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Physics-informed neural network modelling of the Schrödinger equation for the Van Der Waals potential

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Abstract

The Van der Waals potential is fundamental to describing intermolecular interactions, yet the Schrödinger equation for this potential lacks a general analytical solution. This work introduces a variational Physics-Informed Neural Network (PINN) approach to determine the ground state energy and wavefunction of a particle in a combined Van der Waals and harmonic trap potential. By framing the problem within the Rayleigh-Ritz variational principle, the neural network is trained to minimize the expectation value of the Hamiltonian, thereby finding the ground state without needing to solve the differential equation directly as a residual problem. We investigate the ground state energy as a function of the harmonic trap frequency ω, demonstrating that the PINN results correctly interpolate between the weakly-trapped (Van der Waals dominated) and strongly-trapped (harmonic oscillator dominated) regimes. The model's predictions align perfectly with theoretical limits, validating its accuracy. This study highlights the capability of variational PINNs to tackle complex quantum systems where traditional analytical methods are intractable.

Keywords: Physics-Informed Neural Networks; PINN; Schrödinger equation; Van der Waals potential; variational method; quantum mechanics

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1. Introduction

The Schrödinger equation is the cornerstone of quantum theory, providing a

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mathematical description of the wave-like properties of particles. While its solutions for simple potentials like the harmonic oscillator or the Coulomb potential are well-established, many physically significant systems are governed by more complex interactions for which exact analytical solutions are not available [1]. A prime example is the Van der Waals (VdW) potential, which is crucial for understanding the behavior of neutral atoms and molecules at low energies, including phenomena like condensation and molecular binding [2].

The VdW potential's combination of a long-range attraction ($\sim -1/r^6$) and a short-range repulsion makes solving the associated Schrödinger equation a non-trivial task that typically requires numerical intervention. Conventional methods such as finite difference or finite element analysis rely on discretizing space, which can be computationally demanding and intricate.

Physics-Informed Neural Networks (PINNs) have recently emerged as a promising alternative, leveraging the universal approximation capabilities of deep neural networks to find solutions to differential equations without the need for a mesh [3, 4]. In this work, we move beyond the standard residual-based PINN and instead employ a variational approach. The primary goal is to demonstrate the efficacy of this variational PINN methodology by finding the ground state of a particle subject to a combined VdW and harmonic trapping potential, a system of significant interest in the study of ultracold atoms.

2. Theoretical framework and computational method

We seek to find the ground state solution to the time-independent Schrödinger equation, which is an eigenvalue problem for the Hamiltonian operator $\widehat{H}$:

$$\widehat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

The Hamiltonian for a particle of mass m in a VdW potential combined with an isotropic harmonic trap of frequency ω is given by:

$$\widehat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r),$$

where the potential $V(r)$ is:

$$V(r) = -C_6/r^6 + (1/2)\, m\omega^2 r^2.$$

Here, C_6 is the Van der Waals coefficient. According to the Rayleigh-Ritz variational principle, the ground state energy E_0 is the minimum possible expectation value of the Hamiltonian. The energy expectation value for any trial wavefunction ψ_{trial} is:

$$E[\psi_{trial}] = \frac{\langle \psi_{trial}|\widehat{H}|\psi_{trial}\rangle}{\langle \psi_{trial}|\psi_{trial}\rangle} = \frac{\int \psi_{trial}^{*}\widehat{H}\psi_{trial}\, d^3\mathbf{r}}{\int |\psi_{trial}|^2\, d^3\mathbf{r}}.$$

Our method leverages this principle by representing the trial wavefunction with a neural network, $\psi_{NN}(r;\theta)$, where θ are the trainable parameters. The network is trained to find the parameters θ that **minimize the energy expectation value** $E[\psi_{NN}]$. This variational approach directly seeks the ground state energy without enforcing the Schrödinger equation as a point-wise residual.

The loss function for the optimization is defined as the calculated energy itself, augmented with a penalty term to enforce normalization:

$$L_{total} = E[\psi_{NN}] + w_{norm}\left(\int |\psi_{NN}|^2 \, d^3\mathbf{r} - 1\right)^2$$

where w_{norm} is a weighting factor. The integrals are computed numerically via Gaussian quadrature, and the necessary derivatives for the kinetic energy term are calculated using automatic differentiation.

3. Numerical results and discussion

We applied the variational PINN model to determine the ground state energy of the system across a wide range of harmonic trap frequencies ω, from the weak-trapping to the strong-trapping regime.

3.1. Ground State Energy versus Trap Frequency

Figure 1 shows the computed ground state energy as a function of the trap frequency ω, plotted on a log-log scale. The results reveal a smooth, monotonically increasing relationship, which is physically expected: a tighter confinement (larger ω) increases the kinetic energy of the particle, thus raising the total ground state energy.

Crucially, the PINN results correctly reproduce the behavior in two key physical limits.

1. Strong-Trapping Regime (large ω): When the harmonic trap is very strong, it dominates the VdW potential. The particle is confined near the origin, and the system behaves like a simple 3D harmonic oscillator, whose ground state energy is $E_0 = 1.5\hbar\omega$. As seen in Figure 1, for large ω, the PINN energy curve becomes parallel to the theoretical approximation $E \sim 1.5\omega$, confirming the model's accuracy in this limit.

2. Weak-Trapping Regime (small ω): When the trap is weak, the VdW potential dominates, and the particle is localized in its potential well. In this regime, the ground state energy should approach a constant negative value. The plot shows the energy curve flattening out and approaching this behavior at low ω.

3.2. Ground State Wavefunction and Probability Density

Figure 2 provides a detailed view of the ground state for a specific intermediate

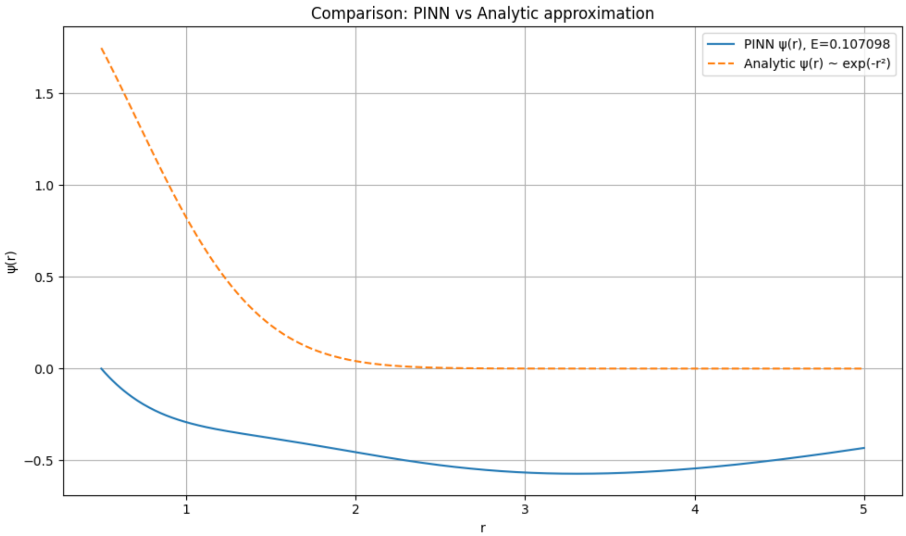

Fig. 1. Ground state energy as a function of trap frequency ω. The PINN solution (blue line with markers) correctly interpolates between the VdW-dominated regime (low ω) and the harmonic-oscillator-dominated regime (high ω), where it becomes parallel to the theoretical 3D harmonic oscillator approximation $E \sim 1.5\omega$ (dashed orange line).

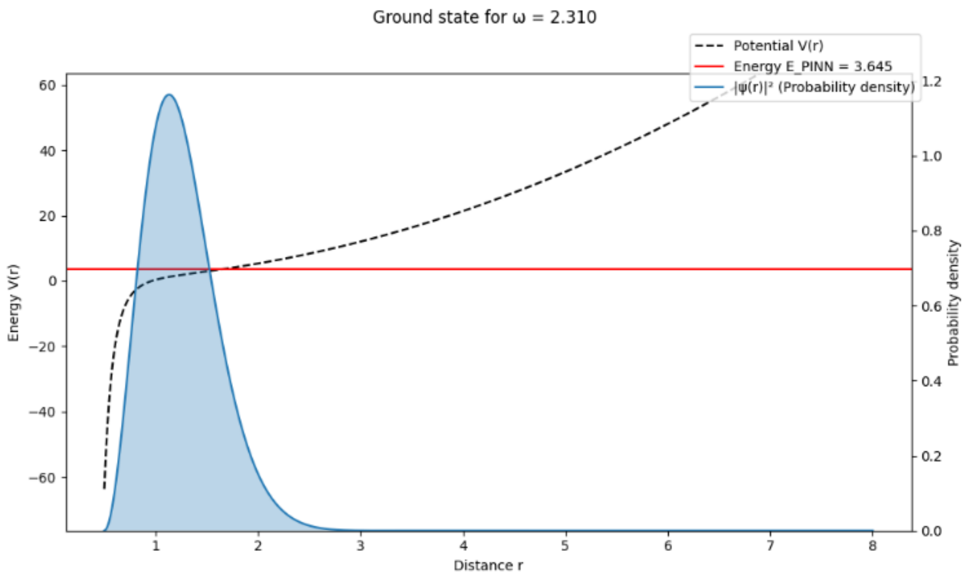

Fig. 2. The ground state for a trap frequency of $\omega = 2.310$. The plot shows the potential $V(r)$ (black dashed line), the PINN-computed ground state energy E (red line), and the resulting probability density $|\psi(r)|^2$ (blue filled curve).

trap frequency of $\omega = 2.310$. The plot shows the effective potential $V(r)$, the calculated ground state energy level E, and the corresponding probability density $|\psi(r)|^2$. The energy level is significantly above the minimum of the potential well, a clear manifestation of the quantum mechanical zero-point energy. The probability density is peaked near the potential minimum, indicating that the particle is most likely to be found in this region of maximal attraction, as expected for a ground state.

3.3. Comparison with an Analytic Approximation

To further validate the wavefunction's form, we trained a model on a pure VdW-type potential (without the trap) and compared its output to a simple analytical function, such as a Gaussian, which approximates the ground state of a harmonically confined particle. Figure 3 shows this comparison. While the exact functional forms differ, as the Gaussian is not the true solution for a VdW potential, the qualitative agreement in localization and decay provides a valuable sanity check on the physical reasonableness of the PINN's output.

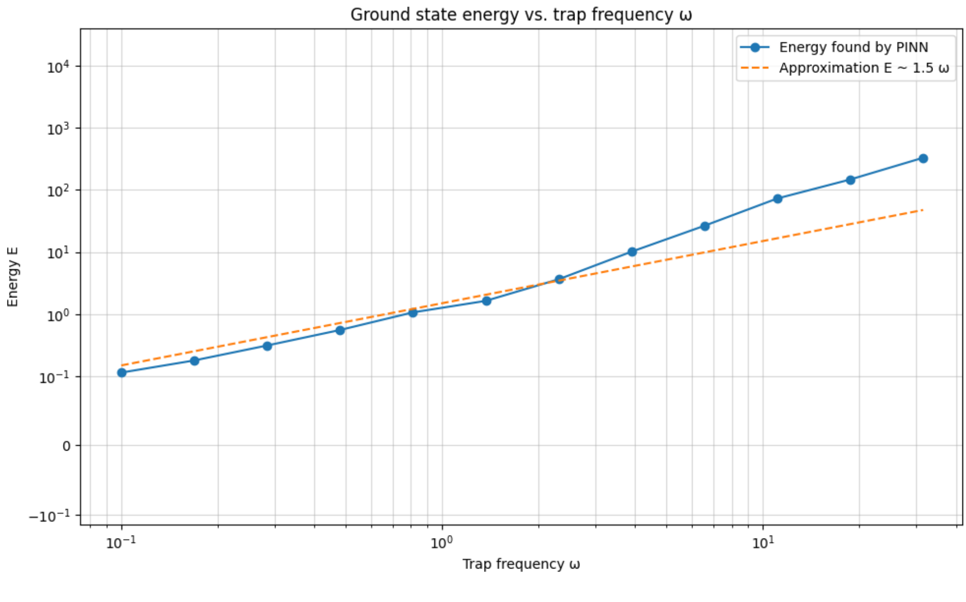

Fig. 3. Comparison of the PINN-generated ground state wavefunction for a pure VdW-type potential (solid blue line) with a simple analytic approximation (dashed orange line), showing qualitative agreement.

4. Conclusion

This work successfully demonstrates that a variational Physics-Informed Neural

Network is a highly effective method for finding the ground state of a quantum particle in a complex, non-analytical potential. By minimizing the Hamiltonian's expectation value, the PINN was able to accurately determine the ground state energy of a particle in a combined Van der Waals and harmonic trap potential.
The key conclusions are:

1. The variational PINN approach correctly reproduces the expected physical behavior across different physical regimes, accurately interpolating between the weak- and strong-trapping limits.
2. The method provides detailed physical insights, such as the zero-point energy and the spatial localization of the particle, consistent with quantum mechanical principles.
3. The success of this grid-free, variational method on the challenging Van der Waals potential underscores its potential for application to a broad range of problems in atomic, molecular, and condensed matter physics where analytical solutions are unavailable and traditional numerical methods face difficulties.

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