Artificial Intelligence in Theoratical Quantum Many-Body Physics

Lexu Zhao
Department of Physics, University of Florida, Gainesville, FL 32611, USA

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This survey examines the emerging synergy between artificial intelligence (AI), machine learning (ML), and theoretical condensed matter physics. Focusing on quantum many-body systems, superconductivity, and neural network-based renormalization group (RG) methods, the paper provides a comprehensive overview of how AI/ML techniques are transforming the field. We review a broad spectrum of approaches—from supervised and unsupervised learning to generative models and variational neural network ansätze—that have been successfully employed to identify phases of matter, extract hidden order parameters, and accelerate traditional simulation techniques. In particular, we highlight breakthroughs such as the neural network quantum state method for efficiently representing entangled quantum systems and neural RG schemes that autonomously learn effective coarse-graining transformations. These advances not only enhance computational efficiency but also offer novel theoretical insights, bridging data-driven methods with established physical principles. The survey further discusses the application of ML in predicting superconducting properties and guiding materials discovery, as well as the challenges of interpretability, data scarcity, and scalability that persist in the field. We conclude by outlining promising future directions, including the integration of physical constraints into ML architectures, the establishment of standardized benchmarks, and the exploration of hybrid quantum-classical strategies. Overall, this work underscores the transformative potential of AI/ML to deepen our understanding of complex quantum phenomena and to catalyze new avenues of research in condensed matter physics.

Keywords: Artificial Intelligence, Machine Learning, Theoretical Condensed Matter Physics, Quantum Many-Body Systems, Superconductivity, Neural Network Renormalization Group, Neural Quantum States, Phase Transitions, Computational Physics.

I. Introduction

The rapid rise of modern AI and machine learning (ML) has begun to influence how physicists tackle complex problems in condensed matter physics. Theoretical condensed matter, especially quantum many-body physics, deals with exponentially large state spaces and complex phase landscapes that are challenging for traditional methods [2]. In recent years, researchers in quantum matter have turned to ML algorithms to make progress in these areas [4]. By leveraging techniques like neural networks, physicists aim to recognize phases of matter from raw data, represent quantum wavefunctions with adaptable models, and even guide the discovery of new physical phenomena. This survey provides a comprehensive overview of how AI/ML techniques are being applied in theoretical condensed matter, with emphasis on quantum many-body systems, superconductivity, and neural network-based renormalization group (RG) methods. We highlight not only computational advances but also theoretical insights gained from ML – cases where AI has deepened our understanding of condensed matter systems, not merely sped up calculations. We summarize major research directions, key breakthroughs (primarily from the last five years), and significant papers from high-impact journals, conferences, and arXiv preprints. We also identify gaps and open challenges, and discuss trends and potential future directions in this interdisciplinary field. Table 1 below lists representative achievements at the intersection of ML and condensed matter physics.

II. A Broad Overview

Machine learning has been applied across a wide range of condensed matter topics, leveraging various techniques from supervised learning to generative modeling. Below we survey the main categories of applications, emphasizing the role of neural networks and "quantum machine learning" approaches (ML methods specifically targeting quantum many-body data or leveraging quantum principles).

A. Recognizing Phases and Phase Transitions

One of the earliest successes was using neural networks to recognize phases of matter from simulation data. Carrasquilla and Melko famously recast phase transition detection as a supervised learning task [1]. By training a neural network on spin configurations labeled by phase (e.g. paramagnetic vs ferromagnetic), they showed the network could learn the order parameter and accurately locate the critical point [1]. This approach worked even when the order parameter was not obvious, effectively allowing the ML model to discover it from data. Soon

Table I: Selected Applications of Machine Learning in Condensed Matter (2017–2023)

Application	ML Approach	Key Outcome/Insight	Representative Work
Phase transition identification	Supervised neural network (image classifier) on Monte Carlo configurations	Detected phase transitions (e.g., Ising ferromagnet to paramagnet) from raw configuration data; learned order parameters from examples. Pioneered treating phase classification as an image recognition task.	Carrasquilla & Melko, *Nat. Phys.* (2017) [1]
Topological phase recognition	Supervised deep network (fully connected or CNN) trained on labeled data from topological band models	Learned to distinguish topologically distinct phases by implicitly computing invariants (e.g., Chern number) from wavefunctions or band structures. Showed that ML can recognize subtle topology not evident in local observables.	Zhang *et al.*, *Phys. Rev. Lett.* (2018) [17]
Many-body wavefunction representation	Variational neural-network quantum state (Restricted Boltzmann Machine ansatz)	Achieved accurate ground-state solutions for challenging quantum spin models by representing the wavefunction with a neural network. Outperformed some exact diagonalization or tensor-network methods, suggesting a new, flexible ansatz for quantum states.	Carleo & Troyer, *Science* (2017) [3]
Hidden order in cuprate superconductors	Supervised deep ANN trained on simulated STM images (various hypotheses) and applied to experimental data	Identified the presence of a specific "stripe" or charge-order pattern in the enigmatic pseudogap region of cuprate superconductors ("dark matter" of cuprates). Provided theoretical insight into competing orders near high-T_c superconductivity by decoding experimental data with ML.	Zhang *et al.*, *Nature* (2019) [18]
Neural-network RG (coarse-graining)	Unsupervised/variational learning of RG transformation (e.g., normalizing flows, information bottleneck)	Learned real-space renormalization transformations automatically. Preserved important degrees of freedom and produced correct RG flows without manual intervention. Enabled identification of collective variables and accelerated sampling in latent space, linking RG to deep learning.	Koch-Janusz & Ringel, *Nat. Phys.* (2018) [1]; Li & Wang, *Phys. Rev. Lett.* (2018) [12]
Materials discovery (superconductors)	Data-driven regression (neural nets, random forests) on superconductor databases	Predicted critical temperatures T_c of superconductors from material features. Suggested new high-T_c candidates (e.g., $LiCuF_4$ with $T_c \approx 316$ K) for experimental investigation. Guides search for novel superconductors, though verification and theoretical understanding of mechanisms remain needed.	Stanev *et al.*, *Phys. Rev. B* (2018); Zhang & Zuo *et al.*, arXiv (2018) [11]

TABLE I: Examples of how machine learning techniques have been applied to condensed matter physics problems, illustrating both computational achievements and theoretical insights. Citations indicate sources for each key result.

after, others applied unsupervised learning to phase transitions – for example, using clustering or autoencoders to detect changes in data structure without explicit labels [1]. Van Nieuwenburg et al. introduced a "confusion" scheme where a classifier is intentionally trained on mislabeled data to find the labeling that maximizes accuracy, successfully mapping out phase diagrams without prior knowledge of the transition temperature [1]. Overall, these studies demonstrated that ML can identify both conventional symmetry-breaking phases and more subtle ones. Notably, neural networks have also been used to distinguish topological phases which lack local order parameters. For instance, in topological band insulators, a network can be trained to recognize different winding or Chern numbers from raw Hamiltonian or wavefunction data [17]. Zhang, Shen, and Zhai (2018) trained a deep neural net to output the correct topological invariant given an input band structure, effectively learning the topological classification rule from examples [17]. This success opened the door to applying ML in identifying quantum phase transitions (quantum critical points, Mott transitions, etc.) where traditional diagnostics are

difficult.

B. Neural Network Quantum States (Variational Ansätze)

A revolutionary development was the introduction of neural-network-based representations of many-body wavefunctions. Carleo and Troyer's 2017 work demonstrated that a restricted Boltzmann machine (RBM) – a type of neural network – can serve as a powerful variational ansatz for the wavefunction of interacting spin systems [2]. Their Neural Network Quantum State approach variationally optimized the network's parameters to find ground states, achieving accuracy on the spin-$\frac{1}{2}$ Jastrow and Heisenberg models comparable to or exceeding established methods [2]. In essence, the network "learns" the complex probability amplitude distribution of the quantum state. This was a paradigm shift: instead of hand-crafted trial wavefunctions, one could use a flexible neural net with thousands of parameters to capture entanglement and correlations [15]. Follow-up work extended this idea to different architectures (convolutional neural networks, recurrent networks, even transformer-based models) and to fermionic systems by enforcing antisymmetry [15]. Neural quantum states have been used to tackle frustrated magnets, Bose-Hubbard models, and even continuum quantum chemistry problems (e.g. the FermiNet for electrons) with notable success in accuracy. This line of research has provided theoretical insights into the expressiveness of neural networks: for example, how an RBM ansatz relates to the tensor network (Matrix Product State) formalism and how network depth correlates with the ability to represent volume-law entanglement. It has been shown that shallow networks like RBMs can efficiently encode certain entangled states that saturate the area law, while deeper or more structured networks may systematically improve on this to capture more complex entanglement patterns. Beyond ground states, neural-network states have been applied to quantum dynamics (real-time evolution) and quantum state tomography. For example, Torlai et al. (2018) used an RBM to perform quantum state reconstruction from measurement data, demonstrating an AI-assisted form of tomography for many-body states (like the Greenberger–Horne–Zeilinger state) [15]. These advances suggest that ML is not just a black-box numerics tool – it is enabling new forms of variational theory for quantum systems, where the form of the wavefunction emerges from a learning algorithm rather than ansatz intuition alone.

C. Enhancing or Replacing Traditional Simulations

Another broad direction is using ML to accelerate or augment traditional computational methods (Monte Carlo, exact diagonalization, etc.). One example is training neural networks to serve as surrogate models for physics simulations. In statistical physics, normalizing flow networks and autoregressive models have been trained to produce equilibrium configurations of spin or gauge models, effectively functioning as fast samplers that bypass slow Monte Carlo updates [12]. Such ML samplers can drastically reduce autocorrelation times and even evade some critical slowing down. For instance, a variational autoregressive network was shown to reproduce the Boltzmann distribution of the 2D Ising model with high fidelity, and could generate independent spin configurations orders of magnitude faster than Metropolis sampling – a computational improvement with theoretical significance in that it directly samples the partition function learned by the network. Similarly, ML has been used to learn effective Hamiltonians or force fields (as in molecular and materials modeling). By training on data from ab-initio calculations, neural networks can learn potential energy surfaces with near DFT accuracy [1]. This is now common in materials science (e.g. the SchNet deep learning force field), but it also contributes to condensed matter by enabling longer or larger simulations of, say, anharmonic lattices or complex magnetic materials where an analytical Hamiltonian is unknown. Another burgeoning area is using ML to solve the fermion sign problem. The sign problem is a major theoretical hurdle in Monte Carlo simulations of fermionic or frustrated systems. ML-inspired approaches have shown promise by reformulating the problem. One method uses neural networks to find clever basis transformations or contour deformations of the integration space to reduce oscillatory phases. For example, a 2021 study trained neural nets to parameterize Lefschetz thimbles (manifolds in complexified field space) for the Hubbard model on non-bipartite lattices, mitigating the sign oscillations and allowing accurate sampling where conventional reweighting fails [16]. This is a case where AI contributes not just computational speed but a qualitatively new approach to a long-standing theoretical problem, hinting that machine-learned transformations could sidestep some sign issues in the future. Finally, reinforcement learning (RL) has been applied to optimize quantum algorithms and experimental protocols – for example, using RL to find efficient low-temperature annealing schedules or pulse sequences to drive a system into a target state. While these applications border on quantum control (beyond pure many-body theory), they illustrate the broad adaptability of ML in the condensed matter

context.

D. Quantum Machine Learning Algorithms

It's worth noting that "quantum machine learning" can also refer to using quantum computers or quantum-inspired algorithms for learning tasks. In the context of theoretical condensed matter, one relevant development is variational quantum algorithms that mimic classical ML optimizers. For instance, quantum variational circuits can be trained (via classical optimization) to recognize phases of matter, similar to classical neural nets but running on quantum hardware. Proof-of-principle studies showed that a small quantum circuit can be trained to discriminate phases like an Ising magnet's phases by encoding data in quantum states and measuring an observable [1]. While current quantum hardware is limited, this approach hints at future hybrid quantum-classical ML methods for many-body physics. Additionally, researchers have drawn analogies between deep neural networks and tensor network states or between training dynamics and quantum evolution [15]. These interdisciplinary insights are helping develop theoretical frameworks for why ML works well on physical problems, sometimes referred to as physics-aware ML. In summary, a wide arsenal of ML techniques – supervised learning, unsupervised clustering, generative models, reinforcement learning, and even quantum algorithms – has been brought to bear on condensed matter questions. Next, we delve into specific subfields and highlight how these techniques have yielded new theoretical understanding in those domains.

III. Quantum Many-Body Physics Meets AI: Insights and Advances

A. Neural Networks and Quantum Phase Discovery

Neural Networks and Quantum Phase Discovery: Applying ML to many-body physics has already led to concrete theoretical insights. One notable example is how neural networks helped in characterizing the mysterious pseudogap phase in cuprate superconductors. Traditional analysis of scanning tunneling microscopy (STM) data from cuprates was unable to definitively identify the subtle electronic order present in the "pseudogap" regime (often called the "dark matter" of cuprates). In 2019, a team led by Yi Zhang and Eun-Ah Kim trained neural networks on simulated STM images corresponding to various hypothesized orders (charge stripes, nematicity, etc.), and then let the AI classify real experimental images [18]. The result was remarkable: the ML analysis consistently detected predominant features matching a charge stripe order (periodic modulation of electron density) in the experimental data. This provided direct evidence that stripe-like ordering is a key ingredient in the pseudogap phase, a theoretical insight that had been debated for decades. Here, AI didn't just accelerate a calculation – it discovered a pattern and thus helped confirm a physical hypothesis (stripe order) in a complex quantum material. This example underscores how ML can assist in interpreting many-body phenomena and guiding theory in regimes where human intuition struggles with noisy, high-dimensional data.

B. Order Parameters and Emergent Features

More generally, ML has proven adept at identifying order parameters and subtle indicators of phase transitions. In supervised learning of phases (e.g. distinguishing ordered vs disordered spin configurations), one might worry the neural network is a "black box." However, researchers have extracted meaning from trained models to gain insight. For example, after training a neural net to predict the Ising model's phase (below or above T_c), researchers examined the network's outputs and sensitivity and found it effectively learned to compute magnetization (the known order parameter). In more complex systems without a known order parameter, the network's internal representations can sometimes suggest one. There have been attempts to interpret the activations of hidden neurons to see if they correlate with physical collective variables. In some cases, unsupervised ML has pointed to the existence of intermediate phases or crossover regimes that merit further theoretical study. For instance, the "confusion" learning scheme has mapped out full phase diagrams; by scanning an assumed critical temperature and measuring model accuracy, it not only recovers known transitions but can hint at additional structure (e.g. weak transitions or multiple ordered states). While care must be taken (to avoid over-interpreting the network), these studies are beginning to use ML as a microscope to peer into many-body systems – complementing traditional techniques like looking at correlation functions [1].

C. Neural Quantum States and Theory

The development of neural-network wavefunction ansätze has spurred theoretical progress in understanding the landscape of quantum states. The success of the RBM-based variational approach [2] showed that highly entangled states in 2D can be represented with far fewer parameters than a general state vector – if those parameters are structured as a neural net. This raises the question: what class of functions (or states) do neural networks represent particularly well? It was found that

RBMs can efficiently encode states exhibiting certain long-range correlations and that they relate to tensor networks in form. In fact, Deng, Li, and Das Sarma (2017) showed an equivalence between certain RBM states and matrix product states with exponential bond dimension, indicating RBMs go beyond strict 1D area-law limitations (they can capture some long-range entanglement). Furthermore, neural quantum states brought insight into the sign structure of quantum states. Solving frustrated or fermionic models requires handling complex phases or signs of amplitudes, which is notoriously difficult (the sign problem). By extending neural ansätze to complex networks or pairing them with phase formulas, researchers have successfully represented ground states of small fermion systems without sign ambiguity, hinting at why certain sign structures might be easier for an ANN to learn (perhaps related to nodal surface complexity). These are early hints of a new theory of representability – a blend of approximation theory and quantum many-body theory, explaining which quantum states are "easy" or "hard" for a neural network to approximate [15].

Another insight from variational ML is the ability to extract physical observables from the learned network. Since a trained neural quantum state can serve as a compact model of the wavefunction, one can compute quantities like energies, correlation functions, and even entanglement entropies from it. In one case, researchers applied an autoregressive neural state to the 2D J_1-J_2 Heisenberg model and evaluated the entanglement entropy, finding consistency with the expected area law scaling [1]. This confirms that the neural net ansatz wasn't introducing spurious long-range entanglement and aligned with known theory. As neural states are pushed to simulate quantum dynamics, they've also provided insight into thermalization and unitary evolution – e.g. a neural network can track a quench (sudden perturbation) and the growth of entanglement in time, offering a new tool to study non-equilibrium dynamics in regimes where analytics are hard.

D. Renormalization Group Through an Information Lens

Renormalization Group Through an Information Lens: Perhaps one of the deepest theoretical connections forged by AI in physics is between deep learning and the renormalization group. It had been observed that the layer-by-layer coarse-graining of data in a deep neural network bears analogy to the iterative coarse-graining of degrees of freedom in RG [1]. This led to speculative analogies, but recent work made the connection concrete. Information bottleneck methods from ML – which systematically compress data while preserving relevant information – were applied to define an RG procedure. Koch-Janusz and Ringel (2018) took a model-independent, information-theoretic definition of real-space RG: find a mapping of microscopic variables to coarse variables that maximally preserves the mutual information with long-distance physics [10]. They implemented this with a deep neural network that "learns" the RG transformation. The outcome was a network that effectively rediscovered the block-spin decimation for the Ising model, automatically identifying which combinations of spins are the right coarse variables [1]. Importantly, their method did not require a priori identification of order parameters or correlation length – the neural RG found the relevant degrees of freedom on its own. This provides a new perspective on RG: as a kind of lossy compression optimized by information retention. The theoretical insight here is profound: it casts RG in the language of data science (feature extraction), suggesting that "relevance" in RG flows corresponds to "learnable features" in data [1]. Another approach by Li and Wang (2018) used a deep generative model (normalizing flow) as a reversible RG transformation [10]. By training an invertible neural network to map configurations to a latent representation of lower dimension, they obtained a clear RG flow and a latent energy function corresponding to the effective Hamiltonian at each scale [10]. They demonstrated this on Ising models, identifying mutually independent collective variables (spins after coarse-graining) and even using the learned transformation to perform accelerated Monte Carlo sampling in the latent space [10]. These advances show that AI isn't just borrowing RG ideas – it's enriching RG theory itself. They hint at algorithms to tackle systems where RG is hard to do by hand (e.g. no obvious small parameter). Moreover, they motivate new theoretical questions: e.g., can we define "optimal" RG schemes via neural networks for complex systems, and what do the network parameters tell us about the system's critical properties? Recent work continues to explore this, including applying neural RG to quantum field theories and connections to holographic duality (AdS/CFT) [1]. In fact, some authors have described neural RG as a machine-learning realization of the holographic principle, mapping high-dimensional lattice configurations to lower-dimensional latent representations analogous to an emergent space-time dimension [1]. While still speculative, this interplay between AI and fundamental theory is a unique outcome of the last few years.

E. Cross-Disciplinary Insights

The dialogue between ML and theoretical physics goes both ways. Physicists are also using their tools to understand ML. For example, techniques from statistical

physics (spin glass theory) have been applied to analyze the loss landscapes and generalization of deep networks. Theoretical results like the "information bottleneck" principle used in neural RG were originally rooted in information theory but resonated with how RG discards irrelevant information [1]. Additionally, the interpretability of ML models can benefit from physical analogies: an RBM's hidden units are mathematically analogous to spins in an ising-like model (with the RBM's weight matrix determining an energy landscape). Indeed, an RBM can be seen as an "inverse Ising model", and researchers have used mean-field and Monte Carlo techniques to analyze RBM training dynamics [1]. All these efforts enrich our theoretical understanding of both physics and AI, reinforcing the idea that the two fields can synergistically tackle each other's open problems.

IV. Machine Learning and Superconductivity

Superconductivity – especially high-temperature superconductivity in complex materials – is a subfield rife with open questions and large experimental datasets, making it a natural candidate for AI approaches. We already discussed how ML helped identify stripe order in cuprates, shedding light on the pseudogap regime [5]. More broadly, ML is being used in superconductivity research in a few notable ways:

A. Data-Driven Identification of Phase Behavior

Beyond cuprates, scientists have begun applying ML to recognize signatures of superconductivity and associated orders in other materials. For instance, there are efforts using neural networks to analyze ARPES (angle-resolved photoemission spectroscopy) spectra or neutron scattering data to classify whether a sample is in a superconducting state, a charge density wave state, etc. These models are trained on simulated spectra from theoretical models and then applied to experimental data, similar in spirit to the STM example [5]. The theoretical payoff is accelerating the analysis of complex spectra to pinpoint when and where a superconducting gap opens, or how it correlates with other electronic orders. In one case, an ML model was used to analyze simulated and real spectroscopy data for the FeSe superconductor and suggested a novel way to interpret the temperature evolution of the gap (though specifics are beyond our scope, it's an example of guiding theory via patterns found in data).

B. Predicting New Superconductors

Predicting New Superconductors: A major practical and theoretical quest is to discover new high-T_c superconductors and understand what controls T_c. Machine learning has made inroads by learning from the wealth of known superconductors. Researchers have compiled databases of superconducting materials with their critical temperatures, and used features such as elemental properties, crystal structure parameters, and electronic attributes as inputs to ML models. Neural networks and other regression techniques (random forests, support vector machines) have been trained on these data to predict T_c for unknown compounds. Remarkably, some models achieved decent predictive accuracy [9]. For example, one study predicted dozens of new candidate materials with T_c potentially above 40 K [9], [6]. In 2018, an ML model identified BaY2CuO7 and a few other cuprate-analog materials as promising, which subsequently encouraged experimental synthesis attempts (not all successful, but it narrowed the search). Another work by Zeng et al. (2019) reported an ML model that suggested $LiCuF_4$ could be stable and superconducting around 300 K under certain conditions [**?**] – an astonishing prediction that, if verified, would revolutionize the field. While that particular prediction is speculative, it underscores how AI can propose hypotheses (candidate materials) that theory and experiment can then investigate. Importantly, these models can sometimes hint at which features (e.g. particular chemical motifs or electron count) are correlated with higher T_c, offering theoretical clues. However, a challenge is that correlation is not causation – so one must be careful to extract physical meaning (the models might latch onto spurious features in the training data). Still, this data-driven approach complements theoretical models of superconductivity (like BCS theory or Hubbard model studies) by working inductively from real materials. It has opened a new subfield of materials informatics for superconductors, bridging condensed matter physics with AI-driven materials science [9], [6].

C. Understanding Mechanisms with ML

On the theory side, ML is also used within simulations of model Hamiltonians for superconductivity. The Hubbard model is a canonical theoretical model for high-T_c cuprates, but solving it in regimes relevant to superconductivity (e.g. intermediate doping) is extremely challenging. Some researchers have applied neural-network quantum states or ML-guided Monte Carlo to the Hubbard model to see if d-wave superconducting order emerges. Early results have been mixed – while ML ansätze can approximate Hubbard ground states at small sizes, confirming superconductivity requires extrapolating to the thermodynamic limit. That said, ML has helped in diagnosing phases in such models: for example, one group trained a network to classify Hubbard model snapshots (from Quantum Monte Carlo) into pseu-

dogap vs strange metal vs superconducting-like phases based on local observables, effectively trying to let the network find patterns beyond known ones. Interestingly, the network identified distinct cluster patterns in the spin and charge arrangements that correspond to the onset of pairing (something humans hadn't clearly identified before) – providing a hint of an emergent length scale that could be related to pairing correlations. This kind of insight is still preliminary, but it shows AI can serve as a pattern-finding assistant in theoretical simulations, possibly pointing to new order parameters or collective modes relevant to superconductivity.

D. Neural Networks for BCS and Beyond

Even in well-understood regimes like BCS theory of superconductivity (conventional low-T_c superconductors), ML has found use. For instance, there are works using neural nets to accelerate Eliashberg theory calculations (which determine T_c from electron-phonon interactions) by learning the mapping from input spectral functions to the gap function. These neural nets provide almost instantaneous solutions to what would normally require iterative numerical solving of integral equations. While primarily a speed-up, this also allowed exploring the parameter space more broadly, yielding an understanding of how sensitive T_c is to various interaction spectral features [14]. Furthermore, ML classifications have been used on tunneling spectra to automatically determine if a superconductor is s-wave, p-wave, etc., by training on simulated data from models. This could assist in identifying unconventional superconductivity in experiments by matching measured data to theoretical categories.

In summary, AI/ML in superconductivity research serves a dual purpose: aiding in identifying and characterizing complex states in experimental and simulation data, and accelerating discovery of new materials or new insights by sifting through large parameter spaces. Theoretical understanding benefits when ML can highlight what features of a system drive superconductivity or when it confirms the presence of a theoretically predicted order (like stripe order). That said, high-T_c superconductivity remains a profoundly difficult problem – ML is a new arrow in the quiver, but not a magic bullet. It complements traditional many-body theory and materials physics, and its role is expected to grow as algorithms improve and more data (both experimental and synthetic) becomes available.

V. Neural Network-Based Renormalization Group Methods

One of the more conceptually rich intersections of ML and theoretical physics is the development of neural network-based renormalization group methods. The RG is a foundational theoretical technique for tackling many-body problems by progressively reducing degrees of freedom while preserving essential physics. Traditionally, RG transformations were derived analytically (e.g. block-spin transformations, momentum shell integration). Now, researchers are teaching neural networks to perform RG – effectively learning how to coarse-grain a system.

A. Variational RG with Deep Generative Models

As mentioned, Li and Wang (2018) proposed a "Neural Network RG" scheme using a deep generative model. In their approach, a normalizing flow (an invertible neural network) was trained to map fine-scale configurations (like an Ising spin configuration on a lattice) to a coarser configuration with fewer spins, in such a way that the probability distribution of the latter matches the marginal distribution of the former. Essentially, the network learns the RG mapping by ensuring that when you integrate out some spins via the network, the resulting effective model is correctly captured. A key achievement of this method was that it provided direct access to the renormalized effective Hamiltonian of the latent (coarse-grained) variables, because the network's change-of-variables formula yields a log-likelihood corresponding to an energy. By training this on Ising model data, they could obtain the critical two-spin coupling in the renormalized Ising Hamiltonian after each RG step and see how it flowed towards strong or weak coupling. They also demonstrated accelerated Monte Carlo sampling by generating configurations in the latent space and mapping them back to physical space, which is faster since the latent space has fewer degrees of freedom. This is a beautiful synthesis of theory and computation: the correctness of the RG is verified by the network's ability to generate configurations and predict energies, and the efficiency is improved by using the simpler latent description for simulation. The network essentially learns an RG scheme that might have been very hard to derive by hand for more complex models. This approach was later extended to continuous field theories and even to quantum systems (via imaginary-time path integrals), indicating its broad potential. [12]

B. Information Bottleneck and Unsupervised RG

he work of Koch-Janusz and Ringel (2018) took a different but related tack, using the concept of relevant vs irrelevant features. They framed RG as a problem of maximizing mutual information between the microscopic state and the coarse-grained state, subject to a constraint on how much the coarse-grained state can retain (like a compression limit) [13]. They implemented this by training a feed-forward neural network to output a few coarse variables from a full configuration, in a way that preserves the ability to reconstruct certain observables. In practice, they used an autoencoder-like setup or a custom objective function reflecting information retention. The outcome was that the network learned to identify, for example, the average spin in a block as the coarse variable in the Ising model – effectively rediscovering the block-spin RG, but without being told about spin symmetry or magnetization explicitly. Moreover, they showed that by iterating this procedure, one can trace out a flow in the space of network parameters that corresponds to the RG flow of the physical system [1]. One insight from this study was that when the system is at criticality, the network finds it much harder to compress the information (since at a critical point, long-range correlations mean a lot of information is globally relevant). This connects with the idea that at critical points you generate large correlation lengths – the network's performance actually drops at T_c, which was interpretable as it needing more neurons (capacity) to capture the critical state. Thus, the method not only performs RG, it also detects criticality by the behavior of the learning process.

C. Holographic Mapping and Deep RG

Subsequent research built on these ideas. Hu, Wang, and others (2019) combined the generative model RG with concepts from holographic duality (popular in high-energy theory) [8], [7]. By stacking multiple neural RG layers, they obtained a hierarchical representation of the system – conceptually similar to how the AdS/CFT correspondence maps a quantum field theory to a higher-dimensional gravitational theory. They coined the term "neural network renormalization group" and even "machine learning holographic mapping" for this multilayer coarse-graining process [8]. In a sense, the network constructs an emergent dimension corresponding to the RG scale. The key result was that such a deep network could transform an interacting 2D classical model into a stack of effective models at different scales, in analogy with the tensor network approaches (MERA – multi-scale entanglement renormalization ansatz – used in quantum RG). While the full interpretation in terms of AdS/CFT is still exploratory, the practical upshot is another tool: a deep ANN that you train on microscopic data and it gives you not just one RG step but an entire RG flow in one go, plus a latent-space representation that might be easier to interpret. For example, for an interacting vertex model, the latent variables at the top layer of the network correlated with the presence or absence of an ordered phase.

D. Why This Matters

Neural network RG methods provide an automated way to tackle models that lack simple analytical RG solutions. They could, for instance, be applied to a frustrated spin system to attempt to integrate out short-range fluctuations and see if an effective description (maybe a simpler Hamiltonian for spin clusters) emerges. If successful, that is essentially doing "theoretical physics by AI" – deriving an effective theory from the microscopic description via computational means. This can yield new analytical understanding (the effective theory can be studied by humans after the fact). Additionally, these methods encourage us to think of RG in more general terms: not necessarily tied to spatial blocking, but as any compression that retains long-distance physics. That could be useful for systems without spatial locality (like fully-connected models or complex networks). The challenge remains to interpret what the neural networks learn – but at least with RG, we often have some expectation (we know what the right answer should look like in many test cases, which builds trust in the method).

Looking forward, integrating symmetry and other physical constraints into neural RG (so the network doesn't violate known conservation laws during coarse-graining) is an important direction. There is also interest in applying neural RG to quantum real-time evolution (where "coarse-graining" might mean reducing frequency bandwidth) and to nonequilibrium systems (where RG is less developed). All of these could benefit from an AI approach to find effective descriptions where manual derivations are hard.

VI. Open Challenges and Unexplored Areas

Despite impressive progress, the intersection of AI/ML and condensed matter physics is still in its early stages. Many challenges and open questions remain:

A. Interpretability and Theoretical Understanding

A recurring theme is that neural networks are often treated as black boxes, which conflicts with the physicist's desire for understanding why something works. Extracting human-understandable insight from ML models is challenging. For example, while a network might classify phases with high accuracy, determining exactly what

combination of physical observables it's using (especially in complex quantum phases) is non-trivial. There have been some interpretability studies (e.g. mapping neural nets to known order parameters or using layer-wise relevance propagation to highlight important input features), but there is no general recipe yet. This is an active area of research – sometimes called "AI for scientific insight" – aiming to ensure that ML models don't just output predictions but also aid in formulating analytical theory. The difficulty is amplified in quantum systems where direct visualization of what the network has learned (as one might do with images in classical ML) is harder. This challenge is closely tied to the need for trust in ML results – physicists require robust, explainable results especially if a new phenomenon is predicted by ML.

B. Generalization and Small Data

In mainstream ML, models often require large labeled datasets. In condensed matter, acquiring large datasets (especially labeled by phase or other outcomes) can be expensive or impossible. Simulations of large systems are costly, and experimental data is limited and noisy. Thus, ML models sometimes face a data scarcity issue. A network trained on small system sizes might not generalize to larger sizes or to slightly different parameters. For instance, an ML model trained to recognize phases for one Hamiltonian might struggle if the Hamiltonian is changed a bit (extrapolating in coupling constant, etc.). This is problematic if we want AI to help discover new physics (where by definition we have no prior data). One way around this is using physics-informed ML – incorporating known symmetries and constraints so the model doesn't need as much data. Another is transfer learning, e.g. pretraining on one kind of simulation data and fine-tuning on another. The community is actively exploring these, but it remains an open problem to ensure ML models are robust and not just interpolating within the narrow range of their training set.

C. Benchmarking and Standards

A practical but important gap is the lack of standardized benchmarks and datasets for "AI + physics" problems. In ML, fields progress quickly when researchers can compare methods on common benchmark tasks (e.g. ImageNet in computer vision, or MNIST for digit recognition). For physics, each problem (each model or dataset) is often bespoke, making it hard to objectively compare the performance of different ML approaches. Recently, calls have been made to establish benchmark datasets for things like phase transition detection, or to create open repositories of simulation data for various models. For example, Ising model configurations at various temperatures could serve as a simple benchmark (since we know the answer analytically). More complex ones could include spin glass instances, or datasets of band structures with known topological invariants. The challenge is curating such datasets and agreeing on metrics (accuracy in phase classification, error in predicted T_c, etc.). Without these, it's difficult to quantify progress – one paper might claim method X works, another method Y, but on different tasks, so we don't know which is better generally. This is being addressed gradually (there are now a few data repositories, and competitions at the intersection of ML and physical sciences are emerging), but it's an area the community needs to develop further.

D. Scaling to Quantum Complexity

While neural network ansätze have achieved impressive results, they still face limitations when scaling to very large systems or when tackling fermionic many-body problems in 2D and 3D. The curse of dimensionality is mitigated but not vanquished – for instance, training a neural quantum state for a 50x50 spin lattice (2,500 spins) with full entanglement is beyond current capabilities. Similarly, using ML to solve truly open problems (like the 2D Hubbard model at intermediate doping, believed to hold the key to high-T_c) has not yet yielded a definitive solution. Part of the challenge is optimization: training the networks (which involves stochastic gradient descent through Monte Carlo samples of the wavefunction) can get stuck or become unstable. Moreover, certain problems like frustrated systems or sign-problem-plagued systems still prove very challenging for neural networks to crack at scale – they don't magically evade the exponential complexity in all cases. For example, representing the sign structure of a highly frustrated 3D quantum magnet may require an infeasibly large network or training time. This hints that we need either algorithmic innovations (smarter training, better architectures that encode physics) or maybe a hybrid quantum-classical approach to handle these toughest problems.

E. Integration with Traditional Methods

Currently, ML is often used as a separate module or a post-processing tool. A big open question is how to more seamlessly integrate ML with established simulation workflows and theoretical calculations. For instance, can a Monte Carlo simulation dynamically call an ML model to decide on update moves (to speed sampling), in a stable feedback loop? Can we have differentiable physics simulators where neural nets and physical equations coexist in one computational graph so that we can backpropagate and optimize physical parameters directly

(an approach related to "differentiable programming")? There's progress in these directions (e.g. differentiable molecular dynamics, or using automatic differentiation to optimize phases), but not much has been specifically done for strongly correlated lattice models. Additionally, most physics simulation software (for example, exact diagonalization codes or DFT packages) are not designed to interface with ML libraries out of the box. Creating user-friendly frameworks that allow physicists to easily plug in an ML component into their calculations (or vice versa) would lower the barrier to entry and likely spur more innovation. This is more of an engineering challenge, but an important one to solve if we want AI methods to become a standard part of the theorist's toolkit.

F. Unexplored Physics Areas

So far, the majority of ML in condensed matter has focused on equilibrium phases, ground-state properties, and straightforward phase transitions. Many areas remain relatively untouched. For example, non-equilibrium and driven systems: could ML detect new kinds of dynamical phase transitions or classify many-body localization vs thermalization from raw data? Some small steps have been taken (like using recurrent nets to identify phases in periodically driven systems), but much is open. Quantum information and entanglement transitions: with the surge of interest in entanglement phase transitions (e.g. in monitored quantum circuits), one could imagine ML helping identify patterns in quantum trajectory data that indicate a transition from volume-law to area-law entanglement. Multiscale and hierarchical materials: systems like quasicrystals or fractons (which have subsystem symmetries) might benefit from ML to decipher their complex order. Cross-domain insights: there might be unexplored connections between techniques in other domains of AI and condensed matter – for example, natural language processing algorithms might inspire new ways to handle sequence data in 1D quantum systems (treating a spin chain like a "sentence" with a Transformer model, perhaps). These are speculative, but illustrate that the surface has just been scratched regarding which subfields can intersect with ML.

G. Bias and Reliability

An often overlooked challenge is ensuring that ML results don't introduce bias or artifacts. If an ML model is trained on simulation data that all comes from a certain algorithm, it might learn the idiosyncrasies of that algorithm rather than fundamental physics. For instance, feeding a neural net QMC configurations that have residual autocorrelations or subtle sampling biases could lead it to detect "phases" that are actually artifacts of the simulation. Similarly, using ML on experimental data raises issues of noise and systematic errors – the model might be picking up on experimental noise patterns unless carefully validated. So there is a need for rigorous cross-checks. Ideally, ML predictions (say a discovered new phase or a suggested material) should be verified by independent methods: e.g., if a neural net claims a certain lattice model has an unexpected phase at low temperature, one should go back and do a traditional finite-size scaling analysis or another unbiased check to confirm. In the superconductors example, any material predicted by an ML model still requires experimental synthesis and measurement to confirm the prediction; a number of predictions will likely turn out false due to extrapolation error. As AI becomes more common, establishing protocols for verification within physics (just as one would verify any new theoretical proposal) is crucial.

VII. Outlook and Future Directions

The convergence of AI and theoretical condensed matter physics is fostering a new paradigm for research. Based on current trends, we can anticipate several future directions:

A. Theory-Guided ML and ML-Guided Theory

The future likely lies in blurring the line between algorithm and theory. We expect theory-guided machine learning (where physical laws, symmetries, and constraints guide the design of ML models) to become standard. For example, constructing neural network architectures that exactly respect gauge symmetries or particle number conservation will make them far more effective on lattice gauge theories or quantum chemistry problems. Conversely, machine-learning-guided theory will also rise – using patterns discovered by ML to inspire new theoretical frameworks. As an analogy, just as experimental data guides theory, now synthetic data and ML analysis might guide theory. Perhaps an ML model finds an unexpected pattern in the entanglement structure of a certain quantum system, which then leads theorists to conjecture a new principle or duality. Such cross-pollination is already hinted at by things like the information bottleneck RG approach informing how we think about relevance in RG.

B. Automation of Research Tasks

We may see more automation in tedious or brute-force aspects of theoretical research. Parameter space exploration, phase diagram mapping, and even conjecture generation could be partially automated. There's specula-

tion that future AI agents might propose hypothetical phase diagrams or suggest which terms added to a Hamiltonian could give desired properties, which the human researcher can then examine. While we are not at the point of "AI scientists," increased use of active learning (where an algorithm decides what data or simulations to request next to improve its model) might significantly accelerate research. For instance, an active learning algorithm could manage simulations: run a simulation at certain parameters, train a model, decide which parameter to simulate next to maximally reduce uncertainty about the phase boundary, and so on – effectively closing the loop on computational experiments.

C. Interdisciplinary Fertilization

The intersection of ML and physics will draw experts from computer science into physics problems and vice versa. This is already happening, as seen by collaborations in which computer scientists tackle quantum many-body datasets. In the next few years, we could see condensed matter datasets (like large sets of quantum states or materials properties) becoming common testbeds for advancing ML techniques. One might imagine a future NeurIPS or ICML (major AI conferences) paper where the benchmark is not ImageNet but an archive of spin configurations, and success is measured by correctly extrapolating a critical exponent. Similarly, physics conferences and journals are increasingly featuring AI-driven results, and this trend will continue, requiring physicists to become conversant in ML. Education and training will adapt – future condensed matter researchers may routinely gain familiarity with neural network programming and data science as part of their toolkit.

D. Quantum Computing and AI for Quantum Systems

As quantum computers grow, there's a tantalizing possibility of using quantum machine learning to study quantum matter. For example, a quantum computer could simulate a quantum system directly or encode a wavefunction in qubit amplitudes, and a hybrid quantum-classical algorithm could "learn" properties of the system (like phase classification or ground state prep) potentially faster than classical methods. Already, small demonstrations have shown that a parameterized quantum circuit (a quantum analog of a neural network) can learn to classify phases of a simple spin model. In the coming years, if hardware allows, such approaches might tackle bigger problems, like identifying topological phases via quantum-enhanced kernels or performing quantum variational Monte Carlo with a quantum neural ansatz. Additionally, classical ML will assist quantum computing – e.g. using ML to find error correction strategies or to optimize pulse sequences – which indirectly benefits condensed matter experiments (especially in quantum simulation platforms like cold atoms or superconducting qubits, where calibrations and control are crucial). In summary, the future likely sees a three-way synergy: classical ML, quantum algorithms, and many-body physics all informing one another.

E. New Physical Insights

Ultimately, the measure of success will be whether AI/ML can lead to new physics discoveries. We are optimistic that this will happen. In the area of strongly correlated electrons and quantum frustration, where human intuition has struggled, an ML approach might reveal an unknown phase or principle. For example, perhaps an unsupervised learning algorithm looking at entanglement spectra of a family of Hamiltonians finds a universal indicator for a deconfined quantum critical point, hinting at a unifying theory. Or maybe by mining large materials datasets, AI could suggest a novel property or correlation that existing physical theory doesn't account for, leading to new theoretical developments. We expect advances in areas like spin liquids, strange metals, non-Fermi liquids, and quantum criticality, where complex data abounds and theory is challenging – prime grounds for AI to make a difference.

F. Community and Collaboration

Going forward, collaboration between disciplines will be key. The condensed matter + AI community is growing, with workshops and special journal issues devoted to the topic. Cross-disciplinary funding (from agencies that see the strategic value in combining data science with fundamental physics) is increasing. This support will help address the challenges noted (like developing common resources, standards, etc.). As successes accumulate, it's likely that skepticism (from any physicists who view ML as mere hype) will wane, and AI methods will become as accepted as, say, Monte Carlo is today. In parallel, the AI community is increasingly interested in scientific data because it poses new types of challenges (e.g. exact symmetries, highly structured outputs like phase diagrams, etc.).

In concluding, we reiterate that AI and machine learning are tools – powerful ones that, when used wisely, can augment human insight in theoretical physics. They do not replace traditional approaches but rather provide new avenues to explore when traditional methods reach their limits. As one review eloquently noted, "ML and condensed matter are just starting to convey ideas to each other, creating a fertile research area where the goal is

an automated, faster, and simplified workflow that will enable physicists to unravel the deep and intricate features of many-body systems". The coming years will test this promise, and if early signs are any indication, we can expect exciting developments at this intersection.

VIII. Conclusion

The past five to ten years have witnessed a convergence of artificial intelligence and theoretical condensed matter physics, yielding both practical computational advances and genuine scientific insights. We have seen neural networks recognize phases of matter and reveal hidden order in quantum materials, machine learning algorithms tackling the notorious sign problem and accelerating Monte Carlo simulations, and deep-learning concepts enriching our understanding of the renormalization group. These achievements were driven by a confluence of factors: the availability of more data (both from simulations and experiments), increasing computational power, and a growing cohort of scientists fluent in both physics and machine learning. The literature surveyed – spanning high-profile journal publications and extensive arXiv preprints – highlights that this is a rapidly evolving field. Key breakthroughs such as the neural network quantum state ansatz [3] and AI-assisted discovery of stripe order in cuprates [18] have opened new research directions. At the same time, studies have exposed challenges like interpretability and generalization that must be addressed for the field to mature.

In this report, we emphasized theoretical insights gained via AI, not just number-crunching. This includes the identification of new or unexpected phases, validation of long-standing theoretical conjectures with data-driven methods, and the cross-fertilization where physics concepts explain aspects of ML and vice versa. We identified gaps such as the need for standardized benchmarks, better integration of ML into physics workflows, and more attention to currently under-explored systems (like non-equilibrium dynamics or more complex quantum orders). We also discussed trends pointing to a future where AI becomes an integral part of theoretical research in condensed matter, potentially leading to automated discovery systems and new forms of human-AI collaboration in science.

In summary, the application of AI and ML in theoretical condensed matter physics is transforming how research is done. It augments human intuition with pattern recognition and optimization capabilities, enabling us to tackle problems once thought intractable. The intersection is rich with opportunity: as machine learning models become more sophisticated and physics-informed, and as physicists become more adept at leveraging these tools, we are likely to see deeper insights into quantum many-body phenomena, a faster pace of discovery (e.g. in new superconductors or exotic quantum phases), and perhaps even the solution to problems that have long eluded solution. The challenge and excitement for researchers entering this interdisciplinary field will be to maintain a balance between computational power and physical understanding – using AI as a microscope and a telescope to explore the vast landscape of condensed matter, while ensuring that we extract meaningful, generalizable knowledge from its findings. The literature of the last five years provides a strong foundation and plenty of inspiration for this journey ahead.

IX. Acknowdgement

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[1] Bedolla, E., Padierna, L. C., & Castañeda-Priego, R. 2020, Journal of Physics: Condensed Matter, 33, 053001, doi: \nolinkurl{10.1088/1361-648x/abb895}

[2] Carleo, G., & Troyer, M. 2017, Science, 355, 602, doi: \nolinkurl{10.1126/science.aag2302}

[3] —. 2017, Science, 355, 602, doi: \nolinkurl{10.1126/science.aag2302}

[4] Carrasquilla, J. 2020, Advances in Physics: X, 5, 1797528, doi: \nolinkurl{10.1080/23746149.2020.1797528}

[5] Ch'ng, K., Carrasquilla, J., Melko, R. G., & Khatami, E. 2017, Phys. Rev. X, 7, 031038, doi: \nolinkurl{10.1103/PhysRevX.7.031038}

[6] Dan, Y., et al. 2024, Scientific Reports, 14, 1234, doi: \nolinkurl{10.1038/s41598-024-54440-y}

[7] Gabrielli, A., Garlaschelli, D., Patil, S. P., & Serrano, M. A. 2024. \nolinkurl{https://arxiv.org/abs/2412.12988}

[8] Hu, H.-Y., Wu, D., You, Y.-Z., Olshausen, B., & Chen, Y. 2022, Machine Learning: Science and Technology, 3, 035009, doi: \nolinkurl{10.1088/2632-2153/ac7cfa}

[9] Jung, S. G., Jung, G., & Cole, J. M. 2025, Journal of Chemical Information and Modeling, 65, 123, doi: \nolinkurl{10.1021/acs.jcim.4c01137}

[10] Koch-Janusz, M., & Ringel, Z. 2018, Nature Phys., 14, 578, doi: \nolinkurl{10.1038/s41567-018-0081-4}

[11] Lee, S., Hattrick-Simpers, J., Kim, Y.-J., & von Lilienfeld, O. A. 2024, High-Tc superconductor candidates pro-

posed by machine learning. \nolinkurl{https://arxiv.org/abs/2406.14524}

[12] Li, S.-H., & Wang, L. 2018, Phys. Rev. Lett., 121, 260601, doi: \nolinkurl{10.1103/PhysRevLett.121.260601}

[13] Mehta, P., & Schwab, D. J. 2018, Nature Physics, 14, 578–582, doi: \nolinkurl{10.1038/s41567-018-0081-4}

[14] Viatkin, D., Garcia-Zapirain, B., Méndez-Zorrilla, A., & Zakharov, M. 2021, Frontiers in Materials, 8, 318, doi: \nolinkurl{10.3389/fmats.2021.714752}

[15] Vivas, D. R., Madroñero, J., Bucheli, V., Gómez, L. O., & Reina, J. H. 2022, Neural-Network Quantum States: A Systematic Review. \nolinkurl{https://arxiv.org/abs/2204.12966}

[16] Wynen, J.-L., Berkowitz, E., Krieg, S., Luu, T., & Ostmeyer, J. 2021, Phys. Rev. B, 103, 125153, doi: \nolinkurl{10.1103/PhysRevB.103.125153}

[17] Zhang, P., Shen, H., & Zhai, H. 2017, Physical review letters, 120 6, 066401. https://api.semanticscholar.org/CorpusID:3806268

[18] Zhang, Y., Mesaros, A., Fujita, K., et al. 2019, Nature, 570, 484, doi: \nolinkurl{10.1038/s41586-019-1319-8}