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Machine Learning-Driven Prediction of Phase Transitions in Advanced Condensed Matter Systems: *A Review of Methods, Applications, and Open Challenges*

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Abstract

The identification and characterization of phase transitions is one of the oldest and most central problems in condensed matter physics, traditionally approached through order parameters, free-energy expansions, renormalization-group analysis, and direct numerical simulation. Over the past decade, machine learning (ML) has emerged as a complementary and, in some regimes, transformative methodology for this task. Supervised classifiers can learn to distinguish phases directly from raw configurations without an a priori order parameter; unsupervised and self-supervised techniques such as principal component analysis, autoencoders, and learning-by-confusion can locate transition points with minimal or no labeled data; and generative and variational architectures, including neural-network quantum states, now approximate ground-state wavefunctions of strongly correlated systems well beyond the reach of exact diagonalization. This paper reviews the theoretical foundations of phase transitions relevant to machine-learning applications, surveys the principal families of algorithms used to detect and classify phases, and examines their application across classical spin systems, percolation, topological and quantum phases, strongly correlated electron systems, and experimentally measured spectroscopic data. Representative case studies are discussed, including convolutional and graph-neural-network classifiers of lattice configurations, explainable-ML detection of thermodynamic transitions in photoemission spectra, and deep-learning-guided discovery of high-temperature superconductors. The review closes with a critical discussion of persistent challenges interpretability, data scarcity in correlated-electron experiments, generalization across Hamiltonians, and the reliability of learned order parameters near criticality and outlines directions for future research, including physics-informed architectures, uncertainty quantification, and closed-loop integration with autonomous experimentation.

Keywords: *machine learning; phase transitions; condensed matter physics; neural networks; unsupervised learning; quantum phase transitions; graph neural networks; superconductivity; critical phenomena.*

1. Introduction

Phase transitions the qualitative reorganizations of matter that occur as a control parameter such as temperature, pressure, or doping crosses a critical value are among the most universal phenomena in physics. From the boiling of water to the onset of ferromagnetism, superconductivity, and the many exotic orders realized in quantum materials, phase transitions link microscopic interactions to macroscopic, often technologically consequential, behavior. The conventional theoretical toolkit for characterizing a transition centers on the identification of an order parameter, the construction of a Landau free-energy functional, and, near criticality, renormalization-group analysis of universality classes. Numerically, these ideas are typically implemented through Monte Carlo (MC) sampling, molecular dynamics (MD), exact diagonalization, tensor-network methods, or density-functional theory (DFT), each of which becomes computationally prohibitive as system size, dimensionality, or the degree of quantum entanglement grows.

Machine learning offers a fundamentally different strategy: rather than deriving an order parameter analytically, a model is trained to recognize patterns in configurations, correlation functions, or spectra that distinguish one phase from another. The seminal demonstrations by Carrasquilla and Melko and by Wang showed that simple neural networks and principal component analysis, respectively, could recover the critical temperature of the two-dimensional Ising model directly from spin configurations, without being told the Hamiltonian or the existence of magnetization as an order parameter [1], [2]. These results catalyzed a rapidly growing literature applying supervised, unsupervised, and generative learning to an increasingly broad set of physical systems, including percolation, topological phases without local order parameters, frustrated magnets, disordered and many-body-localized systems, and strongly correlated electron models relevant to high-temperature superconductivity [3]–[6].

The appeal of ML-based approaches is threefold. First, they can operate directly on high-dimensional, raw data spin configurations, electron-density snapshots, or spectroscopic line shapes without requiring a hand-crafted feature or order parameter, which is particularly valuable for topological or hidden orders that lack a simple local order parameter. Second, once trained, inference is computationally cheap, enabling rapid scanning of large parameter spaces such as multi-dimensional phase diagrams or chemical composition spaces in materials discovery. Third, ML models can be applied directly to noisy, finite, and incomplete experimental data for example, scanning tunneling spectra or angle-resolved photoemission spectroscopy (ARPES) maps where a closed-form theoretical order parameter may be unknown or difficult to extract [7], [8].

This review is organized as follows. Section 2 summarizes the theoretical background of classical and quantum phase transitions relevant to ML applications. Section 3 surveys the major families of machine-learning methodologies used for phase classification, including supervised, unsupervised, and generative approaches, and the neural architectures convolutional, graph, and recurrent networks, together with variational and neural-network-quantum-state methods that instantiate them. Sections 4 through 6 examine applications organized by physical domain: classical statistical-mechanics models, quantum and topological phases, and correlated-electron systems including superconductors, with attention to both simulation-based and experimental-data-driven studies. Section 7 discusses several case studies in greater depth. Section 8 critically examines open challenges, including interpretability, data scarcity, and generalization. Section 9 outlines promising future directions, and Section 10 concludes.

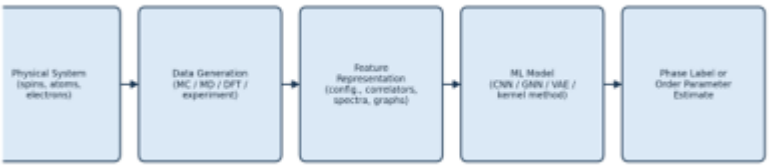

Figure 1. Generic pipeline for machine-learning-driven phase-transition prediction: a physical system is sampled to generate configurational, dynamical, or spectroscopic data; this data is mapped into a feature representation; a model is trained on the representation; and the trained model outputs a phase label, a learned order parameter, or an estimated critical point.

2. Theoretical Background: Phase Transitions in Condensed Matter Physics

2.1 Classical Phase Transitions and Order Parameters

In the Landau paradigm, a continuous (second-order) phase transition is associated with the spontaneous breaking of a symmetry, characterized by an order parameter that vanishes in the disordered phase and grows continuously below a critical temperature Tc. The two-dimensional Ising model, with its exact solution and well-characterized critical exponents, has served as the principal benchmark system for ML-based phase-classification methods because ground-truth values of Tc and the associated universality class are known analytically, allowing rigorous validation of learned predictions [1], [2], [9]. Continuous symmetry-breaking transitions in two dimensions, by contrast, may proceed via the topological Berezinskii–Kosterlitz–Thouless (BKT) mechanism, which involves the

unbinding of vortex–antivortex pairs rather than conventional long-range order, posing a qualitatively harder target for order-parameter-free learning methods [6].

Percolation theory provides a second canonical testbed: as the occupation probability of sites or bonds on a lattice is increased, the system undergoes a transition from a regime of only finite clusters to one containing a spanning, system-size cluster. Because percolation is a purely geometric transition without an energetic Hamiltonian, it is frequently used to test whether ML classifiers are sensitive to structural connectivity rather than only to energetic correlations [3].

2.2 Quantum and Topological Phase Transitions

Quantum phase transitions occur at zero temperature as a non-thermal control parameter such as an external field, pressure, or carrier doping is tuned across a quantum critical point, driven by competition between non-commuting terms in the Hamiltonian rather than thermal fluctuations. Many quantum phases of interest, including topological insulators, quantum spin liquids, and fractional quantum Hall states, are not distinguished by a local order parameter at all but rather by global topological invariants, ground-state degeneracy, or patterns of long-range entanglement. This absence of a conventional order parameter has motivated the use of ML methods capable of learning discriminative features directly from wavefunction snapshots, entanglement spectra, or correlation functions, without requiring the invariant to be specified analytically in advance [10]–[12].

2.3 Correlated-Electron Systems and Superconductivity

Strongly correlated electron systems, including cuprate and iron-based high-temperature superconductors, heavy-fermion compounds, and moiré superlattices, present some of the richest and least understood phase diagrams in condensed matter physics, typically featuring intertwined orders such as antiferromagnetism, charge-density-wave order, nematicity, and superconductivity in close proximity. Because these systems generally cannot be solved exactly and are subject to the fermionic sign problem in quantum Monte Carlo simulation, both classical numerical methods and ML surrogates face substantial challenges; conversely, the complexity and subtlety of the relevant spectroscopic and transport signatures make this domain a particularly active target for ML-based pattern recognition applied directly to experimental data [7], [13], [14].

3. Machine Learning Methodologies for Phase Classification

Machine-learning approaches to phase-transition detection can be organized broadly into supervised, unsupervised/self-supervised, and generative or variational categories, summarized schematically in Figure 2. This taxonomy reflects not only algorithmic differences but also differing assumptions about the availability of labeled data and prior physical knowledge.

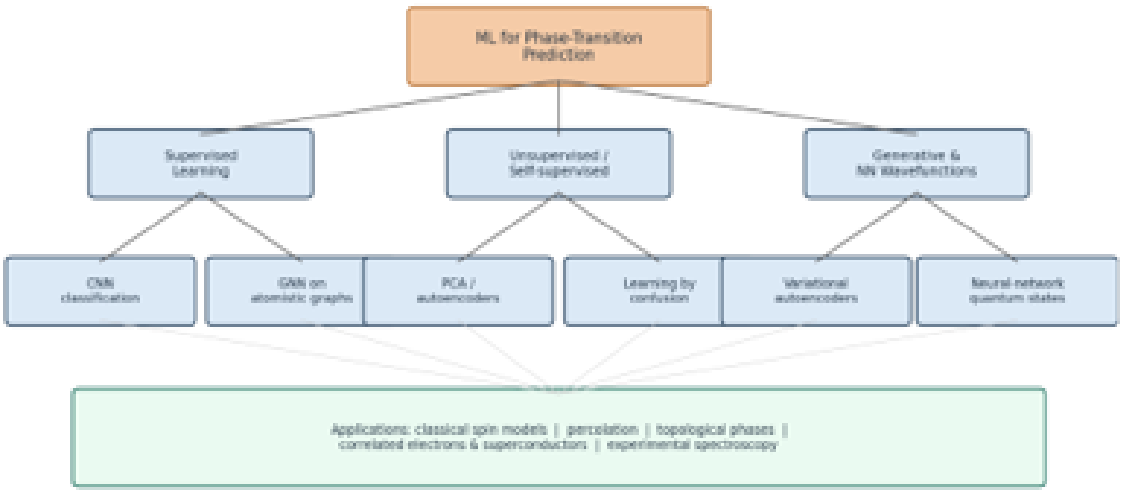

Figure 2. Taxonomy of machine-learning approaches applied to phase-transition prediction, organized by learning paradigm and representative application domains.

3.1 Supervised Learning Approaches

Supervised approaches train a classifier commonly a convolutional neural network (CNN) operating on lattice configurations, or a graph neural network (GNN) operating on atomistic or molecular graphs to map configurations sampled deep within known phases to their corresponding phase labels. Once trained on configurations sampled far from the transition, where phase identity can be assigned with high confidence, the classifier is applied to configurations across the full parameter range; the point at which classification confidence is maximally ambiguous, or at which the predicted phase label crosses over, is taken as an estimate of the critical point [1]. This strategy has been extended using GNNs that operate directly on atomistic graphs with learned, symmetry-respecting (equivariant) representations, enabling near-DFT-accuracy prediction of formation energies and related properties while remaining tractable at the length and time scales needed to resolve phase transitions, interfacial diffusion, and fracture in realistic materials [15].

3.2 Unsupervised and Self-Supervised Learning

Unsupervised methods aim to detect a phase transition without requiring pre-labeled configurations. Principal component analysis (PCA), for example, can reveal an order parameter as the dominant direction of variance in a dataset of configurations, as demonstrated for the Ising model and later extended to variational autoencoders capable of capturing more complex, nonlinear order parameters [4]. A related self-supervised strategy, learning by confusion, deliberately trains a classifier using intentionally mislabeled data under many candidate transition points and identifies the true critical point as the one at which classification accuracy is worst, exploiting the idea that only the correct partition of the data is genuinely learnable [5]. Quantum loop topography and related feature-engineering schemes extend these ideas to topological phases lacking a conventional local order parameter, by constructing input features from loop or string operators that are sensitive to topological order even though they are constructed from local measurements [10].

3.3 Generative Models and Neural-Network Quantum States

A third family of methods uses generative or variational architectures to represent probability distributions or quantum wavefunctions directly. Variational autoencoders learn a compressed latent representation of configurations from which anomalies in the reconstruction error or latent-space structure can signal a transition [4]. In the quantum many-body setting, neural-network quantum states parameterize the amplitudes of a many-body wavefunction using a neural network trained variationally to minimize the expectation value of the Hamiltonian, providing a numerically exact-in-principle method that has been used to discover quantum phase transitions in fermionic systems without an assumed ansatz, and to describe systems including moiré superlattices, dense hydrogen, and chiral superconductivity that are difficult to treat with conventional quantum Monte Carlo due to sign-problem limitations [11], [12], [16]–[18].

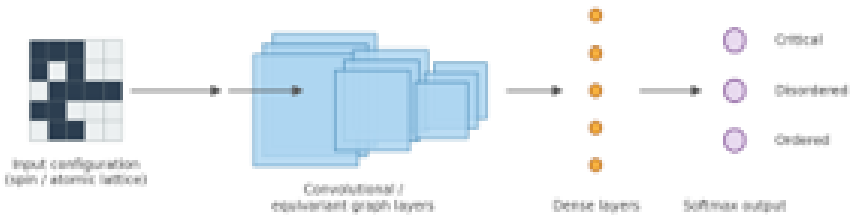

Figure 3. Schematic convolutional/graph-neural-network classifier: a latticZe configuration is processed through convolutional or equivariant graph layers, reduced through dense layers, and mapped to a softmax output over candidate phase labels.

3.4 Feature Representations and Order-Parameter Interpretation

Regardless of learning paradigm, the choice of input representation strongly influences both performance and interpretability. Raw configuration snapshots preserve the most information but may require large networks to

extract relevant correlations; hand-engineered features such as two-point correlators, structure factors, or entanglement entropies embed prior physical knowledge and can improve sample efficiency and interpretability at the cost of generality. Figure 3 illustrates schematically how a trained classifier's output probability behaves as a continuous function of the tuning parameter, tracking — though not always coinciding exactly with — the behavior of a conventional order parameter across the transition.

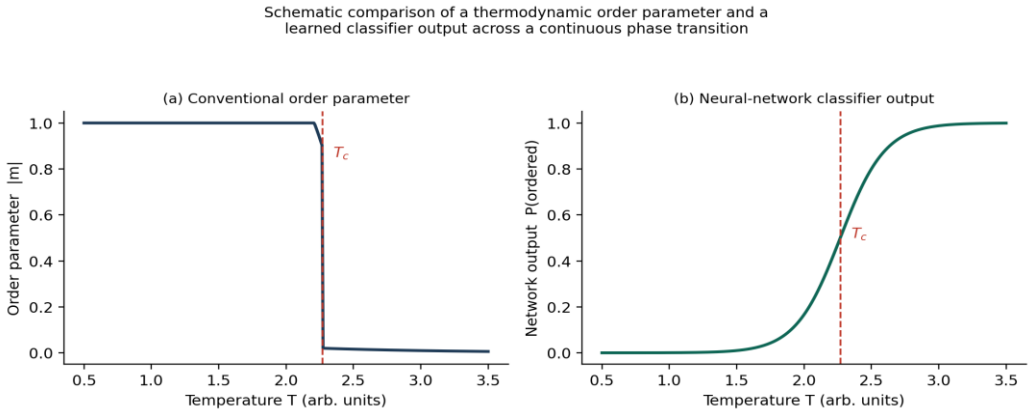

Figure 4. Schematic comparison of (a) a conventional thermodynamic order parameter and (b) a neural-network classifier output as functions of temperature across a continuous phase transition; both exhibit a sharp crossover near the critical temperature Tc, though the learned quantity need not be a true thermodynamic order parameter.

4. Applications to Classical Statistical Systems

Classical spin models remain the primary proving ground for new ML methodologies because their exact or numerically well-converged solutions provide ground truth against which learned predictions can be validated. Beyond the ferromagnetic Ising model, ML techniques have been applied to the two-dimensional J1–J2 Ising model, which introduces competing nearest- and next-nearest-neighbor interactions and a correspondingly richer phase diagram including striped and disordered regimes, and to the three-dimensional Anderson model of localization, in which disorder rather than temperature drives a metal-insulator transition [9]. A recent large-scale study applied both classical statistical techniques and supervised/unsupervised ML to two-dimensional site percolation and to percolation embedded within the three-dimensional Ising model, systematically comparing lattice-based and dynamically generated off-lattice networks; the authors found that off-lattice geometries were harder to classify accurately because they lacked the fixed correlated structure of regular lattices, and released an open-source toolset of trained models for community use [3].

These classical benchmarks have also been used to probe the theoretical underpinnings of why ML classifiers succeed. Several works have shown a formal connection between the features extracted by simple neural networks or PCA and known order parameters or their nonlinear analogues, such as the squared magnetization for the Ising model, lending physical interpretability to what would otherwise be treated as a black-box classifier [2], [4]. Other studies have used confusion-based and regression-based schemes to estimate critical exponents and to quantify the uncertainty associated with ML-derived critical points, an important step toward treating learned quantities with the same statistical rigor as conventional finite-size-scaling analysis [9].

5. Applications to Quantum and Topological Phases

Quantum phase transitions pose distinct challenges because the relevant states are ground states of many-body Hamiltonians, often with substantial entanglement, and because many of the phases of interest (topological insulators, fractional quantum Hall states, quantum spin liquids) lack a local order parameter altogether. Early work demonstrated that neural networks trained on entanglement spectra or wavefunction snapshots could distinguish topologically distinct phases and detect topological phase transitions from entanglement-based features without prior knowledge of the relevant topological invariant [10]. Fermionic neural-network quantum states have subsequently been used to discover quantum phase transitions directly from variational ground-state

optimization, without assuming a particular order parameter or symmetry-breaking pattern in advance, and have been extended to describe emergent Wigner phases in moiré superlattices and the broken-symmetry phase of dense solid hydrogen under pressure [11], [12], [16], [18].

A parallel line of work has applied ML directly to experimental quantum-simulator data. Artificial neural networks trained on quantum-gas-microscope snapshots have been used to identify quantum phase transitions and to analyze non-equilibrium dynamics in cold-atom systems, demonstrating that ML-based phase identification is not restricted to simulated data but can operate on genuinely noisy, finite-statistics experimental measurements [19], [20]. More recently, attention-based architectures adapted from natural-language processing have been applied to variational ansätze for chiral superconductivity, illustrating the continued cross-pollination between advances in mainstream deep learning and quantum many-body methods [17].

6. Correlated-Electron Systems, Superconductivity, and Experimental Data

6.1 Machine Learning and Experimental Spectroscopy

A persistent obstacle in correlated-electron research is the scarcity of high-quality experimental data spanning a phase transition, since synthesizing and measuring samples across a full phase diagram is costly and time-consuming. A 2020 study led by researchers at Emory University and Yale University addressed this limitation by applying explainable machine learning to photoemission spectroscopy data to detect thermodynamic phase transitions in quantum materials, reporting that the approach could identify clear spectral signals of a transition and reduce the time required to characterize complex quantum phases from months to minutes, with particular relevance to the study of low-dimensional superconductors [7]. In a related direction, ML has been used to analyze multidimensional response data relaxation to applied voltage and thermal stimuli in relaxor ferroelectric crystals, producing a temperature-bias phase diagram without requiring the order parameter to be measured or even known in advance, illustrating how ML can substitute for an explicit constitutive model when the underlying physics is only partially understood [8].

6.2 Machine Learning and Superconductor Discovery

Machine learning has also been applied to the forward problem of predicting whether a candidate material will superconduct, and at what critical temperature. Graph-neural-network and other deep-learning surrogates have been trained to predict the Eliashberg electron-phonon spectral function directly from crystal structure, bypassing the need for expensive first-principles phonon calculations for each new candidate and achieving mean absolute errors of a few kelvin on the predicted critical temperature across hundreds of dynamically stable materials [14], [21]. Complementary BCS-inspired screening pipelines combine density-functional-theory pre-screening with deep-learning surrogates to prioritize candidate compounds for more expensive first-principles or experimental follow-up, and generative or reinforcement-learning-guided search strategies have reportedly identified candidate hydride superconductors with predicted transition temperatures competitive with known high-Tc hydrides, illustrating the shift from purely evaluative ML models toward generative, inverse-design workflows in this domain [13], [22].

Table 1. Summary of representative machine-learning methods for phase-transition prediction, organized by physical domain.

Domain	Representative Method	Target Quantity	Key Reference(s)
Classical Ising / percolation	Supervised CNN; PCA; learning by confusion	Critical temperature / percolation threshold	[1], [2], [3], [4], [5]
Topological / quantum phases	Quantum loop topography; entanglement-based CNN; fermionic NNQS	Topological invariant; quantum critical point	[10], [11], [12]

Cold-atom quantum simulators	Supervised ANN on microscope snapshots	Phase boundary from experimental snapshots	[19], [20]
Correlated-electron spectroscopy	Explainable ML on ARPES / relaxor response data	Thermodynamic transition; phase diagram	[7], [8]
Superconductor discovery	GNN / deep-learning surrogates for Eliashberg function; generative inverse design	Critical temperature Tc; candidate compounds	[13], [14], [21], [22]

7. Case Studies

7.1 Convolutional Classification of the Two-Dimensional Ising Model

The canonical demonstration trains a CNN on spin configurations sampled well above and well below the known critical temperature of the two-dimensional Ising model, using MC-generated configurations at each temperature. The network, given no information about the Hamiltonian or the existence of magnetization as an order parameter, learns to output a high-confidence ordered/disordered classification when trained on configurations far from Tc, and its output probability transitions sharply near the true critical temperature when applied across the full temperature range, closely tracking the finite-size-scaling behavior of the magnetization [1], [2]. This case study remains the standard benchmark for new architectures and for studies of data efficiency, such as recent work examining how well a CNN trained only on configurations at a single high-temperature reference point can still resolve the critical region when compared against training on configurations spanning both sides of the transition [9].

7.2 Explainable Machine Learning of Photoemission Spectroscopy

In contrast to simulation-based studies, this case study begins directly from experimental ARPES data on correlated quantum materials, where the number of measured spectra spanning a transition is inherently limited. The reported approach combines an explainable-ML architecture with domain-specific feature engineering to detect subtle spectral changes associated with a thermodynamic phase transition, with the stated aim of reducing characterization time for candidate quantum materials, including low-dimensional superconductors, from months of manual analysis to minutes of automated inference [7]. The emphasis on explainability is notable: rather than treating the model purely as a black-box classifier, the authors sought to identify which spectral features drove the classification, aligning the ML output with physically interpretable signatures that a domain scientist could independently verify.

7.3 Graph-Neural-Network-Guided Superconductor and Materials Discovery

A third case study illustrates the shift from phase classification toward generative materials design. Equivariant graph-neural-network force fields and property predictors, trained on large materials databases, now achieve formation-energy errors near several millielectronvolts per atom and enable molecular-dynamics simulation at near-quantum accuracy but classical computational cost, allowing direct simulation of diffusion, phase transitions, and fracture processes at device-relevant time and length scales [15]. Building on this capability, deep-learning surrogates for the electron-phonon spectral function have been used to screen hundreds of candidate compounds for superconductivity, and generative search strategies have been reported to identify candidate hydride superconductors, illustrating a broader trend in which GNNs are used not only to classify or predict properties of existing materials but to propose new, experimentally viable candidates in a closed loop with first-principles validation [13], [14], [21].

8. Challenges and Limitations

8.1 Interpretability and Physical Meaning

A recurring criticism of ML-based phase classification is that a trained model's decision boundary need not correspond to a genuine thermodynamic singularity; a classifier can achieve high accuracy by exploiting features correlated with, but not identical to, the true order parameter, particularly away from the thermodynamic limit. Efforts to connect learned features analytically to known order parameters, and the development of explainable-ML techniques that expose which input features drive a classification, are partial responses to this concern, but a general theory connecting model architecture to the physical content of what is learned remains incomplete [2], [4], [7].

8.2 Data Scarcity and the Sign Problem

Many of the most scientifically interesting correlated-electron systems are precisely those for which both experimental data and classical simulation are limited — experimental phase diagrams are expensive to measure at fine resolution, and quantum Monte Carlo simulations of fermionic systems are frequently obstructed by the sign problem. This tension motivates two complementary strategies evident in the literature: developing ML methods that are explicitly data-efficient and robust to small or noisy datasets, and developing variational neural-network-quantum-state methods that sidestep the sign problem by directly optimizing a many-body wavefunction ansatz rather than relying on stochastic sampling of amplitudes with indefinite sign [7], [11], [16].

8.3 Generalization Across Hamiltonians and Finite-Size Effects

A model trained to detect a phase transition in one Hamiltonian or at one system size does not automatically generalize to a different model or a different lattice geometry; the percolation study discussed in Section 4, for instance, found that off-lattice, dynamically generated network geometries were classified less accurately than fixed regular lattices, underscoring that structural assumptions embedded in training data can limit transferability [3]. Finite-size scaling, essential in conventional critical-phenomena analysis for extrapolating apparent transition points to the thermodynamic limit, has not yet been fully integrated into ML-based workflows in a standardized way, and the statistical uncertainty of ML-derived critical points and exponents is often reported inconsistently across studies [9].

8.4 Benchmarking and Reproducibility

Because much of the methodological literature validates new ML techniques on well-understood classical models with known analytic solutions, there is a risk that reported successes do not transfer cleanly to the higher-dimensional, less-well-characterized quantum and correlated-electron systems that motivate the field's broader ambitions. The release of open-source toolkits and pretrained models for standard benchmark systems is a positive step toward reproducibility, but community-wide benchmarking standards analogous to those in mainstream machine learning are still emerging in this subfield [3].

9. Future Directions

- Physics-informed architectures: embedding known symmetries, conservation laws, and equivariances directly into network architecture, as already practiced in equivariant GNNs for materials property prediction, to improve data efficiency and out-of-distribution generalization for phase-transition detection [15].
- Uncertainty quantification: extending regression-based and Bayesian ML approaches to provide calibrated confidence intervals on learned critical points and exponents, enabling direct comparison with the statistical rigor of finite-size-scaling analysis [9].
- Integration with autonomous and closed-loop experimentation: coupling ML-based phase classification with automated synthesis and measurement platforms, so that regions of a phase diagram identified as ambiguous or scientifically interesting can be targeted for further measurement without manual intervention [13].

- Foundation models for condensed matter data: extending large pretrained graph- and transformer-based architectures, already used for general-purpose materials property prediction and structure generation, toward multi-task models capable of transferring across Hamiltonians, lattice geometries, and experimental modalities [13], [15].
- Hybrid quantum-classical and neural-network-quantum-state methods: further development of variational wavefunction ansätze capable of treating fermionic sign-problem-afflicted systems, with continued cross-pollination from attention-based and other architectures originally developed for natural-language processing [16], [17].
- Standardized benchmarking: community-adopted benchmark suites spanning classical, topological, and correlated-electron systems, with transparent reporting of uncertainty, to enable fair comparison across the rapidly diversifying set of proposed methods.

10. Conclusion

Machine learning has evolved from an initially speculative application to condensed matter physics into an established and diverse methodological toolkit for the detection, classification, and characterization of phase transitions. Supervised classifiers, unsupervised and self-supervised feature-learning techniques, and generative or variational architectures each offer distinct advantages depending on the availability of labeled data, the presence or absence of a conventional order parameter, and whether the target system is amenable to classical simulation or requires a direct quantum-mechanical treatment. Applications now span the full range from textbook classical spin models, used primarily for methodological validation, to genuinely open problems in topological matter, strongly correlated electron systems, and superconductor discovery, increasingly incorporating real experimental data rather than simulation output alone. Nonetheless, significant challenges remain around interpretability, data scarcity in the most scientifically interesting quantum systems, generalization across Hamiltonians and system sizes, and the standardization of benchmarking practices. Addressing these challenges through physics-informed architectures, principled uncertainty quantification, and closer integration with autonomous experimentation represents a promising and active direction for the continued development of this field.

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