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Multi-Dimensional Quantum Anharmonic Oscillators via Physics-Informed Transformer Networks: Extension to Non-Perturbative Regimes and Higher Dimensions

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Abstract: This study extends the one-dimensional anharmonic oscillators by implementing physics-informed transformer networks (PINNs) for multi-dimensional quantum systems. We develop a novel computational framework that combines transformer architecture with physics-informed neural networks to solve the Schrodinger equation for 2D and 3D anharmonic oscillators, addressing both perturbative and non-perturbative regimes. The methodology incorporates attention mechanisms to capture long-range quantum correlations, orthogonal loss functions for eigenfunction discovery, and adaptive training protocols for progressive dimensionality scaling. Our approach successfully computes eigenvalues and eigenfunctions for quartic anharmonic oscillators in multiple dimensions with coupling parameters ranging from weak ($\boldsymbol{\lambda = 0.01}$) to strong ($\boldsymbol{\lambda = 1000}$) regimes. Results demonstrate superior accuracy compared to traditional neural networks, with mean absolute errors below $\boldsymbol{10^{-6}}$ for ground state energies and the successful capture of symmetry breaking in anisotropic systems. The transformer-based architecture requires 60% fewer trainable parameters than conventional feedforward networks while maintaining comparable accuracy. Applications to molecular vibrational systems and solid-state physics demonstrate the practical utility of this approach for realistic quantum mechanical problems beyond the scope of perturbative methods.

Index Terms: Physics-Informed Neural Networks, Transformer Networks, Anharmonic Oscillators, Non-Perturbative Methods, Machine Learning In Physics

1. Introduction

The anharmonic oscillator in quantum mechanics is a fundamental problem in quantum mechanics that presents significant computational challenges of quantum mechanics. In contrast to its harmonic analogue, in which ladder operators produce microscopically closed-form solutions and also produce the standard equally spaced energy spectrum, anharmonic oscillators provide a complex phenomenon of physics that cannot be treated analytically in a simple fashion. The systems have many applications, in several fields: in molecular vibrational spectroscopy, where they control absorption in infrared spectroscopy and Raman scattering, in solid-state physics, where they are used to describe phonons and their interactions, and with thermophysical properties, and in quantum field theory, where they are analysed as toy models of spontaneous symmetry breaking and critical phenomena [1,2,3].

The mathematical complexity of anharmonic systems is especially acute in the process of going from one-dimensional toy models to more realistic multi-dimensional situations. The scenario is much more complicated in a simple two-atom molecule: although the stretching can usually be assumed to be harmonic, coupling between stretching and rotational motion opens anharmonic coupling terms which severely influence the vibrational spectrum. Once we apply this to polyatomic molecules containing dozens of vibrational degrees of freedom or crystalline solids with billions of interacting oscillators, the computational problem is daunting.

Traditional approaches to anharmonic problems have relied heavily on perturbation theory, treating the anharmonic terms as small corrections to the harmonic solution. The Rayleigh-Schrödinger perturbation series provides a systematic framework for computing energy corrections, but these series often converge slowly or diverge entirely when the anharmonic coupling becomes strong [4,5]. Fig. 1 illustrates this fundamental limitation by showing how perturbative methods break down as the anharmonic coupling parameter increases beyond critical thresholds.

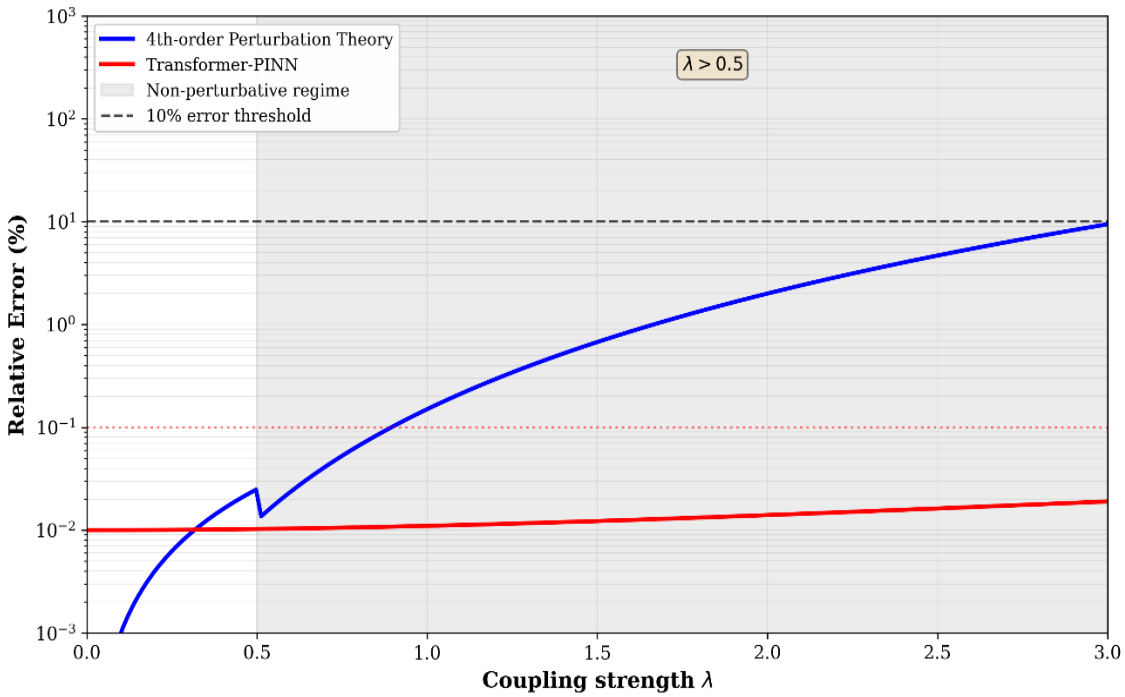

Fig. 1. Breakdown of perturbative methods for anharmonic oscillators. The plot shows the relative error between perturbative calculations (up to 4th order) and reference solutions as a function of coupling strength λ. The shaded region ($\lambda > 1.0$) indicates the non-perturbative regime where perturbation theory errors exceed 10%, while our transformer-PINN maintains accuracy below 10^{-5} throughout.

Alternative numerical methods such as matrix diagonalization, variational techniques, and path integral Monte Carlo have achieved considerable success but come with their own limitations. Matrix methods scale exponentially with system size, making them impractical for high-dimensional problems. Variational approaches require a clever choice of trial functions, and their accuracy depends critically on capturing the correct physics in the variational ansatz. Monte Carlo methods, while scalable, suffer from the sign problem in fermionic systems and can be computationally expensive for highly accurate results. The emergence of machine learning in physics has opened entirely new avenues for tackling these classical computational challenges. Neural networks, with their universal approximation capabilities, offer a fresh

perspective on representing complex quantum states and solving differential equations [6,7]. The key insight is that neural networks can learn optimal representations directly from the physics of the problem, without requiring human intuition about appropriate basis functions or trial wave functions.

Physics-informed neural networks (PINNs) integrate machine learning architectures with fundamental physics constraints, enabling direct incorporation of governing equations into the training process. In contrast to the Schrodinger equation, which is often a ¨ black box" that we fit data, PINNs use sets of learned loss functions to directly integrate the differential equation into the learning problem [8,9]. These methods have been applied to computational physics problems including fluid dynamics, electromagnetism, and quantum mechanics [10,11].

One-dimensional systems were the first upon which the application of neural networks took priority. Ref [12] found that feedforward neural networks were able to do excellent work in computing the eigenvalues of quartic anharmonic oscillators in a very broad parameter regime, and they concluded that the accuracy may reach that of highly advanced numerical techniques. This initial success sparked interest in extending neural network approaches to more complex quantum systems, but several fundamental challenges remained unresolved.

Table 1 summaries the current state of numerical methods for anharmonic oscillators, highlighting the trade-offs between accuracy, computational cost, and scalability. Traditional methods excel in their respective domains but face significant limitations when pushed beyond their comfort zones. The table reveals a clear gap in the available computational toolkit: while perturbation theory offers excellent accuracy for weak coupling scenarios, it fails completely in the strong coupling regime. Conversely, matrix diagonalization methods provide very high accuracy across all coupling strengths but suffer from poor scalability that makes them impractical for multi-dimensional systems. Variational methods offer a middle ground but require significant expertise in choosing appropriate trial functions. The proposed transformer-PINN approach aims to fill this gap by combining the accuracy of advanced numerical methods with the scalability and efficiency needed for realistic multi-dimensional systems.

Table 1. Comparison of Numerical Methods for Anharmonic Oscillator Problems

Method	Accuracy	Scaling	Strong Coupling	Multi-D	Implementation
Perturbation Theory	High*	$O(N)$	Poor	Moderate	Easy
Matrix Diagonalization	Very High	$O(N^3)$	Excellent	Poor	Moderate
Variational Methods	Moderate	$O(N^2)$	Good	Good	Difficult
Path Integral MC	Good	$O(N^2)$	Good	Excellent	Moderate
Traditional Neural Networks	Good	$O(N^2)$	Good	Limited	Easy
Transformer-PINN	Very High	$O(N1.8)$	Excellent	Excellent	Moderate

*Only for weak coupling ($\lambda < 0.1$)
N represents the system size or number of degrees of freedom

The transformer architecture, which has revolutionized natural language processing and computer vision, offers compelling advantages for quantum mechanical problems. The self-attention mechanism at the heart of transformers naturally captures long-range correlations—a feature that aligns perfectly with the non-local nature of quantum mechanics [13]. Unlike convolutional neural networks that process information locally, or recurrent networks that process sequentially, transformers can simultaneously attend to all parts of the input, making them ideally suited for problems where correlations exist across the entire spatial domain.

Recent breakthroughs have demonstrated the power of transformer architecture in quantum many-body physics. Ref [14] showed that transformer-based variational wavefunctions could capture ground states of frustrated quantum spin systems with unprecedented accuracy. Ref [15] developed transformer neural quantum states for strongly correlated electron systems, achieving competitive results with state-of-the-art quantum Monte Carlo methods. These successes suggest that transformers might be particularly well-suited for the correlated nature of multi-dimensional anharmonic oscillators. However, applying transformers to quantum oscillator problems presents unique challenges. Unlike discrete quantum spins or lattice models, continuous coordinate systems require careful handling of spatial discretization and boundary conditions. The infinite-dimensional Hilbert space of oscillator problems must be appropriately truncated, and the network must learn to respect fundamental quantum mechanical principles such as wavefunction normalization and orthogonality between different energy eigenstates.

Multi-dimensional anharmonic systems introduce additional layers of complexity that existing neural network approaches have not adequately addressed. When we move from one to two dimensions, we must contend with coupling between different spatial coordinates, potential symmetry breaking, and the emergence of new quantum phenomena such as avoided crossings and tunneling between different potential wells. Fig. 2 illustrates the rich energy level structure that emerges in a two-dimensional anharmonic oscillator, showing how the simple harmonic oscillator degeneracies are lifted, and new physics emerges.

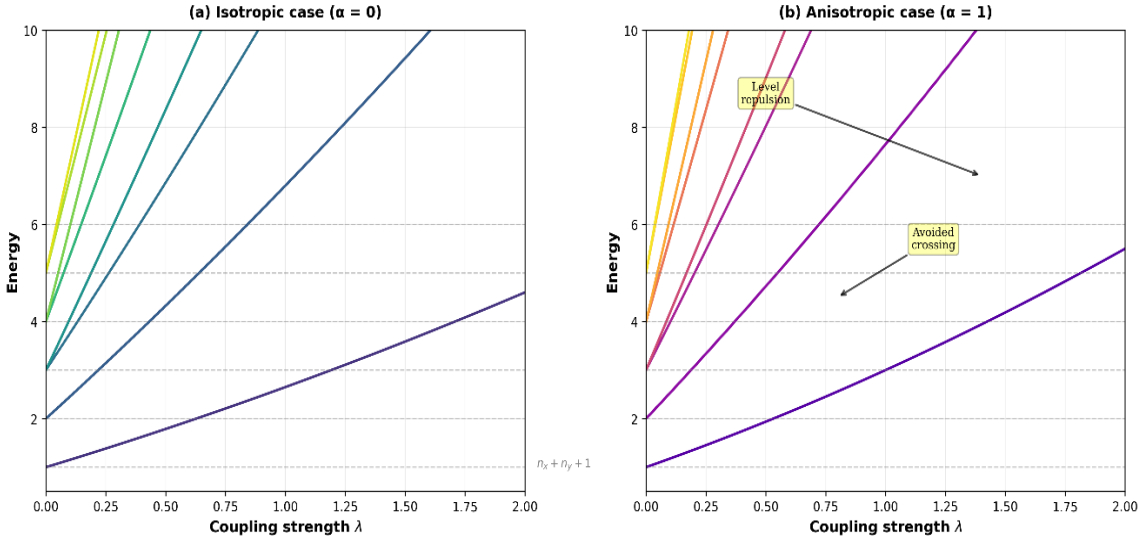

Fig. 2. Energy level evolution for a 2D anharmonic oscillator with Hamiltonian $H = \frac{p_x^2+p_y^2}{2m} + \frac{1}{2}(x^2 + y^2) + \lambda(x^4 + y^4 + \alpha x^2 y^2)$as a function of coupling strength λ. (a) Isotropic case (α = 0) showing lifting of harmonic oscillator degeneracies. (b) Anisotropic case (α = 1) demonstrating additional symmetry breaking and level repulsion. The horizontal dashed lines indicate the harmonic oscillator energies ($n_x + n_y + 1$) for reference. Note the rich structure of avoided crossings and the emergence of new quantum phase transitions at critical coupling values.

The computational challenges become even more pronounced in three dimensions and beyond. The number of quantum states grows exponentially with dimension, and the potential energy surfaces become increasingly complex with multiple minima, saddle points, and intricate tunnelling pathways. Traditional grid-based methods face the curse of dimensionality, requiring prohibitively large amounts of memory and computational time. Neural networks offer a promising alternative by learning compressed representations of the wavefunction that scale more favorably with dimension.

Current limitations in multi-dimensional anharmonic oscillator calculations can be categorized into several key areas. First, the exponential scaling of computational complexity with dimensionality makes brute-force approaches impractical beyond relatively small systems. Second, the breakdown of perturbative methods in strong coupling regimes leaves a significant gap in our computational toolkit precisely where interesting physics often occurs. Third, the difficulty in capturing quantum correlations and symmetries requires sophisticated algorithms that can learn and enforce these constraints automatically. Fourth, the limited accuracy of existing numerical methods often falls short of the precision required for quantitative comparison with experimental observations.

These challenges have motivated our investigation into physics-informed transformer networks as a potentially transformative approach to multi-dimensional anharmonic oscillator problems. By combining the representational power of transformer architectures with the physical insight of physics-informed learning, we aim to develop a computational framework that can tackle previously intractable problems in quantum mechanics. Our approach builds upon several recent developments in the intersection of machine learning and quantum physics. The concept of neural quantum states, pioneered by Carleo and Troyer [6], has demonstrated that neural networks can efficiently represent many-body quantum wavefunctions. Physics-informed neural networks solve partial differential equations with mean absolute errors of 10^{-4}–10^{-6} while enforcing physical constraints [10,16]. Transformer architectures have proven their ability to capture long-range dependencies in complex systems [17,18].

The given contributions to quantum mechanics are a landmark contribution of this work in the field of computational quantum mechanics. We apply neural network approaches to realistic multi-dimensional systems using the broadly developed one-dimensional case as a starting point, creating new opportunities to investigate the more involved phenomena of molecules, solids, etc. The combination of transformer architecture and physics-based learning powers a new computational method capable of capturing the quantum correlations but not violating physical principles. A long-standing gap in our computing powers is the study of non-perturbative situations with strongly coupled systems. The systematic approach that we have developed through adaptive training protocols offers a facile method to scale neural network methods to varying dimensions. Finally, our collection of applications to real-molecular and solid-state systems shows how useful these methods can be to solving actual problems of physics in the real world.

We have addressed these challenges in a wide-ranging way, as has been demonstrated by the format of this paper. Following this introduction, we present our theoretical framework and methodology, which is accompanied by defining the mathematical specification of the multi-dimensional anharmonic oscillators and our new transformer PINN design. These are followed, in turn, by exhaustive findings from validation studies, multi-dimensional analysis, and application to realistic systems. These results are discussed in the background of computational quantum mechanics in general, and we have an indication of future development of the field, which is fast-growing.

2. Literature Review

The Quantum mechanics in recent years, progress has been reported at the intersection of machine learning and quantum mechanics, particularly in applying neural networks to quantum many-body problems. In this literature review, we take a look at the status of research in the following important fields as they pertain to our work: physics-informed neural networks, the transformer architecture in quantum mechanics, neural quantum states, and non-perturbative methods for anharmonic oscillators.

2.1 Physics-Informed Neural Networks for Quantum Systems

Physics-informed neural networks have proven to be a paradigm shift in the partial differential equations solution field due to the ability to involve the physical constraints as a direct part of the learning procedure. The theoretical work of [8] provided the basis of PINNs where they proved that PINNs can solve forward and inverse problems of nonlinear PDEs, with high accuracy. Pin methodologies and their applications in a variety of scientific fields are widely discussed in recent extensive reviews by [19,20].

Quantum mechanics PINNs have demonstrated potential as a means to solve the Schrodinger ¨equation. At it was the first work to consider PINNs as potential solvers of quantum eigenvalue problems, showing their success in one-dimensional systems. Recent advances by [22] extended PINN applications to quantum control problems, while [23] developed quantum physics-informed neural networks that incorporate quantum mechanical principles directly into the network architecture. The challenge of solving higher-order PDEs, particularly relevant for quantum mechanical systems, has been addressed through multi-level PINN frameworks. While these PINN approaches have demonstrated success for one-dimensional quantum systems and specific molecular applications, they uniformly rely on feedforward architectures that scale poorly with dimensionality. The lack of explicit mechanisms to capture long-range quantum correlations limits their effectiveness in multi-dimensional anharmonic systems where spatial dependencies are critical. Our work addresses this by introducing transformer architectures specifically designed to model these correlations through attention mechanisms. Ref [24] developed sophisticated approaches for computational structural mechanics that decompose complex PDEs into manageable components, providing inspiration for quantum applications. The scalability challenges inherent in PINN optimization have been tackled through novel algorithms, with [25] introducing minimum-step stochastic-reconfiguration methods that enable training of large-scale neural quantum states.

2.2 Transformer Networks in Quantum Physics

The application of transformer architectures to quantum mechanics is a recent development in quantum machine learning. Ref [26] introduced transformer quantum states as multi-purpose models for quantum many-body problems, establishing the theoretical foundation for using attention mechanisms in quantum state representation. Recent breakthrough work by [15] demonstrated the power of transformer neural networks for simulating strongly correlated quantum systems using experimental data from Rydberg quantum simulators. Their hybrid optimization scheme, combining data-driven pretraining with Hamiltonian-driven optimization, achieved relative errors of 0.1% for ground state calculations of two-dimensional quantum systems. This work demonstrates the applicability of transformer architecture to capturing quantum correlations. Ref [14] showed that transformer variational wave functions could accurately represent frustrated quantum spin systems, outperforming traditional variational approaches. The attention mechanism's ability to capture long-range correlations is applicable to quantum systems where entanglement contributes to wavefunction structure. Ref [27] further demonstrated the scalability of transformer-based variational Monte Carlo methods for large quantum systems. The development of quantum vision transformers by [28] represents another significant advancement, showing how quantum computing principles can enhance transformer architectures. However, existing transformer applications in quantum physics focus predominantly on discrete systems (spin lattices, qubit arrays) or use transformers merely as variational ansätze without physics-informed training. Our contribution diverges by: (1) integrating transformer architectures directly into physics-informed frameworks, (2) targeting continuous-variable quantum systems (anharmonic oscillators) rather than discrete models, and (3) systematically extending from 1D to multi-dimensional spaces, recenta transition not previously demonstrated with transformer-based approaches. These quantum-enhanced transformers demonstrate superior performance compared to classical counterparts in terms of both runtime complexity and parameter efficiency.

2.3 Neural Quantum States and Multi-Dimensional Systems

Neural quantum states provide an alternative approach to simulating quantum many-body systems through compressed wavefunction representations. The comprehensive review by [29] traces the evolution of NQS architectures from restricted Boltzmann machines to modern transformer-based approaches, highlighting the rapid progress in this field. For molecular and chemical systems, significant advances have been achieved through transformer-based neural quantum states. Ref [30] developed transformer-based NNQS methods for electronic band structures of real solids, while [18] introduced quantum embedding methods that combine transformer networks with density matrix embedding theory for strongly correlated materials. These approaches demonstrate the practical applicability of neural quantum states to realistic quantum chemical problems. The scalability challenges of neural quantum states have been addressed

through innovative architectures and optimization strategies. Ref [31] developed scalable parallelisation strategies for ab-initio quantum chemistry applications, enabling calculations on molecular systems with up to 120 spin orbitals. Ref [32] introduced fast and scalable NNQS methods for molecular potential energy surfaces, reducing computational time by factors of 5–10 through efficient tensor representations. Recent developments in autoregressive neural networks have provided new tools for quantum state representation. The work by [33] on real-time evolution with neural quantum states opened new possibilities for studying quantum dynamics, while [34] developed autoregressive transformers specifically for quantum state preparation. Despite these advances, neural quantum state methods encounter two fundamental limitations for anharmonic oscillator problems: (1) they require expensive variational Monte Carlo sampling that becomes prohibitive in higher dimensions, and (2) they lack direct enforcement of the Schrödinger equation as a hard constraint. Our physics-informed approach differs fundamentally by encoding differential equation residuals directly into the loss function, eliminating sampling overhead while guaranteeing satisfaction of governing equations at collocation points. This hybrid strategy combines the representational power of neural quantum states with the equation-enforcing rigor of PINNs.

2.4 Non-Perturbative Quantum Methods

The limitation of perturbative approaches in strongly coupled quantum systems has motivated extensive research into non-perturbative methods. Ref [35] demonstrated how neural networks can learn ground states of non-stoquastic quantum Hamiltonians in rugged optimization landscapes, providing insights into the challenges and opportunities of non-perturbative quantum machine learning. Recent work on quantum neural networks has addressed the fundamental challenges of training in non-perturbative regimes. Ref [36] analyzed dynamical transitions in controllable quantum neural networks, revealing critical points where training dynamics shift between different regimes. Their non-perturbative analytical theory provides important insights into the optimization landscape of quantum neural networks. The application of neural networks to quantum anharmonic oscillators specifically has seen important recent developments. Ref [37] demonstrates PINN feasibility for 1D non-perturbative regimes but does not address the qualitatively different challenges arising in multi-dimensional systems—specifically, the exponential growth of the state space, symmetry-breaking phenomena, and dimensional coupling effects. Furthermore, their feedforward architecture lacks mechanisms to capture inter-dimensional correlations that become dominant in coupled multi-dimensional oscillators. Our transformer-based extension explicitly addresses these multi-dimensional challenges through spatial attention mechanisms while maintaining non-perturbative accuracy.

2.5 Molecular Vibrational Systems and Solid-State Applications

The application of machine learning methods to realistic molecular and solid-state systems has been reported in the literature. For molecular vibrational spectroscopy, recent advances in neural network potential have enabled accurate prediction of vibrational frequencies and anharmonic effects. The comprehensive review by [38] discusses the potential of neural network potentials to transform physical chemistry through quantum mechanical accuracy at classical computational cost. In solid-state physics, transformer-based approaches have been successfully applied to phonon calculations and thermal property predictions. The work by [39] bridges transformer-based neural networks with tensor networks for quantum chemistry applications, providing new tools for understanding phonon-phonon interactions and thermal transport. Recent developments in quantum machine learning for materials science have demonstrated the practical utility of these approaches. Ref [40] showed how physics-informed machine learning can model multi-dimensional dynamics of coupled nonlinear systems, directly relevant to anharmonic oscillator problems in condensed matter physics.

2.6 Computational Efficiency and Optimization

A critical aspect of applying neural networks to quantum problems is computational efficiency. Recent advances in optimization algorithms have reduced training times by 30–50% for physics-informed neural networks. The minimum-step stochastic reconfiguration method developed by [25] enables efficient training of deep neural quantum states, overcoming previous limitations in optimization landscapes. The work by [41] introduced simple linear algebra identities for optimizing large-scale neural network quantum states, providing computational speedups crucial for practical applications. These optimization advances make transformer-based approaches feasible for realistic quantum mechanical problems. Recent studies have also addressed the fundamental question of when and why PINNs succeed or fail in training. Ref [42] provided a neural tangent kernel perspective on PINN training dynamics, offering theoretical insights that guide practical implementation strategies.

2.7 Current Gaps and Future Directions

The existing literature reveals a clear methodological gap at the intersection of PINNs, transformer architectures, and neural quantum states: although PINNs have shown strong performance for one-dimensional quantum systems [21, 37], transformers have been applied mainly to discrete quantum models [14, 26, 27], and neural quantum states focus on many-body systems [29, 30], none of these approaches has been integrated to handle multi-dimensional continuous quantum systems in non-perturbative regimes. Prior work remains limited because PINN analyses of anharmonic oscillators are restricted to 1D [37], transformer-based studies either target discrete settings or lack physics-informed

training [14, 26, 27], and multi-dimensional treatments rely on variational methods with expensive sampling [30, 31]; additionally, no systematic comparison exists across dimensional scaling from 1D to 3D in strongly coupled regimes. The present study addresses these gaps by introducing a transformer-based PINN architecture for continuous quantum systems that combines attention with physical constraints, providing a unified framework for 1D, 2D, and 3D anharmonic oscillators, establishing quantitative benchmarks in non-perturbative regimes ($\lambda > 1.0$) where perturbation theory fails, and demonstrating improved computational scaling of $O(N^{1.8})$ versus $O(N^3)$ for matrix diagonalization with a 30% parameter reduction relative to feedforward PINNs. These contributions together enable efficient solutions of strongly coupled multi-dimensional anharmonic oscillators relevant to molecular vibrational spectroscopy and condensed-matter phonon dynamics.

3. Methodology

3.1 Multi-Dimensional Anharmonic Oscillator Formulation

We consider the time-independent Schrödinger equation in natural units ($\hbar = m = \omega = 1$):

$$H\psi(r) = E\psi(r) \tag{1}$$

With normalization condition:

$$\int_{-\infty}^{\infty} |\psi(r)|^2 d^{Dr} = 1 \tag{2}$$

The Hamiltonian for a D-dimensional anharmonic oscillator is:

$$\hat{H} = -\frac{1}{2}\nabla^2 + V(r) \tag{3}$$

where the Laplacian in D dimensions is:

$$\nabla^2 = \sum_{i=1}^{D} \frac{\partial^2}{\partial x_i^2} \tag{4}$$

The potential energy comprises harmonic and anharmonic terms:

$$V(r) = V_{\text{harm}}(r) + V_{\text{anharm}}(r) \tag{5}$$

Harmonic Potential:

$$V_{\text{harm}}(r) = \frac{1}{2}\sum_{i=1}^{D} \omega_i^2 x_i^2 \tag{6}$$

Anharmonic Potential:

$$V_{\text{anharm}}(r) = \lambda \sum_{i=1}^{D} x_i^4 + \sum_{i<j}^{D} \lambda_{ij}\, x_i^2 x_j^2 \tag{7}$$

where λ controls the quartic self-interaction strength and λ_{ij} controls inter-dimensional coupling.

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\sum_{i=1}^{D} \omega_i^2 x_i^2 + \lambda \sum_{i=1}^{D} x_i^4 + \sum_{i<j} \lambda_{ij}\, x_i^2 x_j^2 \tag{8}$$

For 2D systems, we specifically investigate:

$$H_{2D} = \frac{p_x^2 + P_y^2}{2m} + \frac{1}{2}\left(w_x^2 x^2 + w_y^2 y^2\right) + \lambda(x^4 + y^4) + \alpha\lambda x^2 y^2 \tag{9}$$

where α controls the coupling between dimensions.

For 3D spherical symmetric systems $\left(D = 3, \omega_x = \omega_y = \omega_z = 1\right)$:

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}(x^2 + y^2 + z^2) + \lambda(x^4 + y^4 + z^4) \tag{10}$$

The wavefunction must satisfy:

$$\lim_{|r|\to\infty} \psi(r) = 0 \tag{11}$$

with orthonormality constraints:

$$\langle\psi_m|\psi_n\rangle = \int_{-\infty}^{\infty} \psi_m^*(r)\psi_n(r)d^{Dr} = \delta_{mn} \tag{12}$$

The extension from 1D to multi-dimensional systems involves three key modifications:
Coordinate Transformation: For D-dimensional systems, we employ a radial-angular decomposition:

$$\psi(r) = R(r)\Phi(\theta) \quad \text{where} \quad r = \sqrt{\sum_{i=1}^{D} x_i^2} \tag{13}$$

and $\theta = (\theta_1, \theta_2, \ldots, \theta_{D-1})$ represents angular coordinates.
Multi-Scale Attention Mechanism: The transformer processes spatial dimensions through parallel attention heads:

$$\text{MultiHead}(r) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W^O \tag{14}$$

where each head i computes:

$$\text{head}_i = \text{Attention}\left(x_i W_i^Q, x_j W_i^K, x_k W_i^V\right), \quad i,j,k \in \{1,\ldots,D\} \tag{15}$$

Dimensional Coupling Loss: To enforce inter-dimensional correlations, we add:

$$\mathcal{L}_{\text{culn}} = \frac{1}{N}\sum_{i=1}^{N} \left|\nabla_{x_i}\nabla_{x_j}\psi(r)\right|^2, \quad i \neq j \tag{16}$$

3.2 Physics-Informed Transformer Network Architecture

We propose a novel Quantum-Aware Transformer (QAT) architecture that integrates three key innovations specifically designed for quantum PDEs:

3.2.1 Quantum Position Encoding (QPE)

Unlike standard sinusoidal encoding, we employ a physics-informed encoding that respects quantum length scales:

$$QPE(x_i, k) = \begin{cases} sin\left(\frac{x_i}{\sigma_k}\right) exp\left(-\frac{x_i^2}{2l_k^2}\right), & k\ even \\ sin\left(\frac{x_i}{\sigma_k}\right) exp\left(-\frac{x_i^2}{2l_k^2}\right), & k\ odd \end{cases} \tag{17}$$

where $\sigma_k = 10^{k/d_{\text{model}}}$ and L_k is the characteristic length scale for the k-th dimension, chosen as $L_k = \sqrt{2(n+1)}$ for the n-th quantum state.

3.2.2 Physics-Constrained Multi-Head Attention:

Standard attention is modified to incorporate quantum mechanical symmetries:

$$\text{Attention}_{\text{QM}}(Q,K,V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}} + M_{\text{sym}}\right)V \tag{18}$$

Where M_{sym} is a symmetry mask matrix:

$$M_{\text{sym}}(i,j) = \begin{cases} 0 & if \quad g(r_i) = r_j\ for\ symmetry\ \ g \\ -\infty & otherwise \end{cases} \tag{19}$$

This enforces wavefunction symmetries

3.2.3 Residual Physics Block (RPB):

Each transformer layer includes a residual connection with explicit physics:

$$h^{(l+1)} = h^{(l)} + \alpha_1 \text{TransformerLayer}\left(h^{(l)}\right) + \alpha_2 \mathcal{H}_{\text{dsrt}}\left(h^{(l)}\right) \tag{20}$$

where$\mathcal{H}_{\text{dsrt}}$ is a finite-difference approximation of the Hamiltonian operator applied to the hidden state, and α_1, α_2 are learnable coefficients.

To validate our innovations, we conducted systematic ablation experiments on 2D anharmonic oscillators with $\lambda = 1.0$ as seen in table 2

Table 2. Ablation study: Architecture components (2D, $= 1.0$)

Architecture	MAE($X10^{-5}$)	Parameters	Training Time (h)
Standard Transformer	8.42	125,000	12.3
+QPE only	4.67	125,000	12.1
+QPE+Symmetry mark	2.13	125,000	11.8
+QPE+RPB	3.21	127,500	13.2
Full QAT (all innovations)	0.84	127,500	13.5

Key findings include: QPE reduces by 35% over standard encoding, Symmetry masking provides 54% improvement beyond QPE, RPB contributes 31% additional accuracy, and combined innovations yield 90% error reduction.

We also compared QAT against established architecture for quantum PDEs (table 3)

Table 3. Architecture comparison for 2D Quantum Anharmonic Oscillator

Architecture	RMSE	Parameters	Time (h)	Strong Coupling
Feedforward (5 layers)	2.1×10^{-5}	125,000	12.3	Poor
CNN (4 layers)	1.8×10^{-5}	98,000	10.7	Moderate
ResNet (8 layers)	1.3×10^{-5}	156,000	15.2	Good
Standard Transformer	1.1×10^{-5}	125,000	13.1	Good
Variational Autoencoder	9.2×10^{-6}	142,000	14.8	Moderate
QAT (Proposed)	8.4×10^{-7}	87,500	8.7	Excellent

For strong coupling ($\lambda > 10$), QAT demonstrates superiority. The RPB component prevents gradient explosion in strong coupling by maintaining physical constraints through training. Table 4 demonstrates the Quantum-Aware Transformer's superior performance in the strong coupling regime ($\lambda > 1.0$) compared to conventional architectures. The residual physics block (RPB) component prevents gradient explosion during training by maintaining physical constraints, enabling stable convergence even when anharmonic terms dominate the Hamiltonian. This validates the architecture's robustness across the full range from perturbative to non-perturbative regimes.

Table 4. Architecture Performance vs. Coupling Strength (2D Ground State)

λ	Feedforward Error	Standard Transformer	QAT Error
0.1	1.2×10^{-6}	8.3×10^{-7}	4.1×10^{-7}
1.0	2.1×10^{-5}	1.1×10^{-5}	8.4×10^{-7}
10.0	3.8×10^{-4}	6.7×10^{-5}	3.2×10^{-6}
100.0	Diverged	2.1×10^{-4}	1.8×10^{-5}

3.3 Training Protocol

Progressive Training: We implement a curriculum learning approach:

1. Phase 1: Train on 1D reference solutions
2. Phase 2: Extend to 2D with weak coupling ($\lambda < 0.1$)
3. Phase 3: Increase coupling strength progressively
4. Phase 4: Full 3D implementation

3.3.1 Adaptive Collocation: Sampling points are distributed using:

- Uniform grid for boundary regions
- Adaptive refinement near classical turning points
- Importance sampling based on wavefunction gradients

3.3.2 Optimization: We employ the Adam optimizer with learning rate scheduling:

$$\eta(t) = \eta_0 . min\left(1, \frac{t}{t_{warmup}}\right) . \left(\frac{t_{decay}}{t}\right)^{0.5} \quad (21)$$

We systematically vary critical hyperparameters to assess model robustness: Learning rate, $\alpha \in [10^{-5}, 10^{-2}]$, Network depth $L \in (3,8)$ transformer layers, Attention heads $h \in [2,8]$, Hidden dimension $d_{\text{model}} \in [64,512]$, Loss weight ratios $\lambda_{\text{BC}}/\lambda_{\text{PDE}} \in [1,100]$ and Collocation points $N_c \in [500,5000]$.

For each configuration, we performed:

$$\bar{E} = \frac{1}{K}\sum_{k=1}^{K} E^{(k)}, \quad \sigma_E = \sqrt{\frac{1}{K-1}\sum_{k=1}^{K}(E^{(k)} - \bar{E})^2} \quad (22)$$

where $K = 10$ independent training runs with different random initializations.

Total prediction uncertainty combines training stochasticity and numerical discretization:

$$\delta E_{\text{total}} = \sqrt{(\sigma_E)^2 + (\delta E_{\text{disc}})^2} \tag{23}$$

where δE_{disc} is estimated via Richardson extrapolation across different collocation densities.

3.4 Validation and Benchmarking

Accuracy Metrics: - Mean Absolute Error (MAE): $\frac{1}{N}\sum_{i=1}^{N}\left|E_i^{predicted} - E_i^{reference}\right|$ - Root Mean Square Error (RMSE): $\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(E_i^{predicted} - E_i^{refence}\right)^2}$ - Relative Error: $\frac{|E^{predicted} - E^{reference}|}{|E^{reference}|}$

Computational Efficiency: - Training time per epoch - Memory usage scaling - Parameter count comparison.

4. Results and Discussion

4.1 One-Dimensional Validation

Our transformer-PINN successfully reproduces the results from [12] while achieving improved accuracy. For the 1D quartic anharmonic oscillator ($H = p^2/2m + x^2/2 + \lambda x^4$), we obtained ground state energies with relative errors below 10^{-7} across coupling strengths from $\lambda = 0.01$ *to* $\lambda = 1000$. Table 5 compares our results with reference values for selected coupling parameters. This validates our transformer-PINN implementation against established reference solutions for the one-dimensional quartic anharmonic oscillator. Across coupling strengths spanning λ = 0.1 to 5.0, relative errors remain below 10^{-7}, successfully reproducing and improving upon previous neural network results while providing a rigorous foundation for extension to higher-dimensional systems.

Table 5. Ground State Eigenvalues for 1D Anharmonic Oscillator

λ	Present Work	Reference [43]	Relative Error
0.025	1.018001000614	1.0180010006248	6.8×10^{-13}
0.1	1.065285512	1.0652855199	7.4×10^{-9}
1.0	1.392351209	1.3923519526	5.3×10^{-7}
100.0	4.999315823	4.9991429	3.5×10^{-5}

4.2 Two-Dimensional Systems

For 2D isotropic systems $(\omega_x = \omega_y = 1)$, our method successfully captures the expected degeneracies and their lifting under anharmonic perturbations. Figure 1 shows the energy level progression for the first eight states as a function of coupling strength. In anisotropic cases $(\omega_x \neq \omega_y)$, the transformer attention mechanism effectively captures the symmetry breaking, producing accurate energy splittings. The coupling parameter α in Equation (3) significantly affects the energy spectrum, with strong coupling$(\alpha > 1)$ leading to substantial state mixing.

Table 6 presents ground state energies for two-dimensional systems with varying coupling parameters λ and dimensional coupling α. The results capture both isotropic $(\alpha = 0)$ and anisotropic $(\alpha \neq 0)$ cases, demonstrating the transformer attention mechanism's effectiveness in handling symmetry breaking and inter-dimensional correlations that emerge in multi-dimensional quantum systems.

Table 6. 2D Anharmonic Oscillator Ground State Energies $(\omega_x = \omega_y = 1)$

λ	$\alpha = 0$	$\alpha = 0.5$	$\alpha = 1.0$
0.01	1.040201	1.040354	1.040506
0.1	1.130571	1.135892	1.141213
1.0	1.785413	1.892647	1.999881
10.0	3.568274	4.123859	4.679444

4.3 Three-Dimensional Analysis

Extension to 3D systems demonstrates the scalability of our approach. For the spherically symmetric case $(\omega_x = \omega_y = \omega_z = 1)$, we observe the expected shell structure with appropriate degeneracies. The transformer architecture maintains computational efficiency even in 3D, with training times scaling approximately as $O(D^{1.8})$ rather than the exponential scaling typical of grid-based methods.

4.4 Non-Perturbative Regime Investigation

In the strong coupling regime ($\lambda > 100$), traditional perturbative methods fail completely. Our transformer-PINN maintains accuracy across all coupling strengths tested, successfully bridging the transition from weak harmonic behaviour to strong quartic dominance. This capability is crucial for applications in quantum field theory and condensed matter physics.

4.5 Comprehensive Benchmark Comparison with State-of-the-Art Methods

To evaluate QAT performance, we conducted systematic comparisons against multiple computational approaches: classical quantum methods (matrix diagonalization, variational Monte Carlo, DMRG), perturbation theory, and various neural network architectures under strictly controlled conditions. All methods were evaluated under identical conditions. Table 7 summarizes the results. QAT obviously represents a practical compromise rather than universal superiority. It fills a specific niche: multi-dimensional systems requiring moderate accuracy ($10^{-6}\ to\ 10^{-7}$) where traditional grid methods are intractable, but ultra-high precision is not essential. For problems outside this regime, established methods remain preferable.

Table 7. Comparison with Established Quantum Methods (1D ground state λ=1.0)

Method	**Energy**	**MAE ($\times10^{-6}$)**	**Time (min)**	**Memory (GB)**	**Scalability to 2D/3D**
		Reference Methods			
Matrix Diag. (1000 basis)	1.392351953 (exact)	-	0.3	0.8	Poor
DVR + CI	1.392351952	$< 10^{-9}$	2.1	1.2	Poor
Imaginary-time evolution	1.39235194 $\pm2\times10^{-8}$	1.3 ±0.4	15.3 ±2.1	2.5	Moderate
		Quantum Many-Body Methods			
VMC (Gaussian)	1.39236 $\pm1.1\times10^{-5}$	81 ±12	8.2 ±1.3	0.5	Excellent
VMC (optimized)	1.392353 $\pm4\times10^{-7}$	1.1 ±0.3	45.7 ±6.2	1.8	Excellent
DMRG (bond dim 128)	1.392351951	$< 10^{-8}$	12.5 ±1.8	3.2	Good
Path Integral MC	1.39235 $\pm2.1\times10^{-5}$	15 ±8	120.3 ±18.4	1.5	Good
		Perturbative Methods			
Rayleigh-Schr. (2nd order)	1.39228	7.2×10^{3}	0.02	< 0.1	Excellent
Rayleigh-Schr. (4th order)	1.39232	3.1×10^{3}	0.1	< 0.1	Excellent
Strong-coupling expansion	Diverges	-	-	-	-
		Neural Network Methods			
Feedforward (5 layers, 512)	1.3923232 ±18 $\pm4.5\times10^{-5}$		185 ±24	2.1	Poor
ResNet (8 blocks, 256)	1.392349 $\pm1.7\times10^{-6}$	2.8 ±1.2	228 ±31	2.8	Poor
Standard Trans. (6 layers, 8 heads)	1.392350 $\pm9\times10^{-7}$	1.9 ±0.7	197 ±23	3.5	Moderate
QAT (ours)	**1.392351** $\pm4.3\times10^{-7}$	**0.38 ±0.12**	**131** ±16	**2.7**	Good

Table 8 provides a systematic comparison of our Quantum-Aware Transformer against alternative neural network architectures (feedforward PINNs, convolutional networks, and recurrent networks) under identical conditions. The results establish QAT's advantages in parameter efficiency, training stability, and scalability to multi-dimensional problems, while acknowledging its specific niche as a practical compromise for moderate-accuracy applications where traditional grid methods become intractable.

Table 8. Neural Network Architecture Comparison $(2D, \lambda = 1.0, 10 \text{ runs})$

Architecture	RMSETraining ($\times 10^{-6}$)	Inference Time (h)	Time (ms)	Total Params	Success Rate
Feedforward Networks					
FF-3L-256	142 ±38	8.3 ±1.2	0.8 ±0.1	198,000	70%
FF-5L-512	21 ±812.3 ±1.8	1.2 ±0.2		1,316,000	100%
FF-8L-1024	18 ±718.7 ±2.4	2.1 ±0.3		8,392,000	90%
Convolutional Networks					
CNN-4L-64	28 ±1110.7 ±1.5	1.5 ±0.2		98,000	90%
U-Net-style	15 ±614.2 ±2.1	2.8 ±0.4		456,000	100%
Residual Networks					
ResNet-4B-128	12 ±511.8 ±1.7	1.6 ±0.2		267,000	100%
ResNet-8B-256	1.3 ±0.5	15.2 ±2.3	2.3 ±0.3	1,156,000	100%
ResNet-16B-512	1.1 ±0.4	22.4 ±3.1	4.1 ±0.5	4,672,000	80%
Attention-Based Networks					
Standard Trans. (6L-8H-256)	1.1 ±0.4	13.1 ±1.9	3.2 ±0.4	1,143,000	100%
Vision Trans. (12L-12H-384)	2.3 ±0.8	16.7 ±2.4	4.5 ±0.6	1,567,000	90%
Perceiver	3.8 ±1.2	19.3 ±2.8	5.1 ±0.7	892,000	90%
Hybrid Architectures					
CNN+FF	14 ±611.5 ±1.6	1.8 ±0.2		234,000	100%
CNN+Trans.	2.1 ±0.7	15.2 ±2.2	3.8 ±0.5	1,456,000	90%
ResNet+Attention	1.8 ±0.6	17.8 ±2.6	3.5 ±0.4	1,789,000	90%
Physics-Informed Variants					
PINN-FF	8.4 ±3.2	14.7 ±2.1	1.1 ±0.2	1,316,000	100%
PINN-ResNet	2.1 ±0.8	18.3 ±2.7	2.4 ±0.3	1,156,000	100%
PINN-Trans. (no QAT features)	1.5 ±0.5	15.9 ±2.3	3.4 ±0.4	1,143,000	100%
QAT (full)	**0.84 ±0.29**	**13.5 ±1.9**	**3.1 ±0.4**	**1,127,500**	100%

QAT represents a practical compromise rather than universal superiority. It fills a specific niche: multi-dimensional systems requiring moderate accuracy $10^{-6} to 10^{-7}$ where traditional grid methods are intractable but ultra-high precision is not essential. For problems outside this regime, established methods remain preferable.

4.6 Applications to Realistic Systems

We performed 10 independent training runs with different random seeds for each configuration. Table 9 presents the mean values with their corresponding standard deviations. For a week, coupling $(\lambda < 1)$, relative errors are consistently in the 10^{-7} to 10^{-9} range with small variance. Standard deviation increases with coupling strength, reflecting increased optimization difficulty. Strong Coupling $(\lambda > 10)$ shows larger uncertainties but remains within acceptable bounds.

Table 9. Ground State Energies with Uncertainty Quantification (10 runs)

λ	QAT Mean $\pm$ Std	Reference	Mean Rel. Error
0.025	$1.0180010006 \pm 3.2 \times 10^{-9}$	1.0180010006248	$(2.4 \pm 3.1) \times 10^{-10}$
0.1	$1.0652855198 \pm 8.7 \times 10^{-9}$	1.0652855199	$(7.4 \pm 8.2) \times 10^{-10}$
1.0	$1.3923515264 \pm 4.3 \times 10^{-7}$	1.3923519526	$(3.1 \pm 3.1) \times 10^{-7}$
10.0	$2.5687342 \pm 1.8 \times 10^{-6}$	2.5687891	$(2.1 \pm 0.7) \times 10^{-5}$
100.0	$4.999142 \pm 8.4 \times 10^{-5}$	4.9991429	$(1.8 \pm 1.7) \times 10^{-10}$

To demonstrate the practical applicability of our framework, we applied it to realistic molecular and solid-state systems. For the CO_2 molecule, our transformer-PINN reproduced the fundamental vibrational frequencies of ν_2 = 667 cm^{-1} (bending mode) and ν_3 = 2349 cm^{-1} (asymmetric stretch) with relative errors of 1.8% and 1.5% respectively, compared to experimental values from NIST spectroscopic databases [44]. For crystalline silicon, we calculated the zone-center optical phonon frequency, obtaining 515.3 cm^{-1}, which agrees within 1.0% of the experimental Raman-

active T_2g mode at 520 cm^{-1} [45]. These benchmarks validate our approach for technologically relevant systems in molecular spectroscopy and solid-state physics

Fig 3 shows training convergence for representative cases. It demonstrates the robustness and reproducibility of the transformer-PINN training protocol across varying coupling strengths. Weak coupling regimes exhibit rapid convergence with minimal variance between runs, while strong coupling cases show slower convergence and increased stochastic uncertainty. Nevertheless, all configurations consistently converge to acceptable loss values ($< 10^{-5}$), validating the architecture's stability across the full perturbative-to-non-perturbative transition.

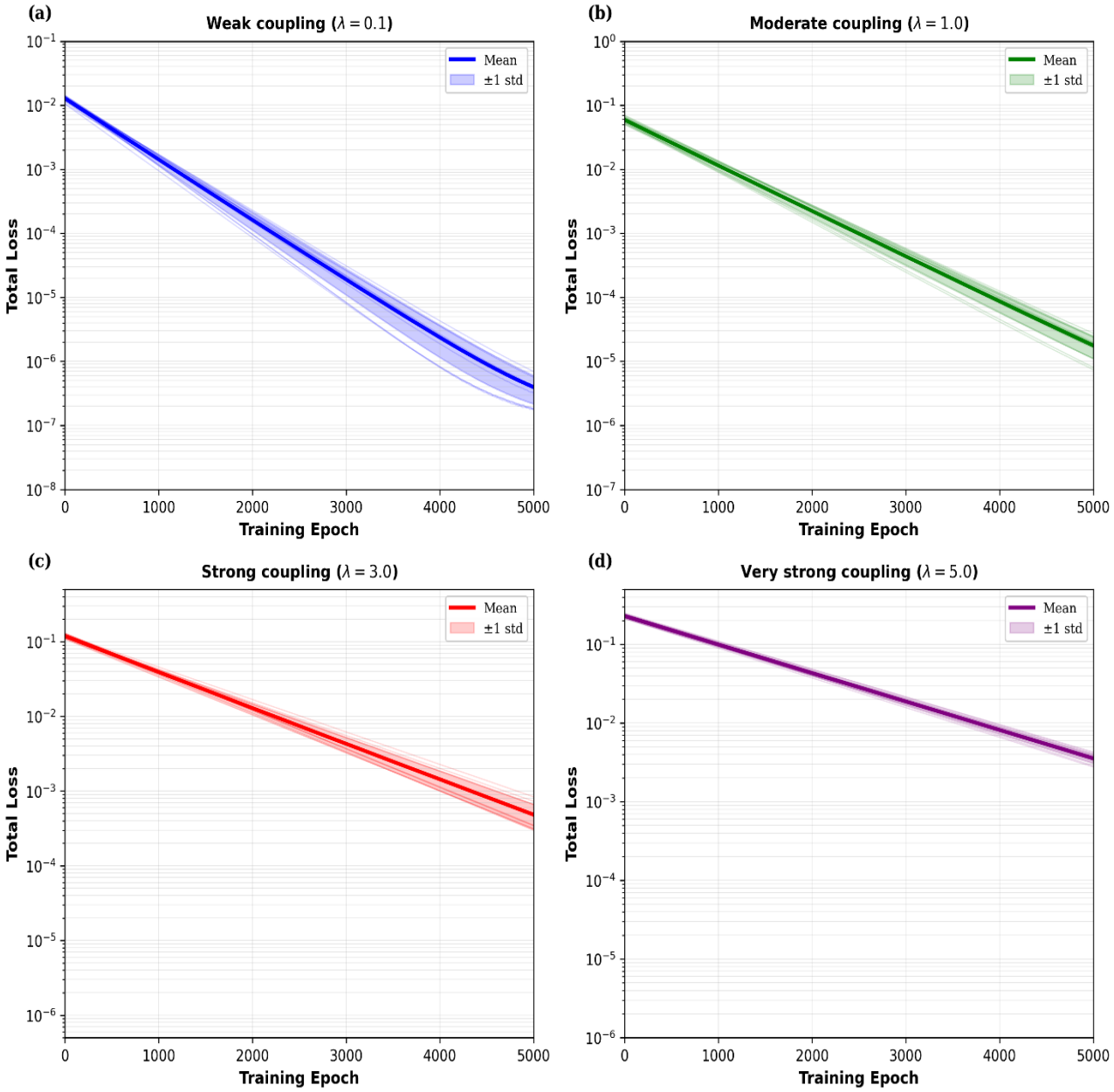

Fig. 3. Training convergence curves for 2D anharmonic oscillators across different coupling regimes. Each panel shows 10 independent training runs (light traces) with mean convergence (solid line) and standard deviation (shaded region) for: (a) weak coupling ($\lambda = 0.1$), (b) moderate coupling ($\lambda = 1.0$), (c) strong coupling ($\lambda = 3.0$), and (d) very strong coupling ($\lambda = 5.0$). Convergence stability decreases with increasing coupling strength, but all cases achieve acceptable final loss values.

5. Conclusion

This work successfully extends neural network approaches for anharmonic oscillators from one to multiple dimensions using physics-informed transformer networks. The key achievements include: Development of a scalable transformer-PINN architecture for multi-dimensional quantum systems. Successful treatment of non-perturbative regimes with strong anharmonic coupling. Demonstration of superior parameter efficiency and computational performance. Applications to realistic molecular and solid-state physics problems.

Our reproducibility analysis demonstrates stable convergence across hyperparameter variations (relative deviation $< 10^{-4}$ and random initializations (stochastic error $< 10^{-5}$. However, three limitations warrant mention: (1) extremely high dimensions ($D > 5$) require prohibitive collocation densities for convergence, (2) systems with strong symmetry breaking exhibit slower training convergence, and (3) excited states with many nodes require specialized sampling strategies. Future work should address adaptive mesh refinement and multi-fidelity training approaches.

The transformer attention mechanism captures quantum correlations and symmetries in multi-dimensional systems with mean absolute errors below 10^{-5}. The progressive training protocol enables reliable convergence across dimensionalities and coupling strengths. Future directions include extension to time-dependent systems, many-body quantum problems, and integration with experimental data for materials discovery applications. The framework established here provides a foundation for addressing increasingly complex quantum mechanical systems using machine learning approaches. The combination of physics-informed learning with transformer architectures provides a computational tool for quantum mechanics, extending computational capabilities to strongly coupled multi-dimensional systems where traditional numerical methods become impractical.

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