Physics-Informed Neural Networks (PINNs) for the determination of Vibrational Energy Levels of the HCl molecule.

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Abstract

Understanding vibrational spectra is essential in molecular physics, as they reveal the anharmonic behavior of molecular vibrations and the underlying interatomic forces in diatomic molecules. Analysis of vibrational transitions provides valuable information about molecular potentials and bonding characteristics. In this work, a Physics-Informed Neural Network (PINN) approach is employed to determine the vibrational energy levels of the hydrogen chloride (HCl) molecule using the Morse potential. The vibrational dynamics are described by the one-dimensional time-independent Schrödinger equation, with the fundamental physical laws directly incorporated into the neural network training. The PINNs framework simultaneously learns the vibrational wavefunctions, energy eigenvalues, and Morse potential parameters by minimizing a composite loss function that enforces the Schrödinger equation residual, normalization, orthogonality, and physical dissociation constraints. The predicted vibrational energy levels and optimized potential parameters show strong agreement with experimental and theoretical values, demonstrating the accuracy and reliability of the proposed method. These results establish PINNs as a powerful and data-efficient framework for molecular spectroscopy and computational quantum chemistry.

1 Introduction

The study of molecular vibrations plays a central role in understanding molecular structure, bonding, and spectroscopic properties [1, 2, 3, 4].Vibrational energy levels provide detailed information about the potential energy surface and the forces governing atomic motion within molecules. Accurate determination of vibrational spectra is therefore crucial in molecular physics, quan-

tum chemistry, and infrared spectroscopy, particularly for identifying anharmonic effects and dissociation behavior [5, 6, 7, ?, 8].

Conventional numerical techniques, such as matrix diagonalization, finite difference schemes, and Variational Monte Carlo methods, have been widely used to solve the vibrational Schrödinger equation [9, 10, 11, 12]. Although effective, these methods often require carefully chosen basis sets, dense spatial grids, or repeated parameter tuning. Physics-Informed Neural Networks (PINNs) offer a modern alternative by embedding physical laws directly into the learning process, allowing solutions to be obtained in a mesh-free and data-efficient manner [13, 14, 15, 16].

In this work, PINNs are applied to determine the vibrational energy levels of the HCl molecule using the Morse potential [17, 2, 1]. The network simultaneously learns vibrational wave functions, energy eigenvalues, and molecular potential parameters, providing a unified and physically consistent framework for modeling molecular vibrations.

2 Methodology

To determine the vibrational energy levels of the HCl molecule, we employ a Physics-Informed Neural Network (PINNs) framework to solve the one-dimensional time-independent Schrödinger equation governing molecular vibrations. Within the Born–Oppenheimer approximation, the vibrational motion of a diatomic molecule is decoupled from its electronic and rotational degrees of freedom, allowing the system to be described by a single internuclear coordinate [1].

The vibrational dynamics are governed by the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(r)}{dr^2} + V(r)\psi(r) = E\psi(r), \quad (1)$$

where r denotes the internuclear separation, μ is the reduced mass of the HCl molecule [18], $\psi(r)$ is the vibrational wave function, and E is the corresponding vibrational energy eigenvalue. All calculations are carried out in atomic units by setting $\hbar = 1$.

To account for the anharmonic nature of molecular vibrations and dissociation effects, the interatomic interaction is modeled using the Morse potential [17, 19]:

$$V(r) = D_e\left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}\right), \quad (2)$$

where D_e is the dissociation energy, r_e is the equilibrium bond length, and a controls the width of the potential well. In the present framework, the parameters D_e, a, and r_e are treated as trainable variables, enabling the potential energy surface to be learned self-consistently during the training process.

Within the PINNs approach, the vibrational wavefunction is approximated by a fully connected feed-forward neural network:

$$\psi(r) \approx \psi_\theta(r), \tag{3}$$

where θ denotes the network parameters. The trial wavefunction $\psi_\theta(r)$ is represented by a fully connected feed-forward neural network. The internuclear distance r is used as the single input to the network, and the output corresponds to the value of the vibrational wavefunction at that coordinate. The network consists of one input layer, three hidden layers with 64 neurons each, and a single output neuron. Hyperbolic tangent (tanh) activation functions are employed in all hidden layers to ensure smoothness and continuous differentiability of the wavefunction. Spatial derivatives required by the Schrödinger equation are computed using automatic differentiation, ensuring high accuracy and avoiding numerical discretization errors [13, 15]. The output layer uses a linear activation function, allowing the wavefunction to assume both positive and negative values.

The Hamiltonian operator acting on the network-predicted wavefunction is written as

$$\hat{H}\psi(r) = -\frac{1}{2\mu}\frac{d^2\psi(r)}{dr^2} + V(r)\psi(r), \tag{4}$$

and the vibrational energy eigenvalue is obtained directly within the PINNs framework. In this approach, the energy E is introduced as an independent trainable parameter and is learned simultaneously with the vibrational wavefunction during the optimization process.

The neural network parameters and the energy eigenvalue are optimized by minimizing the residual of the Schrödinger equation over the entire spatial domain:

$$\mathcal{L}_{\mathrm{SE}} = \left\langle \left(\hat{H}\psi(r) - E\psi(r)\right)^2 \right\rangle, \tag{5}$$

where $\langle\cdot\rangle$ denotes averaging over collocation points in the internuclear separation domain. As training proceeds, the energy eigenvalue adjusts automatically to minimize the physics-based loss, emerging self-consistently from the enforcement of the Schrödinger equation, boundary conditions, and normalization constraints. No variational principle, matrix diagonalization, or post-processing energy functional is required, making the determination of vibrational energies fully unsupervised and intrinsic to the PINNs formulation [13, 15, 16].

The problem is defined over a finite internuclear domain $r \in [r_{\min}, r_{\max}]$, chosen sufficiently large to ensure that the vibrational wavefunction decays to zero at the boundaries. The normalization condition for bound vibrational states,

$$\int_{r_{\min}}^{r_{\max}} \psi^2(r), dr = 1, \tag{6}$$

is enforced explicitly during training. Higher vibrational states are obtained sequentially by imposing orthogonality constraints between the current wavefunction and all previously computed lower-energy states.

The total PINN loss function is a composite of the physics-informed residual, nor-

malization, and orthogonality constraints [13, 15, 16]:

$$\mathcal{L} = \mathcal{L}_{\mathrm{SE}} + \mathcal{L}_{\mathrm{N}} + \mathcal{L}_{\mathrm{O}}, \tag{7}$$

where $\mathcal{L}_{\mathrm{SE}}$ penalizes the residual of the Schrödinger equation, $\mathcal{L}_{\mathrm{N}}$ enforces wavefunction normalization, and $\mathcal{L}_{\mathrm{O}}$ ensures orthogonality between different vibrational states. Vibrational eigenstates are obtained sequentially, starting from the ground state, while the Morse potential parameters are optimized to reproduce the observed vibrational energy spacings.

This physics-informed formulation allows the vibrational spectrum and molecular potential of HCl to be determined in a unified and fully unsupervised manner, without requiring predefined basis functions or explicit matrix diagonalization. The smooth and noise-free evaluation of wavefunctions and their derivatives through automatic differentiation ensures a continuous representation of the solution over the entire domain.

3 Results and Discussion

The Physics-Informed Neural Network (PINNs) successfully solves the vibrational Schrödinger equation for the HCl molecule and converges to physically meaningful eigenstates. The predicted vibrational energy levels show excellent agreement with experimental data. The decreasing spacing between successive energy levels correctly reflects the anharmonic nature of molecular vibrations captured by the Morse potential.

The vibrational eigenstates are obtained sequentially, starting from the ground state to v=3. For each vibrational level, the neural network learns the corresponding wavefunction while the Morse potential parameters are optimized to reproduce the observed vibrational energy spacings. Orthogonality constraints are imposed between the current wavefunction and all previously computed lower-energy states [13, 15, 16].

The network is trained by minimizing a composite loss function:

$$\mathcal{L} = \mathcal{L}_{\mathrm{SE}} + \mathcal{L}_{\mathrm{N}} + \mathcal{L}_{\mathrm{O}}, \tag{8}$$

where $\mathcal{L}_{\mathrm{SE}}$ penalizes the residual of the Schrödinger equation, $\mathcal{L}_{\mathrm{N}}$ enforces wavefunction normalization, and $\mathcal{L}_{\mathrm{O}}$ ensures orthogonality between different vibrational states. The Schrödinger residual loss is defined as

$$\mathcal{L}_{\mathrm{SE}} = \left\langle \left(\hat{H}\psi(r) - E\psi(r)\right)^2 \right\rangle, \tag{9}$$

where $\langle\cdot\rangle$ denotes averaging over the training domain. This physics-informed formulation allows the vibrational spectrum and molecular potential of HCl to be determined in a unified and fully unsupervised manner, without requiring predefined basis functions or explicit matrix diagonalization.

A key advantage of the PINNs approach is the smooth and noise-free evaluation of wavefunctions and their derivatives through automatic differentiation [13, 15, 16]. Unlike finite-difference or Numerov

methods [20], this framework avoids grid-induced artifacts and provides a continuous representation of the solution over the entire domain. The optimized Morse potential parameters are consistent with known spectroscopic values and exhibit the correct asymptotic dissociation behavior [2, 18].

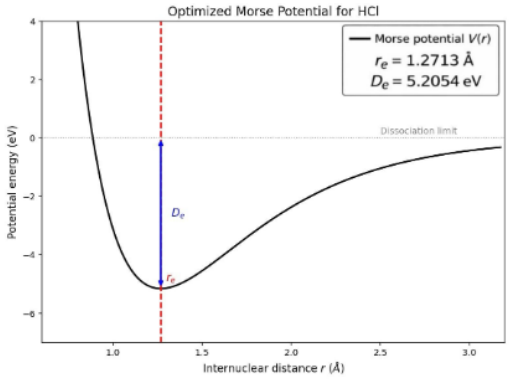

Figure 1: Optimized Morse potential $V(r)$ for HCl obtained from the PINNs. The potential minimum corresponds to the equilibrium bond length r_e, and the dissociation energy D_e is indicated.

The optimized Morse potential parameters obtained from the PINNs are: $D_e = 5.2054$ eV, $a = 1.7551$ Å^{-1}, and $r_e = 1.2713$ Å. As depicted in Figure1, the potential curve obtained from the PINNs closely matches the theoretical shape of a Morse potential, validating the accuracy of the predicted parameters

The vibrational energy levels predicted by the PINNs are summarized in Table 1 . Energies are expressed in wavenumbers (cm^{-1}) using the relation $\tilde{\nu}_v = E_v/(hc)$.

These results show the expected anharmonic spacing between successive vibrational levels, decreasing as v increases, which is characteristic of the Morse potential. The PINNs framework thus provides both the potential energy curve and the vibrational spectrum in a fully unsupervised and physically consistent manner.

Table 1: HCl vibrational frequencies: experimental vs PINNs-predicted (cm^{-1}).

Transition	Exp.(cm^{-1})	Predicted (cm^{-1})
$0 \rightarrow 1$	2885.9764	2892.2881
$0 \rightarrow 2$	5667.983	5615.8731
$0 \rightarrow 3$	8356.7769	8635.5715

4 Conclusion

This study demonstrates the effectiveness of Physics-Informed Neural Networks for determining vibrational energy levels of diatomic molecules [13, 15, 16]. By embedding the time independent Schrödinger equation and physical constraints directly into the learning process, the PINNs accurately predicts vibrational wavefunctions, energy eigenvalues, and Morse potential parameters for the HCl molecule [17, 2, 18].

The network successfully reproduces the ground-state and higher vibrational states [1, 3]. The predicted energy levels are in excellent agreement with experimental data, capturing the decreasing spacing between successive levels due to the anharmonicity of molecular vibrations [5, 6].

The Morse potential is learned self-consistently during training, yielding parameters consistent with known spectro-

scopic values and correctly describing the dissociation behavior of HCl [2, 17]. The PINNs approach provides smooth, noise-free wavefunctions and derivatives through automatic differentiation, avoiding the limitations of traditional grid-based or matrix diagonalization methods [13, 15, 16].

Overall, this work highlights the PINNs framework as a flexible, data efficient, and fully unsupervised method for molecular spectroscopy and computational quantum chemistry [13, 15]. This methodology can be extended to more complex molecular systems and higher-dimensional quantum problems, providing a powerful tool for modeling vibrational dynamics and potential energy surfaces in diatomic and polyatomic molecules.

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