Taken together, these failures indicate that $E(3)$ equivariance, while adequate for non-magnetic systems, systematically suppresses the degrees of freedom that define magnetic order. The resulting errors are not isolated but arise from a common structural deficiency, ensuring that at least one mode of failure manifests in any realistic application [18, 24].

Detection Principles

Detection of these failure modes can be operationalized through a set of architecture-agnostic consistency checks that directly probe the symmetry mismatches identified above, requiring only forward evaluations on carefully constructed inputs. When identical atomic coordinates are paired with distinct spin configurations, such as ferromagnetic and antiferromagnetic orderings, indistinguishable outputs indicate an inability to resolve magnetic structure on a fixed lattice [10, 11]. This limitation extends to systems with known degeneracies: configurations that are energetically equivalent should yield identical predictions, and any systematic splitting signals an artificial lifting of degeneracy incompatible with the underlying energy landscape [6, 22]. A related diagnostic arises from global spin rotations, which leave physical energies invariant in the absence of external fields; deviations in network output under such transformations reveal sensitivity to arbitrary spin frames and a breakdown of rotational symmetry in spin space [18, 24]. The same logic applies to global spin inversion, where consistency under time-reversal symmetry is expected when spin information is not explicitly encoded; discrepancies in this case expose implicit symmetry breaking within the model [20, 21].

Mitigation Principles

Restoring physical fidelity requires architectural extensions that address the underlying symmetry deficiencies while preserving the advantages of equivariant learning. Incorporating magnetic moments as explicit vector features enables the network to distinguish configurations that differ only in spin orientation, provided that message passing respects both spatial $E(3)$ and spin $SU(2)$ transformations [18, 24]. This extension naturally motivates a shift toward magnetic space-group equivariance, where combined spatial and time-reversal operations are treated as intrinsic symmetries of the model [20, 21]. Beyond symmetry representation, the single-valued nature of standard outputs must be relaxed to accommodate degenerate magnetic manifolds; probabilistic or multi-branch outputs allow the model to retain competing configurations rather than collapsing them [6, 22]. A further refinement separates structural and magnetic processing streams, ensuring that spin information is not suppressed by spatial operations before final integration [9, 18]. Introducing temperature as an explicit input extends the framework beyond the zero-temperature limit, enabling the model to capture thermally driven phase transitions and associated changes in magnetic order [7, 10].

Table 2 consolidates the manuscript's contribution by mapping each failure mode to its violated assumption, observable symptom, falsification test, and minimum viable mitigation.

Table 2. Failure-mode diagnostic matrix linking violated assumptions, empirical symptoms, and minimum architectural remedies

Failure mode	Violated underlying assumption	Typical empirical symptom	Minimal falsification test	Why the error is physically serious	Minimal architectural remedy
Ferromagnetic/antiferromagnetic confusion	A single coordinate set uniquely determines ordering type	Iso-structural ferro- and antiferromagnetic materials receive indistinguishable or unstable predictions	Hold coordinates fixed and swap spin pattern from FM to AFM; compare outputs	Misclassifies the application domain itself, confusing permanent-magnet and antiferromagnetic functionality	Add explicit spin-vector inputs coupled to equivalent message passing
Collinear/non-collinear collapse	Spin direction can be ignored or reduced to magnitude	Predictions are insensitive to changes in spin texture despite strong property differences	Keep coordinates fixed and rotate into a non-collinear texture; test output sensitivity/invariance conditions	Erases spin-texture-dependent physics such as anisotropy, coupling pathways, or magnon topology	Represent as a directed object include secondary transformation rules
Temperature dependence blindness	Zero-temperature structure is sufficient for magnetic-state prediction	Ordered and paramagnetic regimes are implicitly treated as the same state when coordinates do not change	Evaluate the model on identical structures across temperature-labeled regimes	Removes the phase-transition axis of the magnetic problem and invalidates finite-temperature use	Introduce temperature as an explicit condition variable thermodynamic character
Degeneracy collapse	One physically correct output exists for each structure	The model returns an arbitrary branch or an averaged state that corresponds to no realizable magnetic configuration	Feed known degenerate magnetic states on the same scaffold and inspect whether the model splits or averages them	Suppresses intrinsic multiplicity and hides switching sensitivity under perturbation	Replenish determinate readout multi-objective probabilistic manifold prediction heads
Artificial symmetry lifting	Learned distinctions reflect physical distinctions	Tiny architectural or initialization changes produce inconsistent preference among near-degenerate states	Re-run across seeds or equivalent degenerate inputs and inspect branch selection stability	Introduces spurious ordering preferences not present in the Hamiltonian	Enforce degeneracy aware to objective symmetry consistency constraints
Magnetic space-group blindness	Ordinary structural	Materials with different	Compare states distinguished only	Prevents proper classification of	Extend equivalent

	symmetry is an adequate proxy for magnetic symmetry	magnetic symmetry classes appear equivalent to the model	by magnetic space-group operations	magnetically inequivalent but structurally similar systems	beyond ordinary groups to magnetic space-groups
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Implications for Magnetic Materials ML

The failure-mode analysis carries immediate consequences for three stakeholder groups in AI-driven materials science.

For model developers, the central lesson is that E(3)-equivariant networks alone are provably insufficient for any task involving magnetic ordering. The architecture must be extended to include spin vectors, magnetic space-group operations, and multi-valued outputs from the outset. Retrofitting these features after training is impossible; the symmetry constraints must be baked into the message-passing layers themselves [1, 2, 18, 24]. Developers should therefore treat magnetic materials as a distinct problem class rather than a simple add-on to non-magnetic potentials.

For benchmark designers, standard structure-to-property datasets are inadequate. Future benchmarks must include iso-structural pairs that differ only in magnetic order, explicit degenerate configurations, and temperature-dependent labels. Tasks should explicitly test the ability to distinguish ferromagnetic from antiferromagnetic states on identical lattices and to preserve hidden degeneracies [4, 5, 8, 10]. Only such stress tests will reveal whether a proposed architecture has overcome the four failure modes identified here.

For practitioners and end users in computational magnetism, the safest default is to avoid unmodified E(3)-equivariant networks for any prediction that depends on magnetic ordering type, net magnetization, or spin texture. Before deployment, every candidate model must pass the four detection principles of Section 7. When standard networks are used for structural relaxation or phonon calculations in magnetic materials, the resulting geometries must still be post-processed with a separate magnetic-aware step; treating the relaxed structure as a direct proxy for magnetic properties is invalid.

Taken together, these implications signal a paradigm shift: magnetic materials machine learning cannot inherit the symmetry toolkit developed for non-magnetic systems. The field must develop a new generation of “magneto-equivariant” architectures that respect the full symmetry group of the magnetic Hamiltonian. Only then can data-driven methods achieve the same transformative impact in magnetism that they have already delivered in structural materials science [9, 25].

Conclusion

Standard E(3)-equivariant networks are highly effective for non-magnetic structure–property prediction, but they are not adequate for magnetic ordering because they omit the very degrees of freedom that define magnetic states. When magnetic order introduces broken time-reversal symmetry, spin-sector structure, and hidden degeneracy, coordinate-only equivariant mappings become non-identifiable and systematically collapse distinct physical configurations. The resulting failures are architectural rather than data-driven, and they cannot be resolved by scale alone. Reliable prediction in computational magnetism therefore requires magnetically aware equivariant models that explicitly represent spin, magnetic symmetry, and multi-branch ground-state structure.

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