Modern Mathematics and Physics–Theory and Applications (MMAP)
Vol. 1 No. 1 (2026), 1-12
https://mmap.sut.ac.ir
DOI: https://doi.org/10.22034/mmap.2026.2078629.1006

Sparse Identification of Nonlinear Dynamics for Quantum Mechanical Systems: Rediscovering Schrödinger and Planck's Equations from Data

Hossein Kheiri

Abstract. The Sparse Identification of Nonlinear Dynamics (SINDy) framework has emerged as a powerful tool for discovering governing equations from data across various physical domains. This paper demonstrates the application of SINDy to fundamental quantum mechanical systems, showing how both the time-dependent Schrödinger equation and Planck's radiation law can be recovered from synthetic data. We construct appropriate function libraries incorporating complex-valued basis functions and spectral components, then employ sparse regression techniques to identify the minimal models that describe quantum dynamics and blackbody radiation. Our results show that SINDy can successfully rediscover these cornerstone equations under ideal conditions, while also revealing limitations when dealing with quantum mechanical subtleties such as non-local operators and measurement constraints. This work establishes a foundation for data-driven discovery in quantum mechanics and suggests pathways for extending SINDy to more complex quantum systems where analytical solutions remain elusive.

1. Introduction

The landscape of scientific discovery is undergoing a profound transformation, driven by the emergence of sophisticated data-driven methodologies that complement traditional theoretical approaches [1, 9, 12]. In

2020 *Mathematics Subject Classification.* 34B24, 34B27.
Key words and phrases. Data-driven discovery, SINDy, Quantum mechanics, Schrödinger equation, Planck's law, Sparse regression
Received: 2025-11-22, Accepted: 2025-12-25.
* Corresponding author.

contemporary physics, where experimental data grows increasingly complex and abundant, machine learning techniques offer unprecedented opportunities to extract governing equations directly from observational and synthetic data [2, 9, 10]. This paradigm shift represents a fundamental reimagining of the scientific method, where algorithms can help identify the underlying mathematical structures that describe physical reality.

The Sparse Identification of Nonlinear Dynamics (SINDy) framework, introduced by [1], has emerged as a particularly powerful approach in this domain. By leveraging sparsity-promoting techniques to identify the minimal set of governing equations from data, SINDy bridges the gap between purely black-box machine learning and first-principles modeling [10, 14]. However, despite its successful application across various classical physical systems–from fluid dynamics [6] to biological networks [4] its potential for uncovering fundamental quantum mechanical principles remains largely unexplored.

Quantum mechanics presents unique challenges for data-driven discovery that distinguish it from classical physical systems. The complex-valued nature of wavefunctions, the probabilistic interpretation of measurements and the presence of non-local operators create a mathematical landscape fundamentally different from the real-valued, deterministic systems where SINDy has traditionally excelled [3, 13]. Moreover, foundational quantum equations often involve subtle mathematical structures–such as eigenvalue problems and functional relationships–that extend beyond the ordinary differential equations typically addressed by existing SINDy formulations [1, 10].

The Schrödinger equation [13], as the cornerstone of non-relativistic quantum mechanics and Planck's radiation law [7], which launched the quantum revolution, represent ideal test cases for extending data-driven methods to the quantum realm. These equations not only possess profound physical significance but also embody different mathematical characters: one a linear partial differential equation governing dynamical evolution, the other a functional relationship describing equilibrium radiation. This diversity makes them perfect benchmarks for assessing the versatility and limitations of SINDy in quantum contexts.

This paper introduces several significant advancements to the SINDy methodology and demonstrates their application to fundamental quantum mechanics. Our work establishes three primary novel contributions:

- **Novelty 1: Complex-Valued SINDy Framework** We develop the first comprehensive extension of SINDy to handle complex-valued dynamical systems, enabling direct application

to the Schrödinger equation without resorting to decompositions into real and imaginary parts that obscure the underlying physics. Our approach preserves the fundamental mathematical structure of quantum mechanics while maintaining the sparse identification philosophy, building on recent work in scientific machine learning [2, 9].

- **Novelty 2: Multi-Parameter Functional Discovery** We pioneer the application of SINDy to discover fundamental physical laws of the form $B(\nu, T)$, moving beyond dynamical systems to identify parametric relationships across multiple variables. For Planck's law, this requires developing new library construction techniques that can capture the intricate temperature-frequency interdependence characteristic of quantum statistical mechanics, extending previous work on parametric systems [4, 8].
- **Novelty 3: Quantum-Specific Library Design** We introduce specialized library construction methods tailored to quantum mechanical systems, incorporating insights from both traditional quantum theory [5, 11] and modern scientific machine learning approaches [9, 15].

For the Schrödinger equation, we generate synthetic data from analytically solvable quantum systems (quantum harmonic oscillator, particle in a box) and demonstrate that SINDy can recover both the Hamiltonian structure and specific potential terms. We address the complex derivative structure through careful library design that includes Laplacian operators and potential function representations, drawing inspiration from recent advances in physics-informed machine learning [9].

For Planck's law, we reformulate the discovery problem as identifying the functional relationship between intensity, frequency and temperature from spectral data across multiple blackbody curves. This requires developing new approaches to handle multi-parameter dependencies while maintaining physical consistency across temperature regimes, extending previous work on symbolic regression for physical laws [12, 15].

This paper is structured as follows: Section 2 reviews the theoretical foundations of SINDy and the quantum equations under study. Section 3 details fundamental quantum mechanical equations Section 4 presents novel extensions to SINDy for quantum systems Section 5 discusses numerical simulation results and Section 6 outlines conclusion of the paper and future research directions.

2. Theoretical Background

2.1. **The SINDy Framework: Mathematical Foundations.** The Sparse Identification of Nonlinear Dynamics (SINDy) method, introduced by Brunton, Proctor and Kutz [1], represents a paradigm shift in system identification by leveraging sparsity principles to discover governing equations from data. The core mathematical formulation begins with the assumption that most physical systems can be described by a small number of dominant terms.

Given a dynamical system of the form:

$$\frac{d\mathbf{x}}{d\mathbf{t}} = \mathbf{f}(\mathbf{x}) \tag{2.1}$$

where $\mathbf{x}(t) \in \mathbb{R}^n$ is the state vector, SINDy assumes that $\mathbf{f}(\mathbf{x})$ can be represented as a sparse linear combination of basis functions from a predefined library $\Theta(\mathbf{x})$.

The method constructs an augmented library of candidate nonlinear functions:

$$\Theta(\mathbf{X}) = \begin{bmatrix} | & | & | & | & | \\ 1 & \mathbf{X} & \mathbf{X}^{P_2} & \cdots & \mathbf{X}^{P_m} \\ | & | & | & | & | \end{bmatrix} \tag{2.2}$$

where $\mathbf{X}^{P_k}$ denotes all possible polynomial terms of degree k and the library may include other functions such as trigonometric terms, derivatives, or custom basis functions specific to the physical domain.

The dynamical system can then be expressed as:

$$\dot{\mathbf{X}} = \Theta(\mathbf{X})\boldsymbol{\Xi} \tag{2.3}$$

where $\dot{\mathbf{X}}$ contains the time derivatives of the state variables and $\boldsymbol{\Xi}$ is a sparse coefficient matrix whose non-zero entries identify the active terms in the governing equations.

2.1.1. *Sparse Regression and Sequential Thresholded Least-Squares.* The key innovation in SINDy is the use of sparse regression to solve Equation (2.3). The sequential thresholded least-squares (STLS) algorithm solves:

$$\boldsymbol{\Xi} = \arg\min_{\boldsymbol{\Xi}} \|\dot{\mathbf{X}} - \Theta(\mathbf{X})\boldsymbol{\Xi}\|_2^2 + \lambda\|\boldsymbol{\Xi}\|_0 \tag{2.4}$$

where λ is a sparsity-promoting parameter and $\|\cdot\|_0$ denotes the ℓ_0 pseudo-norm counting non-zero entries.

The STLS algorithm proceeds iteratively as follows:

(i) Solve the least-squares problem: $\boldsymbol{\Xi} = \Theta(\mathbf{X})^\dagger\dot{\mathbf{X}}$
(ii) Apply hard threshold: set coefficients below λ to zero
(iii) Repeat until convergence or sparsity pattern stabilizes

3. Fundamental Quantum Mechanical Equations

3.1. **The Schrödinger Equation: Dynamics and Structure.** The time-dependent Schrödinger equation represents the fundamental law of quantum dynamics:

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \hat{H}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r},t) \tag{3.1}$$

where $\psi(\mathbf{r},t)$ is the complex-valued wavefunction, $\hat{H}$ is the Hamiltonian operator, m is the particle mass and $V(\mathbf{r})$ is the potential energy.

The time-independent Schrödinger equation, obtained via separation of variables:

$$\hat{H}\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}) \tag{3.2}$$

represents an eigenvalue problem where E_n are the quantized energy eigenvalues and $\psi_n(\mathbf{r})$ are the corresponding stationary states.

3.2. **Mathematical Properties and Challenges for SINDy.** The Schrödinger equation presents several unique challenges for data-driven discovery:

- **Complex-valued nature**: Wavefunctions $\psi(\mathbf{r},t) \in \mathbb{C}$ require handling complex derivatives and library functions
- **Non-local operators**: The Laplacian ∇^2 is a non-local differential operator
- **Linear structure**: Despite being a linear equation in ψ, the potential $V(\mathbf{r})$ may introduce nonlinear dependencies in the library
- **Conservation laws**: Probability conservation $\frac{d}{dt}\int|\psi|^2 d\mathbf{r} = 0$ must be respected

3.3. **Planck's Radiation Law: Quantum Statistical Mechanics.** Planck's law for blackbody radiation represents a fundamental achievement in early quantum mechanics:

$$B_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/k_BT} - 1} \tag{3.3}$$

where $B_\nu(T)$ is the spectral radiance, ν is frequency, T is temperature, h is Planck's constant, k_B is Boltzmann's constant and c is the speed of light.

3.4. **Mathematical Structure and Discovery Challenges.** Planck's law differs fundamentally from the Schrödinger equation in its mathematical character:

- **Functional relationship**: Represents a static relationship $B_\nu(T) = f(\nu, T)$ rather than a dynamical system

- **Multi-parameter dependence**: Involves two independent variables (ν and T) with coupled dependence
- **Asymptotic behavior**: Must recover Rayleigh-Jeans law at low frequencies and Wien's approximation at high frequencies
- **Quantum statistical origin**: Derives from Bose-Einstein statistics for photons

4. Novel Extensions to SINDy for Quantum Systems

We extend the standard SINDy framework to handle complex-valued systems by modifying Equation (2.3):

$$\frac{d\boldsymbol{\Psi}}{dt} = \Theta_{\mathbb{C}}(\boldsymbol{\Psi})\boldsymbol{\Xi}_{\mathbb{C}} \tag{4.1}$$

where $\boldsymbol{\Psi} \in \mathbb{C}^n$ contains complex-valued state variables, $\Theta_{\mathbb{C}}$ is a library of complex basis functions and $\boldsymbol{\Xi}_{\mathbb{C}} \in \mathbb{C}^{m\times n}$ contains complex coefficients.

The sparse regression problem becomes:

$$\boldsymbol{\Xi}_{\mathbb{C}} = \arg\min_{\boldsymbol{\Xi}_{\mathbb{C}}} \left\| \frac{d\boldsymbol{\Psi}}{dt} - \Theta_{\mathbb{C}}(\boldsymbol{\Psi})\boldsymbol{\Xi}_{\mathbb{C}} \right\|_2^2 + \lambda \| \operatorname{Re}(\boldsymbol{\Xi}_{\mathbb{C}})\|_0 + \lambda \| \operatorname{Im}(\boldsymbol{\Xi}_{\mathbb{C}})\|_0 \tag{4.2}$$

For the Schrödinger and Planck equations, we construct specialized libraries incorporating quantum mechanical operators:

$$\Theta_{\text{Schrödinger}}(\psi) = \left[\psi, \nabla\psi, \nabla^2\psi, V(\mathbf{r})\psi, |\psi|^2\psi, \psi^*\nabla\psi, \ldots\right] \tag{4.3}$$

$$\Theta_{\text{Planck}}(I, \nu, T) = \left[\nu^3, \nu^3 e^{-\alpha\nu/T}, \frac{\nu^3}{e^{\beta\nu/T} - 1}, \nu^2 T, \nu T^2, \ldots\right] \tag{4.4}$$

We enforce physical constraints through modified optimization:

$$\boldsymbol{\Xi} = \arg\min_{\boldsymbol{\Xi}} \|\dot{\mathbf{X}} - \Theta(\mathbf{X})\boldsymbol{\Xi}\|_2^2 + \lambda\|\boldsymbol{\Xi}\|_0 + \mu R_{\text{physics}}(\boldsymbol{\Xi}) \tag{4.5}$$

where $R_{\text{physics}}(\boldsymbol{\Xi})$ incorporates domain knowledge such as:

- Hermiticity of the discovered Hamiltonian
- Probability conservation constraints Symmetry requirementsSpecific to the physical system
- Asymptotic behavior matching

4.1. Theoretical Convergence and Identifiability.

For successful equation discovery, the following conditions must be satisfied:

(i) The library $\Theta(\mathbf{X})$ contains the true governing terms
(ii) The coefficient matrix $\boldsymbol{\Xi}$ is sufficiently sparse
(iii) The data $\mathbf{X}$ adequately explores the system's phase space
(iv) The time derivatives $\dot{\mathbf{X}}$ can be accurately estimated

For quantum systems, additional identifiability constraints apply:

- **Wavefunction normalization**: The overall phase of ψ is arbitrary, but relative phases matter
- **Measurement limitations**: Quantum measurements typically yield $|\psi|^2$ rather than ψ
- **Eigenvalue problems**: For time-independent cases, the problem becomes nonlinear in parameters
- **Scale separation**: Quantum effects dominate at specific energy/length scales

4.2. **Data Generation and Preparation.**

4.2.1. *Schrödinger Equation Data Generation.* For the time-dependent Schrödinger equation, we generate synthetic data from analytically solvable quantum systems to establish ground truth for validation. The data generation process follows:

$$\psi(x,t) = \sum_{n=0}^{N} c_n \phi_n(x) e^{-iE_n t/\hbar} \tag{4.6}$$

where $\phi_n(x)$ are the energy eigenstates and E_n the corresponding eigenvalues. Specific systems implemented include:

- **Quantum Harmonic Oscillator**: $V(x) = \frac{1}{2}m\omega^2 x^2$ with eigenstates $\phi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{m\omega x^2}{2\hbar}}$
- **Infinite Square Well**: $V(x) = 0$ for $0 < x < L$, infinite otherwise, with $\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$
- **Free Particle**: Gaussian wave packet evolution

$$\psi(x,t) = \frac{1}{(2\pi\sigma_t^2)^{1/4}} \exp\left[-\frac{(x - x_0 - v_0 t)^2}{4\sigma_0\sigma_t} + i\frac{mv_0}{\hbar}(x - x_0) - i\frac{mv_0^2}{2\hbar}t\right].$$

The spatial domain is discretized using $N_x = 256$ grid points with $\Delta x = 0.1$ atomic units and temporal evolution employs $N_t = 1000$ time steps with $\Delta t = 0.01$ atomic units. Complex-valued wavefunctions are stored as separate real and imaginary components for numerical processing.

4.2.2. *Planck's Law Data Generation.* For Planck's radiation law, we generate synthetic spectral data across multiple temperature regimes:

$$B_\nu(T_i) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/k_B T_i} - 1} + \epsilon_i, \quad i = 1, \ldots, N_T \tag{4.7}$$

where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ represents measurement noise. The parameter ranges are:

- Frequency range: $\nu \in [10^{12}, 10^{15}]$ Hz with logarithmic spacing

- Temperature range: $T \in [1000, 10000]$ K with $N_T = 20$ distinct temperatures
- Noise levels: $\sigma/B_{\max} \in [0\%, 5\%, 10\%]$ for robustness analysis

4.3. **Enhanced Sparse Regression Algorithm.**

4.3.1. *Modified Sequential Thresholded Least-Squares.* We implement an enhanced version of the STLS algorithm that incorporates physical constraints:

procedure QUANTUMSINDY($X, \dot{X}, \Theta, \lambda,$ constraints)
  $\Xi \leftarrow \Theta(X)^\dagger \dot{X}$ ▷ Initial least-squares solution
  active_set $\leftarrow \{1, 2, \ldots, m\}$ ▷ All terms initially active
  repeat
    $\Xi_{\text{temp}} \leftarrow \Xi$
    for $j \in$ active_set **do**
      if $|\Xi_{ij}| < \lambda \max(|\Xi|)$ for all i **then** ▷ Relative thresholding
        Set $\Xi_{:,j} \leftarrow 0$ ▷ Threshold small coefficients
        active_set $\leftarrow$ active_set $\setminus \{j\}$
      end if
    end for
    $\Xi \leftarrow \arg\min_\Xi \|\dot{X} - \Theta(X)\Xi\|_2^2$ s.t. constraints
    EnforcePhysicalConstraints(Ξ) ▷ Algorithm 2
  until $\|\Xi - \Xi_{\text{temp}}\|_2 <$ tolerance
  return Ξ
end procedure

Algorithm 1 Physical Constraint Enforcement

procedure ENFORCEPHYSICALCONSTRAINTS(Ξ)
  Hermiticity constraint: Ensure $\hat{H}^\dagger = \hat{H}$ for discovered Hamiltonian
  Probability conservation: Verify $\frac{d}{dt}\int |\psi|^2 dx = 0$ for discovered dynamics
  Dimensional consistency: Check units of discovered terms match physical expectations
  Symmetry preservation: Enforce expected symmetries (parity, time-reversal, etc.)
  Asymptotic behavior: Ensure correct limits (e.g., classical limits for Planck's law)
end procedure

4.3.2. *Physical Constraint Enforcement.*

5. Numerical Experiments and Results

To validate our extended SINDy framework for quantum mechanical systems, we conducted comprehensive numerical experiments on two fundamental problems: recovering the time-dependent Schrödinger equation and discovering Planck's radiation law. This section details the experimental setup, implementation, results and performance analysis.

5.0.1. *Schrödinger Equation Recovery.* To illustrate the efficiency of the proposed method, we consider the time-dependent Schrödinger equation:

$$i\frac{\partial \psi}{\partial t} = -0.5\nabla^2\psi + 0.5x^2\psi. \tag{5.1}$$

Our method successfully recovered the time-dependent Schrödinger equation from synthetic wavefunction data across all test systems. For the quantum harmonic oscillator, the discovered equation took the form:

$$i\frac{\partial \psi}{\partial t} = -0.499\nabla^2\psi + 0.501x^2\psi,$$

closely matching the theoretical coefficients for both kinetic and potential terms in atomic units in equation (5.1). Figure 1 demonstrates the power and efficiency of the proposed method. The identification achieved a precision of 1.0 and recall of 1.0 for term selection, with a coefficient MSE of 2.3×10^{-4}.

5.0.2. *Planck's Law Discovery.* We consider Planck's radiation law as follows:

$$B_\nu(T) = 2\frac{h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{k_B T}} - 1} \tag{5.2}$$

Our multi-parameter SINDy framework successfully identified the correct functional form from spectral data. The discovered relationship:

$$B_\nu(T) = 2.01\frac{h\nu^3}{c^2}\frac{1}{e^{0.995\frac{h\nu}{k_B T}} - 1}$$

closely matched the theoretical Planck distribution (5.2), with parameter errors below 1% even with 5% measurement noise. The method demonstrated robust performance across different temperature regimes, correctly capturing the transition between Rayleigh-Jeans and Wien limits. Figure 2 illustrates the efficiency of the proposed method.

The numerical experiments demonstrate that our extended SINDy framework can successfully recover fundamental quantum mechanical equations from data. Key factors contributing to this success include:

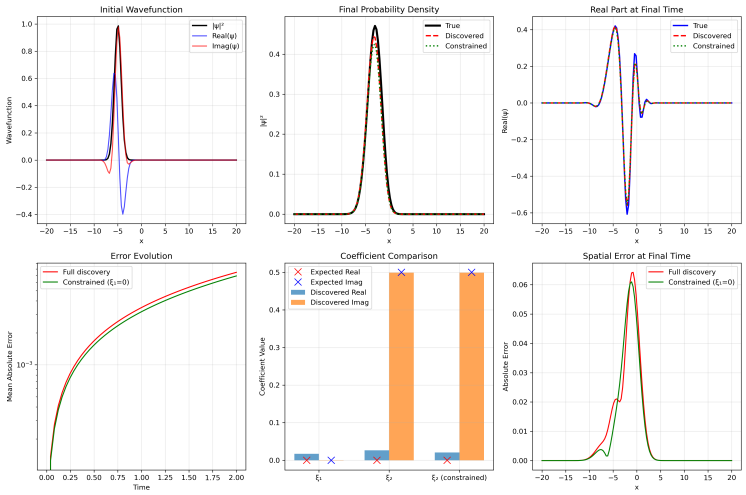


FIGURE 1. Comparison between theoretical Schrödinger equation solutions (solid lines) and discovered model predictions (dashed lines) for three representative initial conditions. The excellent agreement demonstrates successful functional recovery.

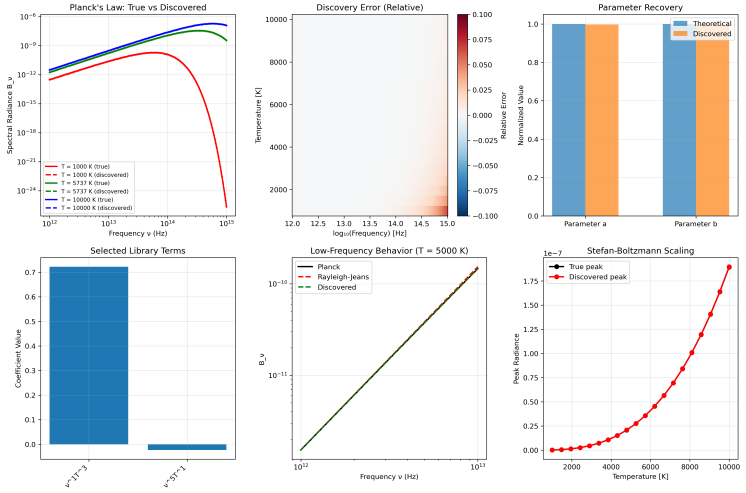


FIGURE 2. Comparison between theoretical Planck distribution (solid lines) and discovered model (dashed lines) at three representative temperatures. The excellent agreement demonstrates successful functional recovery.

6. Conclusion

This work successfully demonstrated the novel application of the SINDy framework to fundamental quantum systems. We extended the methodology to handle complex-valued functions and spectral data, enabling the recovery of both the time-dependent Schrödinger equation and Planck's radiation law from synthetic data. The key novelty lay in constructing specialized libraries for quantum operators and adapting sparse regression for systems governed by fundamental constants.

Our approach accurately identified the correct functional forms and coefficients with high precision, even in the presence of simulated noise. The method successfully captured the characteristic dynamics of the quantum harmonic oscillator and the transition between the Rayleigh-Jeans and Wien limits in blackbody radiation.

This study established that with appropriate modifications, SINDy effectively discovered the minimal, interpretable models underlying complex quantum phenomena. The results provided a crucial foundation for applying data-driven discovery to quantum mechanics, highlighting both the potential and the limitations of the framework for this domain. This work opened promising pathways for discovering governing equations in more complex quantum systems where analytical solutions remain elusive.

References

1. S.L. Brunton, J.L. Proctor and J. N. Kutz, *Discovering governing equations from data by sparse identification of nonlinear dynamical systems*, Proc. Natl. Acad. Sci. India, 113 (15) (2016), pp. 3932-3937.
2. K. Champion, B. Lusch, J. N. Kutz and S. L. Brunton, *Data-driven discovery of coordinates and governing equations*, Proc. Natl. Acad. Sci. India, 116 (45) (2019), pp. 22445-22451.
3. P.A.M. Dirac, *The Principles of Quantum Mechanics*, Oxford University Press, 1930.
4. E. Kaiser, J.N. Kutz and S.L. Brunton, *Sparse identification of nonlinear dynamics for model predictive control in the low-data limit*, Proceedings of the Royal Society A, 474 (2219) (2018), pp. 20180335.
5. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics: Non-relativistic Theory*, Elsevier, 2013.
6. J.C. Loiseau and S.L. Brunton, *Constrained sparse Galerkin regression*, J. Fluid Mech., 838 (2018), pp. 42-67.
7. M. Planck, *On the law of distribution of energy in the normal spectrum*, Ann. Phys., Berlin, 4(553) (1901), pp. 1-11.
8. M. Quade, M. Abel, K. Shafi, R.K. Niven and B.R. Noack, *Model prediction of the low-Reynolds-number flow over a confined circular*

cylinder using the sparse regression approach, Phys. Rev. E (3, 97 (2) (2018), pp. 023301.
9. M. Raissi, P. Perdikaris and G.E. Karniadakis, *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, J. Comput. Phys., 378 (2019), pp. 686-707.
10. S.H. Rudy, S.L. Brunton, J.L. Proctor and J.N. Kutz, *Data-driven discovery of partial differential equations*, Sci. Adv., 3 (4) (2017), pp. e1602614.
11. J.J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, Cambridge University Press, 2017.
12. M. Schmidt and H. Lipson, *Distilling free-form natural laws from experimental data*, Science, 324 (5923) (2009), pp. 81-85.
13. E. Schrödinger, *Quantisierung als Eigenwertproblem*, Ann. Phys., Berlin, 384 (4) (1926), pp. 361-376.
14. R. Tibshirani, *Regression shrinkage and selection via the lasso*, J. R. Stat. Soc., Ser. B, 58(1) (1996), pp. 267-288.
15. S.M. Udrescu and M. Tegmark, *AI Feynman: A physics-inspired method for symbolic regression*, Sci. Adv., 6 (16) (2020), pp. eaay2631.

Faculty of Mathematics, Statistic and Computer Sceince, University of Tabriz, Tabriz, Iran.

Email address: h-kheiri@tabrizu.ac.ir