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A deep learning approach to solve the Schrodinger equation

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الإهداء

بسم الله الرحمان الرحيم

اهدي ثمرة جهدي تخرجي الى

رمز الفداء الى العظيمة فلسطين والى من زكوا بدمائهم من ارض هذا الوطن الحبيب الى شهدائها و اسراها الى من كلل العرق جبينه و من علمني ان النجاح لا ياتي الا بالصبر و الاصرار الى النور الذي انار دربي و السراج الذي لا ينطفي نوره بقلبي ابدا من بذل الغالي و النفيس و استمديت منه قوتي و اعتزازي بداتي

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الى من جعل الجنة تحت اقدامها و سهلت لي الشدائد بدعائها الى الانسانة العظيمة التي لطالما تمنت ان تقر عينها لرؤيتي في يوم كهذا

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الى جدي و جدتي الغاليان اطال الله بعمرهما

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الى اخي الغالي و اخواتي الغاليات

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كوثر و وصال

الى شريكتي في هذا المشروع

بن سالم فاطمة الزهراء

اليكم عائلتي اهديكم هذا الانجاز و ثمرة نجاحي التي لطالما تمنيته ها انا اليوم اكملت و اتممت اول ثماراته بفضله سبحانه و تعالى الحمد لله على ما وهبني و ان يجعلني مباركا و ان يعينني اينما كنت فمن قال انا لها نالها فانا لها و ان ابت رغما عنها اتيت بها الحمد لله شكرا و حبا و امتنانا على البدء و الختام

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العيورات خيرة

DEDICATION

To those I miss in the struggle against difficulties, and whom the world did not allow me to quench my thirst for his kindness, my father, may God have mercy on him and grant him a spacious paradise.

To the one who carried me, weak and weary, and suffered and endured for my sake, to the one whose prayers were the secret of my success, my beloved mother, may God prolong her life.

To the light of my eyes and my refuge in life, my brothers **Ilyes**, **Ramadan**, and **Sallah Edine**.

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To all my family, relatives, and neighbors.

To all my friends whom I cherish their friendship and my colleagues in school, each by name.

To all of them

I dedicate the fruit of my effort and the result of my success, in the belief in the spirit of work and perseverance.

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Abstract

To understand the properties of matter and predict them, it's crucial to solve the Schrodinger equation, where the solution is a wave vector. Many theoretical methods have been explored in this area.The most common ones are those that reduce the cost and time of calculations, especially for complex particle systems. The rapid advancement in computer science and the emergence of new technologies like machine learning have paved a new path towards solving equations like this.
In this work, we propose calculating the fundamental energy of a physical system using the Schrodinger equation with the use of deep learning and proving its efficiency in solving by making a comparison with traditional machine learning techniques.
To apply the theoretical study, we conducted an experimental study on solving the Schrodinger equation using CNN, CNN-LSTM, SVR, RF, and XGBoost structures with relevant datasets for calculating the system's fundamental energy.
The results showed that deep learning can be effective in solving the Schrodinger equation, achieving an error of 0.0063(ev/atom) and an accuracy of 0.9807 . These findings open up new possibilities for enhancing and developing models.

Key words: Schrodinger equation, wave vector, machine learning, fundamental energy, Deep learning.

Résumé

Pour comprendre comment les matériaux fonctionnent et les prédire avec précision,il est essentiel de résoudre l'équation de Schrödinger, dont la solution est un vecteur d'ondes. Différentes approches théoriques ont été explorées dans ce domaine. Les plus courantes sont celles qui réduisent les coûts et le temps de calcul, notamment lorsqu'il s'agit de systèmes de particules complexes. L'évolution rapide de l'informatique et l'émergence de nouvelles technologies telles que l'apprentissage automatique ouvrent de nouvelles perspectives pour résoudre ce type d'équation.

Dans ce travail, nous proposons de calculer l'énergie fondamentale d'un système physique en utilisant l'équation de Schrödinger avec l'utilisation de l'apprentissage profond et de prouver son efficacité dans la résolution en faisant une comparaison avec les techniques traditionnelles d'apprentissage automatique.

Pour appliquer l'étude théorique, nous avons mené une étude expérimentale sur la résolution de l'équation de Schrödinger en utilisant les structures CNN, CNN-LSTM, SVR, RF et XGBoost avec des ensembles de données pertinents pour calculer l'énergie fondamentale du système.

Les résultats ont montré que l'apprentissage profond peut être efficace dans la résolution de l'équation de Schrödinger, avec un erreur de 0.0063(ev/atome) et une précision de 0.9807,ouvrant ainsi de nouvelles perspectives pour l'amélioration et le développement des modèles.

Mots clés: Équation de Schrodinger, vecteur d'onde, apprentissage automatique, énergie fondamentale, apprentissage profond

ملخص

لفهم خصائص المادة والتنبؤ بها ، من الضروري للغاية حل معادلة شرودنجر ، التي يكون حلها متجه الموجة. تم التماس العديد من المناهج النظرية في هذا الموضوع.
الأكثر شيوعا هي تلك التي تقلل من تكلفة ووقت الحساب خاصة عندما يتعلق الأمر بنظام الجسيمات المعقد.
لقد فتح التطور السريع لعلوم الكمبيوتر وظهور تقنيات جديدة مثل التعلم الآلي طريقا جديدا نحو حل مثل هذه المعادلة.
في هذا العمل ، نقترح حساب الطاقة الأساسية لنظام فيزيائي باستخدام معادلة شرودنجر باستخدام التعلم العميق وإثبات كفاءته في الحل من خلال إجراء مقارنة بينه و بين تقنيات التعلم الآلي التقليدية .
لتطبيق الدراسة النظرية، قمنا بإجراء دراسة تجريبية على حل معادلة شرودينجر باستخدام بنية CNN , CNN-LSTM , SVR, RF و XGBoost مع مجموعة بيانات ذات صلة لحساب الطاقة الأساسية للنظام .
أظهرت النتائج أن التعلم العميق يمكن أن يكون فعالاً في حل معادلة شرودينجر، حيث حققنا خطأ 0.0063(ev/atom) ودقة تصل إلى 0.9807 ، هذه النتائج تفتح آفاقًا جديدة لتحسين وتطوير النماذج.

الكلمات المفتاحية:
معادلة شرودنجر ، متجه الموجة ، التعلم الآلي ، الطاقة الأساسية ، التعلم العميق

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List of acronyms

ML Machine Learning

DL Deep Learning

SE Schrödinger Equation

DFT Density Functional Theory

CNN Convolutional Neural Network

LSTM Long Short-Term Memory

R2Score R-Squared Score

CSV Comma-Separated Values

LDA Local Density Approximation

GGA Generalized Gradient Approximation

HF Hartree-Fock

NNQS Neural Network Quantum State

RBM Restricted Boltzmann Machine

VMC Variational Monte Carlo

SE-NET Schrödinger Equation Neural Network

ODE-NET Ordinary Differential Equation Neural Network

TDDFT Time-Dependent Density Functional Theory

KS Kohn-Sham

XC Exchange-Correlation

MSE Mean Squared Error

SVR Support Vector Regression

RF Random Forest

XGBoost eXtreme Gradient Boosting

General Introduction

General Introduction

The emergence of quantum mechanics was a reaction to the difficulties faced by classical physics when it came to interpreting the behavior of objects at the atomic and molecular level, where quantum mechanics showed that small particles follow completely different laws and behavioral patterns from those we know from the classical world and in doing so brought about a revolutionary shift in our understanding of the world in which we live[9].

The Schrödinger equation in quantum mechanics plays the same role as Newton's equation in classical mechanics, and its solution is through access to the wave function, which is a mathematical representation describing the quantum state of the system, because it gives information about the probability of finding a particle in a certain region of space,in addition to other information such as energy, kinetic quantum, and others. In this sense, the wave function represents an essential tool for describing and understanding physical phenomena at the quantum level[10].

Since the publication of Schrödinger's works, physicists have sought many ways to solve this equation, both analytical and numerical. The rapid development of Computer Science and the emergence of new technologies such as machine learning have seen a coup in how to solve these equations[11].In this work, we propose to use and prove the efficiency deep learning in solving the problem of calculating the fundamental energy of a physical system using the Schrodinger equation, by making a comparison between it and machine learning algorithms.

This thesis consists of three chapters:
In the first chapter, we will delve into the origin of the Schrodinger equation, starting with an introduction to the importance of this equation and then moving on to studying its nature, history, and evolution. We will also explain the methodological formulation of the Schrodinger equation and its physical interpretation. In addition, we will discuss the Density Functional Theory (DFT) as a numerical method for solving the Schrodinger equation and because the dataset we use in our study is calculated by DFT.

As for the second chapter, we are embarking on a journey towards advanced convergence of deep learning and quantum mechanics. We discuss how advanced neural network engineering can revolutionize the solution of the Schrödinger equation. First, we explore the limitations and challenges we face in moving from classical methods to deep learning, and then we delve

into the role of deep learning in quantum chemistry and computational quantum mechanics. In addition, we analyze the structures of advanced neural networks of quantum systems, mention the latest state of the art deep learning methods for solving the Schrödinger equation, and finally,we highlight the strengths and weaknesses in it.

In the third chapter,we will discuss the implementation and the results obtained by applying deep learning and machine learning models to solve the Schrodinger equation for the purpose of making a comparison between them. We will start with an introduction to the environment used in the experiments, including software libraries and the configuration of the computing environment. We will explain how to import and process data, preparing it for use in convolutional neural network models (CNN) and (CNN-LSTM). We will provide details on the design and training of the following models:CNN, CNN-LSTM, SVR, RF and XGBoost. Then, we will evaluate, analyze, and compare the results.We conclude with a summary of the main points.

Finally, the conclusion to sum up all that we have seen.

Chapter 1

Chapter 1

Background

1.1 Introduction

One of the latest challenges in classical physics is the inability to explain certain phenomena using classical theories, even with advanced mathematical methods. Such problems often arise in the study of objects that are too small or too large, and classical physics is not able to explain the quantum behavior of particles, such as electrons and atoms. Because they perceive these particles as solid bodies that have specific properties, such as size, location and speed. However, experiments have shown that electrons and atoms can behave unpredictably, such as passing through physical barriers or being in several places at the same time.

As a reaction to this, quantum mechanics appeared, since the latter was able to describe the behavior of particles at the atomic level. It also relied on the idea that particles have wave properties, in addition to their physical properties. The other thing that revolutionized our understanding of the microscopic world and had profound implications in many fields such as chemistry, materials science, quantum physics, etc. It is the emergence of the Schrodinger equation, which allowed scientists to make accurate predictions about the probability of finding particles in different states and also explain their behavior within the quantum system.

In this chapter, we're gonna dig into the origin of the Schrödinger equation and touch on the basic concepts, the mathematical formula, and the physical interpretations of it.Finally,We will discuss density functional theory (DFT) as a numerical approach to solv the Schrödinger equation.

1.2 Basics of the Schrodinger equation

Below we will mention some basic concepts of the Schrodinger equation starting from its history ,its definition , its mathematical formula right up to its physical interpretation and solutions .

1.2.1 History

The development of quantum mechanics marked a paradigm shift in our understanding of the universe at the atomic and subatomic levels, revealing a world governed by probabilistic laws and characterized by wave-particle duality. Below we will delve into the events that led to this transformation and the emergence of the Schrodinger equation.

Quantum mechanics was first proposed by Planck in 1900 and continued to evolve until Einstein introduced the photoelectric effect, demonstrating that Planck's idea could be represented as a de Broglie wave. This ultimately led to the Schrodinger equation,which describes the behavior of quantum bodies and explains the emission and absorption spectrum of hydrogen[12, 13].

- **Planck's quantum theory (1900)**

  In the early 20th century, physicists were grappling with the enigmatic behavior of blackbody radiation, objects that absorb all electromagnetic radiation that falls upon them. While classical physics predicted a continuous spectrum of emitted radiation, observations instead revealed a discrete pattern with specific peaks and valleys. Max Planck, a German physicist, sought to reconcile this discrepancy by introducing the concept of quanta, discrete packets of energy[14].
  Planck's revolutionary hypothesis proposed that energy is not infinitely divisible but rather exists in smallest units, much like atoms or particles. He calculated that the energy of each quantum was directly proportional to the frequency of the emitted radiation. This radical departure from classical physics, where energy was considered continuous, marked a turning point in our understanding of the microscopic world.
  Initially met with skepticism, Planck's quantum theory gradually gained acceptance as it successfully explained various experimental observations. His groundbreaking work laid the foundation for quantum mechanics, paving the way for further discoveries in the field[14].

- **Einstein's photoelectric effect (1905)**

  Building upon Planck's quantum theory, Albert Einstein, a Swiss-German physicist, made a significant contribution to our understanding of light with his explanation of the photoelectric effect. In this phenomenon, when light strikes a metal surface, electrons are ejected, a process known as photoemission.
  Einstein proposed that light is not just a wave but also exhibits particle-like properties,

existing as a stream of particles called photons. Each photon carries a specific amount of energy, or quantum, and when interacting with matter, can transfer that energy to electrons. If the energy of the photon is greater than the minimum energy required to remove an electron from the metal, the electron is ejected from the surface.
Einstein's explanation of the photoelectric effect provided compelling evidence for the quantization of energy and further solidified the quantum revolution. His work highlighted the dual nature of light, challenging the prevailing understanding of light as a purely wave-like phenomenon[15].

- **De Broglie's wave-particle duality (1924)**

Louis de Broglie, a French physicist, took the quantum revolution a step further by proposing the concept of wave-particle duality. He suggested that all particles, including electrons, protons, and neutrons, possess both wave-like and particle-like properties. This revolutionary idea blurred the distinction between these two fundamental concepts. De Broglie's hypothesis was based on the idea that energy and momentum are conserved. He argued that if momentum is conserved, then a particle with a given momentum must also have a wavelength. The wavelength of the particle is given by the following equation:

$$\lambda = h/p \tag{1.1}$$

where:
λ : is the wavelength of the particle
h: is Planck's constant particle
p: is the momentum of the particle

De Broglie's hypothesis was confirmed by experiments that showed that electrons can be diffracted, just like waves. This discovery demonstrated that particles and waves are not mutually exclusive but rather two different aspects of the same reality[16, 17, 15].

- **Schrödinger's equation (1925)**

Erwin Schrödinger, an Austrian physicist, made a significant contribution to quantum mechanics with his development of the wave equation in 1925. This mathematical formulation described the behavior of quantum particles as waves, providing a powerful tool for understanding their properties and interactions[18].

1.2.2 Definition of the schrodinger equation

The Schrödinger equation, a partial differential equation, elucidates the evolution of a quantum system's state over time[19]. Erwin Schrödinger formulated this equation in 1925, inspired by Louis de Broglie's wave hypothesis[15],and published it the following year. Named after its discoverer, it holds significant importance in quantum mechanics.

Analytical solutions of the Schrödinger equation are critical in the study of atoms and molecules. Erwin Schrödinger demonstrated the correctness of this equation by analyzing the hydrogen atom, successfully predicting many of its properties. However, exact solutions can be achieved only for single-electron systems, with hydrogen serving as a fundamental example[20].

1.2.3 Mthematical formula of the schrodinger equation

To obtain the mathematical formula of the Schrodinger equation, we will see how this equation is constructed in its two types (time-dependent and time-independent).

- **Construction of the Schrödinger equation**

The Austrian physicist Erwin Schrödinger used De Broglie's results to establish an equation governing the spatial and temporal evolution of the function of a physical system. To obtain the Schrödinger equation, taking the formula of the de Broglie plane wave :

$$\Psi(\overrightarrow{r},t) = A\exp^{i(\overrightarrow{k}\,\overrightarrow{r}-\omega t)} \tag{1.2}$$

where:
ω: The pulsation and k : the wave vector according to the postulates of quantum mechanics are related to the classical particle by the Planck-Einstein relation [12]:

$$E = \hbar\omega \tag{1.3}$$

and the relationship of L. De Broglie :

$$\overrightarrow{p} = \hbar\,\overrightarrow{k} \tag{1.4}$$

So:

$$\Psi(\overrightarrow{r},t) = A\exp^{i(\overrightarrow{p}\,\overrightarrow{r}-Et)/\hbar} \tag{1.5}$$

We derive the wave relative to time :

$$\frac{\partial\Psi(\overrightarrow{r},t)}{\partial t} = -\frac{i}{h}EA\exp^{i(\overrightarrow{p}\,\overrightarrow{r}-Et)\hbar} = -\frac{i}{h}E\Psi(\overrightarrow{r},t) \tag{1.6}$$

We obtain:

$$E\Psi(\overrightarrow{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\overrightarrow{r},t) \tag{1.7}$$

so:

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \tag{1.8}$$

$\hat{E}$: is the energy operator.
By deriving the wave with respect to space, it comes :

$$\overrightarrow{\nabla}\Psi(\overrightarrow{r},t) = \frac{i}{\hbar}pA\exp^{i(\overrightarrow{p}\,\overrightarrow{r}-Et)\hbar} = \frac{i}{\hbar}p\Psi(\overrightarrow{r},t) \tag{1.9}$$

where:

$$\overrightarrow{\nabla} = \overrightarrow{i}\frac{\partial}{\partial x} + \overrightarrow{j}\frac{\partial}{\partial y} + \overrightarrow{k}\frac{\partial}{\partial z} \tag{1.10}$$

$\overrightarrow{\nabla}$ is the gradient operator, then :

$$\hat{p} = -i\hbar\overrightarrow{\nabla} \tag{1.11}$$

is the impulse operator.
On classical mechanics, the mechanical energy of a free particle is given by :

$$E = E_c = T = \frac{p^2}{2m} \tag{1.12}$$

This quantity appears in the Hamiltonian formulation for a free particle ($V(\overrightarrow{r}) = 0$) of classical mechanics.
By applying the principle of correspondence between the classical values and quantum, for the energy, of the equation (1.7) and (1.12) we obtain :

$$\frac{p^2}{2m}\Psi(\overrightarrow{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\overrightarrow{r},t) \tag{1.13}$$

where:

$$\frac{p^2}{2m}\Psi(\overrightarrow{r},t) = \frac{1}{2m}(-i\hbar\overrightarrow{\nabla})^2\Psi(\overrightarrow{r},t) = -\frac{p^2}{2m}\overrightarrow{\nabla}^2\Psi(\overrightarrow{r},t) \tag{1.14}$$

$\overrightarrow{\nabla}^2 = \Delta$: is the Laplacian

$$-\frac{p^2}{2m}\Delta\Psi(\overrightarrow{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\overrightarrow{r},t) \tag{1.15}$$

The Hamiltonian operator of the system for a free particle is written :

$$\hat{H} = -\frac{p^2}{2m}\Delta \tag{1.16}$$

Using $\hat{H}$, we can simplify the writing of the Schrödinger equation[21, 19], We obtain:

$$\hat{H}\Psi(\overrightarrow{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\overrightarrow{r},t) \tag{1.17}$$

When the particle is immersed in a scalar potential ($V(\overrightarrow{r})$,for example the potential of a harmonic oscillator) according to classical mechanics, the system totale energy is written as follows:

$$E = T + V(\overrightarrow{r}) = \frac{p^2}{2m} + V(\overrightarrow{r}) \tag{1.18}$$

with this new energy value and from equation (1.8) and the operator of impulse $\hat{P}$: , the Schrödinger equation becomes :

$$\left[-\frac{p^2}{2m}\Delta + V(\overrightarrow{r})\right]\Psi(\overrightarrow{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\overrightarrow{r},t) \tag{1.19}$$

the total energy is only the Hamiltonian operator of the system [22]:

$$\hat{H} = -\frac{p^2}{2m}\Delta + V(\overrightarrow{r}) \tag{1.20}$$

where :
i: The numerical value of the imaginary unit i is $\sqrt{-1}$. As an operator, multiplication by i has the effect of causing a 90∘ rotation in the complex plane , moving numbers from the positive real axis to the positive imaginary axis, or from the positive imaginary axis to the negative real axis.
$\hbar$: The modified Planck constant $\hbar$ is the Planck constant h divided by 2.
m: The mass of the particle or system associated with the quantum wavefunction $\psi(x,t)$ is a measure of inertia, that is, resistance to acceleration. In the SI system, mass has units of kilograms[16].
V: is the potential energy of the particle.

The goal of theoretical physicists has been to solve the Schrödinger equation using various mathematical techniques, such as analytical or numerical approaches. The basic equation of quantum mechanics is known as the Schrödinger equation. The majority of quantum systems find it challenging to solve it. There are two types of Schrödinger equations: the time-dependent and time-independent ones [13]:

1.2.4 Physical interpretation of Schrödinger equations

The time-independent solution to the Schrödinger equation will be presented in this section. In classical mechanics, a system's state can be found by solving its equations of motion; however, in quantum mechanics, the state of the system can be determined by solving the Schrödinger equation and identifying its wave function.

- **The wave function**

  A complex function of all particle positions is the wave functionΨ. All system properties are accessible through this knowledge. Its square, $\|\Psi^2\|$ in particular, is related to the probability of finding particles at the locations considered. The operator $\hat{H}$ applied to the function, which could be more clearly represented by Ψ, must be understood as the $\hat{H}\Psi$ operation. The expression $E\Psi$, on the other hand, refers to a simple product of the Ψ function and the real number E. According to mathematics, the Schrödinger equation thus described is equivalent to an "eigenvalue equation" and has an infinite number of solutions known as quantum states. Every quantum state has a corresponding energy E and a wave function Ψ. The lowest energy state is called the ground state, and the other states with greater energies are the excited states.

In short, the wave function is a quantum postulate that describes the motion of quantum particles and contains all the information about the quantum states. It represents the solution to the Schrödinger equation of a quantum system.
The wave function $\Psi(\overrightarrow{r}, t)$ must satisfy the following requirements:

- It needs to go on forever for $\overrightarrow{r}$.

- The $\frac{\partial \Psi}{\partial t}$ derivative has to be continuous; the limit on solutions applies to these restrictions.
- We have to normalize it. This suggests that when $\overrightarrow{r}$ approaches infinity, the wave function approaches zero, meaning:

with : $|\Psi(\overrightarrow{r}, t)|^2$ is the probability density.
A solution associated with an energy E is called an energy eigenstate of energy E. The set of all allowed values of E is called the spectrum of the Hamiltonian[16, 13**?**].

1.3 Density Functional Theory DFT:Numerical approch to solve schrodinger equation

It has been effectively utilized to explain both finite and periodic systems, density functional theory (DFT) is a widely used and rigorously precise quantum many-body theory.A (practically precise) theory of electronic structure, density functional theory (DFT) is based on the electron density distribution n(r), not the many-electron wave function (r1,r2,r3,...).Mainly expressed in terms of the electronic density distribution n(r), density functional theory (DFT) is a theory of electronic ground state structure.All chemical quantities are stated in terms of the electron density n(r), which is the most fundamental parameter in DFT.The Schrodinger equation's parameters in terms of the single-electron wavefunction (Ψ) and the structural parameters derived from the electronic density ($\rho(r)$ concept) compare favorably, and the latter can be used[23, 24, 25].

1.3.1 The evaluation of Born-Oppenheimer

The nuclei will move much slower than the electrons because they are much heavier, thus the movements of the electrons and the nuclei are separable and consequently the kinetic energy of the latter can be neglected, the term of interaction nuclei-nuclei is constant and the term of interaction nuclei-electrons depends only on the positions of the electrons. The equation:

$$H = -\sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 - \sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|R_I - R_J|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i - r_j|} - \sum_{I,i}\frac{Z_I e^2}{|R_I - r_i|} \quad (1.21)$$

represent the Hamiltonian of an N-body system composed of nuclei and electrons , after this approximation becomes :

$$H = -\sum_i \frac{\hbar^2}{2m_i r_i^2} + \frac{1}{2}\sum_{i,j} \frac{Z_i Z_j e^2}{|R_i - R_j|} - \sum_{i,l} \frac{Z_l e^2}{|R_i - r_l|} + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{|r_i - r_j|} \tag{1.22}$$

Or again :

$$H = -\sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_i V_{\text{ext}}(r_i) + \sum_{i \neq j} V_{\text{e-e}}(r_i, r_j) \tag{1.23}$$

The third term in equation (1.34) represents the electron-electron interaction potential, grouping together the effect of the Colombian repulsion between the electrons, the Van der Waals effects (exchange effects) and the repulsion effects due to the Pauli principle (correlation effects).

Despite the simplification brought by the Born-Oppenheimer approximation, the third term in equation (1.23) remains quite complex to calculate analytically. In this thesis, we will present two simplifying methods. The first method, called Hartree-Fock, focuses on the system's wave function, while the second method is based on the value and shape of the electron density[26].

1.3.2 The evaluation of Hartree-Fock

The major difficulty in the application of variational principle to find the ground state of a system is the multidimensional nature of wave vector. The Hartree-Fock method consists in replacing the interaction of each electron with the other electrons by the interaction of an average field created by the nuclei and the rest of the electrons, as if this electron were moving independently in an average field . This representation makes it possible to divide the Hamiltonian into separable terms and equation (1.23) becomes:

$$H = \sum_i h(i) + \sum_{i,j} V(i,j) + V_{IJ} \tag{1.24}$$

Where $\sum_i h(i) = -\sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 - \sum_{i,I} \frac{Z_I e^2}{|R_I - r_i|}$ is the sum of the Hamiltonians of each electron independently. Similarly, the wave function of a complex system with several particles, can be written in the form of a product of wave functions with a single electron and the system energy is equal to the sum of the energies of all the electrons.

$$\Psi(r_i ... t) = \phi_i(r_1)\phi_j(r_2)...\phi_k(r_N) \tag{1.25}$$

It should be noted that the Hartree-fock approximation does not take into account, neither the effects of the correlation, nor the exchange effects, that is to say that the real system energy, in addition to the Hartree energy given by equation (1.26), a corrective term includes the correlation.

$$E_{\text{Hartree}} = \iint \frac{\rho(r)\rho(r')}{|r - r'|}\, dr\, dr' \tag{1.26}$$

$\rho(r)$ is the electron density that can be put in the representation of the mean field in the form:

$$\rho(r) = \sum_{i=1}^{N} |\phi_i(r)|^2 \tag{1.27}$$

Finally, we can rewrite equation (1.23) in the form :

$$H = -\sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_i V_{\text{ext}}(\mathbf{r}i) + \iint \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, d\mathbf{r}d\mathbf{r}' + V\text{xc} \tag{1.28}$$

where Vxc is the potential for exchange and correlation[26].

1.4 The theory of the density functional

Whereas the methods used in the framework of the Hartree-Fock approximation express the energy of the system as a functional of the wave functionψ , those who use DFT from the English Density Functional Theory, express it as an electron density functional $\rho(r)$ of the system.The probability of finding an electron in a unit volume d^3r defined by r , it is therefore, a positive function which depends only on the three coordinates x,y and z space. It cancels out to infinity and its integral over the entire space is N (total number of electrons).
The theory of the density functional responds to the need to find an exact formalism of the quantity $\rho(r)$,this makes it possible, using equation (1.27), to solve the Schrödinger equation in a self-consistent way.
Among the theoretical approaches that have developed formalisms thus making it possible to calculate the electron density, we present in the following those of Hohenberg-Kohn in 1964 and those of Kohn-Sham in 1965[26].

1.4.1 The Hohenberg-Kohn approach

The theory of the density functional DFT is based on the work of Hohenberg and Kohn 1964 which demonstrated that the total energy of the ground state of a system at N interacting particles in an external potential Vext is a functional of its electron density.

$$E_o = E[\rho_0(r)] \tag{1.29}$$

where $\rho(r)$ is the electron density of the ground state, which can be calculated from the Schrödinger equation :

$$\rho_0(r) = N \int \psi^*_{GS}(r, r_2, r_3, \ldots, r_N)\psi_{GS}(r, r_2, r_3, \ldots, r_N)\, dr_2\, dr_3 \ldots\, dr_N \tag{1.30}$$

The total energy of the electronic system can be expressed as :

$$E[\rho(r)] = F_{\text{HK}}[\rho(r)] + \int V_{\text{ext}}(r)\rho(r)\, dr \tag{1.31}$$

Where, $F_{\text{HK}}[\rho(r)] = T[\rho(r)] + V_{\text{e-e}}[\rho(r)]$ is the Hohenberg and Kohn functional,$T[\rho(r)]$is the functional of the kinetic energy of a system of non-interactive particles and $V_{\text{e-e}}[\rho(r)]$ is the

functional of the Colombian electron-electron interaction.
According to the variational principle, the total system energy in a known external potential reaches its minimum value (the ground state energy) when the density $\rho(r)$ corresponds to the density $\rho_0(r)$[26].

$$E[\rho_0(r)] = minE[\rho(r)] \tag{1.32}$$

$$\left.\frac{\delta E[\rho(r)]}{\delta\rho(r)}\right|_{\rho_0} = 0 \tag{1.33}$$

1.4.2 The Kohn-Sham approach

The two Hohenberg-Kohn theorems assert that the external potentialV_{ext} is independent of density and that the functional$F_{\text{HK}}[\rho(r)]$is stained with errors about kinetic energy$T[\rho(r)]$and about the potential$V_{\text{e-e}}[\rho(r)]$.To correct these errors, in 1965 Walter Kohn and Lu Sham developed an approach based on the following two ideas :

- The real electronic system is redefined as a fictitious system of fermions without interaction and of the same electronic density of the ground state (correction on the potential $V_{\text{e-e}}[\rho(r)]$)
- Single-particle orbitals are introduced in order to treat the error in the kinetic energy term (correction on kinetic energy $T[\rho(r)]$)

With these conditions and taking into account that the total number of particles is conserved, The functional F_{HK} is written :

$$F_{\text{HK}}[\rho(r)] = T_s[\rho(r)] + E_{\text{H}}[\rho(r)] + E_{\text{xc}}[\rho(r)] \tag{1.34}$$

Where

$$T_s[\rho(r)] = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int \psi^*(r)\nabla^2\psi(r)\,dr \tag{1.35}$$

is the kinetic energy of the independent particles without interaction, and

$$E_{\text{H}}[\rho(r)] = \frac{1}{2}\int\int \frac{\rho(r)\rho(r')}{|r-r'|}\,dr\,dr' \tag{1.36}$$

is the electrostatic energy, called Hartree's energy. Thus the energy of the ground state of a system can be obtained by minimizing the functional of its energy, and equation (1.31) becomes:

$$\delta\left\{\int V_{\text{ext}}(r)\rho(r)\,dr - \mu\left(\int \rho(r)\,dr - N\right)\right\} = 0 \tag{1.37}$$

The result is :

$$\mu = \frac{\delta F_{HK}[\rho(r)]}{\delta\rho(r)} + V_{\text{ext}}(r) = \frac{\delta T_s[\rho(r)]}{\delta\rho(r)} + V_{KS}(r) \tag{1.38}$$

Where μ is the chemical potential,$V_{\mathrm{XC}}(r)$ is the potential of Kohn-Sham.

$$V_{KS}(r) = V_{ext}(r) + V_H(r) + V_{XC}(r) \tag{1.39}$$

Or again,
$V_{\mathrm{H}}(r) = \frac{\delta E_{\mathrm{H}}[\rho(r)]}{\delta\rho(r)}$ is Hartree's potential, and $V_{\mathrm{xc}}(r) = \frac{\delta E_{\mathrm{xc}}[\rho(r)]}{\delta\rho(\gamma)}$ is the potential for exchange and correlation.
The Schrödinger equation or also called Kohn-Sham equation for a particle in the framework of this approach is written :

$$\left[-\frac{\hbar^2}{2m}\nabla_i^2 + V_{KS}(r)\right]\varphi_i(r) = \varepsilon_i\varphi_i(r) \tag{1.40}$$

This equation can be solved numerically in a self-consistent way (figure 1.1) by starting with a value of the initial density ρ_{initial}, this value corresponds to a potential $V_{\mathrm{KS}}(r)$ which will give a solution to the Kohn-Sham equation which is a new value of the density. This same value will improve the potential$V_{\mathrm{KS}}(r)$ An algorithm repeats this process until convergence is reached[26].

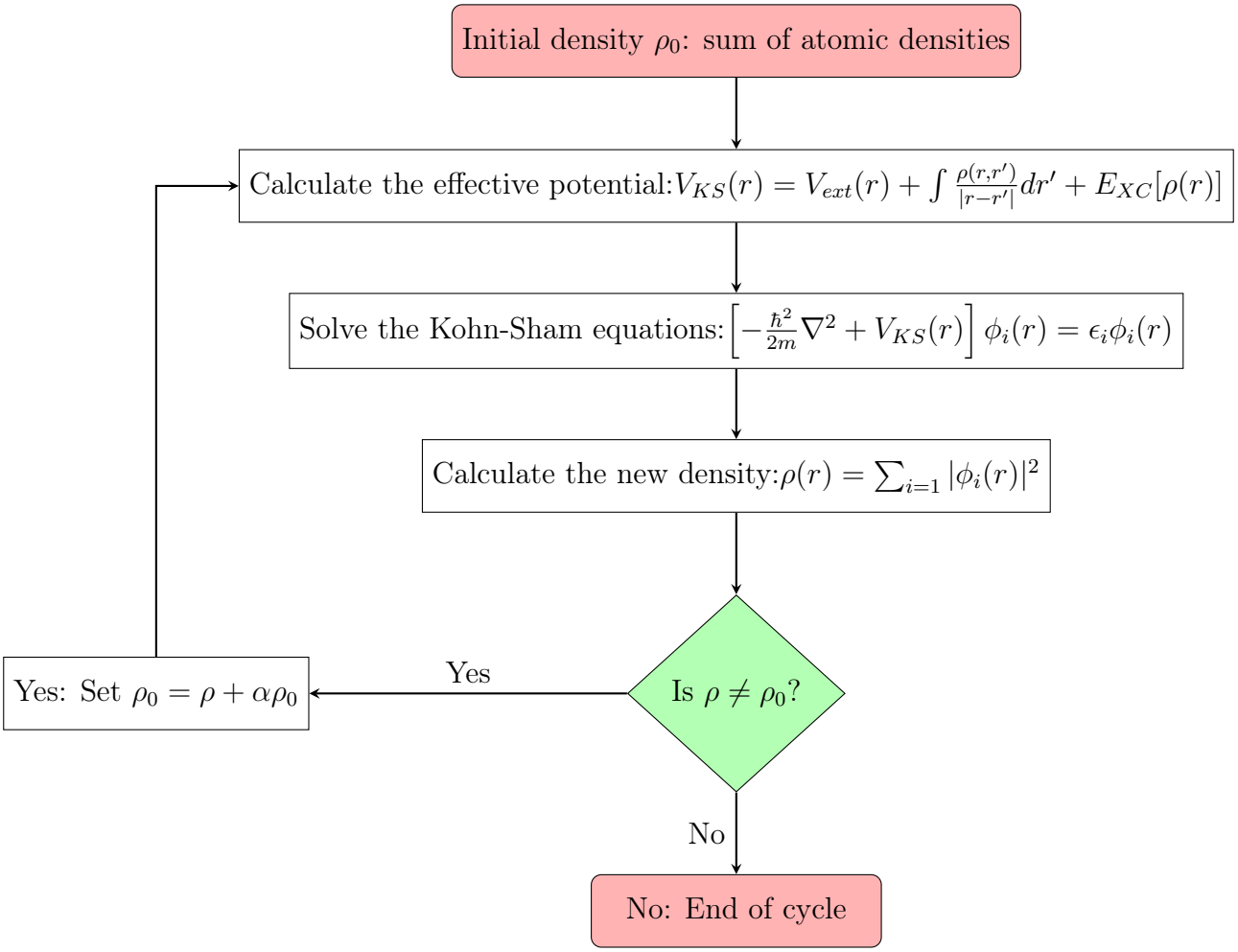

Figure 1.1: Scheme for solving the Kohn-Sham equation.

1.5 The exchange and correlation functionals

In order to solve the Kohn-Sham equations which implicitly depend on exchange and correlation potential $V_{\mathrm{XC}}(r)$, it must find an exact expression of the latter. This expression is unknown, but in practice, to highlight it, approximations are necessary.

1.5.1 Approximation of the local density LDA

Known by the acronym LDA, it is the simplest and most used and which is written in the form :

$$E_{xc}^{\mathrm{LDA}}[\rho(r)] = \int \rho(r)\epsilon_{xc}^{\mathrm{hom}}[\rho(r)]\, dr \tag{1.41}$$

Where $E_{xc}^{\mathrm{hom}}[\rho(r)] = \epsilon_x[\rho(r)] + \epsilon_c[\rho(r)]$ is the exchange-correlation energy of a homogeneous electron gas of densité $\rho(r)$ .The correlation part $\epsilon_x[\rho(r)]$ determined from the numerical results of Ceperley and Alder and analytically for the exchange part

$$\varepsilon_x[\rho(r)] : \quad \varepsilon_x[\rho(r)] = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} \int \rho(r)^{4/3}\, dr \tag{1.42}$$

If we introduce the spin effect, we will have two densities according to the value of spin($Up \uparrow ouDown \downarrow$)and equation (1.41) will be in this case [26]:

$$E_{xc}^{\mathrm{LSDA}}[\rho_\uparrow(r), \rho_\downarrow(r)] = \int \rho(r)\, \varepsilon_{xc}^{\mathrm{hom}}(\rho_\uparrow(r), \rho_\downarrow(r))\, dr \tag{1.43}$$

1.5.2 Generalized gradient approximation GGA

The approximation of the local density or LDA is valid only for densities that vary slowly. Indeed, for a long range where the density begins to be heterogeneous, corrections must be made to the exchange-correlation energy by introducing the density gradient into it. There are several GGA whose general expression is :

$$E_{xc}^{GGA}[\rho_\uparrow(r), \rho_\downarrow(r)] = \int \rho(r)\epsilon_{xc}^{\mathrm{hom}}(\rho_\uparrow(r), \rho_\downarrow(r), \nabla\rho_\uparrow(r), \nabla\rho_\downarrow(r))\, dr \tag{1.44}$$

The different GGA used are generally better suited than the LDA to calculate the length and the binding energy of the molecules, the constant of the crystal lattice, in particular in systems where the charge density varies rapidly. However, the GGA sometimes overestimates, in the case of ionic crystals, the value of the lattice constant compared to experimental data . On the other hand, in the case of systems where the electrons tend to be localized and highly correlated, such as transition metal oxides and rare earth element compounds, both methods (LDA or GGA) have poor performance[26].

1.5.3 Hybrid functions

Hybrid functionals include a series of functionals that mix the two theories of Hartree-Fock and DFT. They aim to improve the expression of the exchange-correlation energy by incorporating the exact part of the exchange energy obtained from the Hartree-Fock method. One of the most used hybrid functional, we find B3LYP .

$$E_{xc}^{B3LYP} = E_{xc}^{GGA} + a\left(E_x^{HF} - E_x^{GGA}\right) \tag{1.45}$$

Where a is a fitting parameter (adjustment with the experimental data)[26].

1.6 Conclusion

In this chapter, we provided a comprehensive exploration of the Schrödinger equation, starting from its historical origins, through the basic concepts, mathematical formula, and physical interpretations of this equation. We also reviewed the density functional theory (DFT) as a numerical method for solving the Schrödinger equation.

In the next chapter, we will address advanced methods for solving the Schrödinger equation using a deep learning approach.

Chapter 2

Chapter 2

State of the art

2.1 Introduction

Schrödinger's equation has long held the secret to the universe's smallest scales, requiring massive computational resources and challenging traditional methods.
Solving this equation, especially for complex quantum systems with multiple interacting particles, has historically been a difficult task. Especially given the increasing complexity of systems, analytical solutions are often unobtainable. Computational methods are crucial to solving the mysteries of quantum mechanics, providing insights into molecular structure and material properties.
In recent years, a paradigm shift has occurred with the emergence of deep learning, a subfield of artificial intelligence, as a transformative tool across various scientific disciplines. Its ability to recognize complex patterns and process large amounts of data, as well as to approximate complex functions, has stimulated interest in applying deep learning methods to solve quantum mechanical problems.

In this chapter, we'll dig into the shift from traditional methods to deep learning in quantum science. We'll explore the limitations and challenges posed by traditional methods, delve into the relationship between quantum mechanics and deep learning, and study the structures of advanced neural networks designed for quantum systems.
Additionally, we'll showcase the latest works that have embraced deep learning to solve the Schrödinger equation,and discussing the pros and cons of deep learning in quantum mechanics.

2.2 From Traditional Methods to Deep Learning

The transition from traditional methods to deep learning is a landmark in the history of artificial intelligence. Deep learning provides immense capabilities for solving complex problems in various fields.

2.2.1 Limitations and challenges of traditional methods

Traditional methods of solving the Schrodinger equation have served us well for decades, such as numerical methods and analytical approximation, but they have many limitations and challenges compared to the use of deep learning techniques that it aims to overcome, among them:

- **Dimensionality (N)**

  The dimensions of a system significantly affect complexity. In general, as the number of dimensions increases, the computational resources required to solve the Schrödinger equation increase significantly. This is because the number of ground states or grid points required to estimate the system grows exponentially with N[27, 28].

- **Interactions**

  Complexity increases further when a system involves interactions between its components. Interactions can lead to entanglements and correlations between different parts of the system and increase the computational effort when simulating dynamics or calculating system properties. For example, in many-body systems, interactions between particles can lead to complex collective behaviors that are difficult to model accurately[29, 30].

- **Intractable Entanglement**

  In the context of the Schrödinger equation, intractable entanglement arises with quantum systems of multiple particles. The equation describes the wave function evolution, where entanglement occurs as states of particles become interdependent. As particle numbers increase, entanglement complexity grows exponentially, rendering accurate description or simulation infeasible with traditional computational methods. This challenge, termed intractable entanglement, impedes understanding and manipulation of complex quantum systems, hindering accurate prediction and analysis of their behavior. Researchers pursue new computational and theoretical approaches like tensor network and variational methods to tackle intractable entanglement and advance understanding and utilization of quantum phenomena. This issue has implications for quantum computing, communication, and simulations, necessitating its resolution for progress in these fields[31].

- **Convergence and Accuracy**

  Achieving convergence and high accuracy with traditional numerical methods can be challenging, particularly for systems with strong spatial variations or complex potentials.Additionally, analytical approximations may introduce errors, especially for systems with non-linear or non-perturbative interactions[32].
  In the context of the Schrödinger equation, the accuracy problem arises from the need to obtain reliable and meaningful results when solving the wave function of a quantum system.
  Accuracy refers to the degree to which calculation results correspond to the actual physical behavior of a quantum system, obtaining a solution that faithfully represents real-world behavior, including energy levels and wave functions. This involves minimizing errors and uncertainties in the numerical methods used to solve the equations to ensure that the results are as close as possible to the true values.

  The challenge with the Schrödinger equation is to achieve a balance between precision and accuracy, which often requires computationally intensive methods to minimize numerical errors.When solving the Schrödinger equation and predicting the behavior of quantum systems, the balance between accuracy and precision is critical to obtaining reliable results[33].

- **Limited Analytical Solutions**

  While analytical solutions exist for some simple systems, such as the hydrogen atom or harmonic oscillator, obtaining analytical solutions for complex systems with arbitrary potentials or interactions is often not feasible. This limitation restricts the applicability of traditional analytical methods[34].

All these constraints and more have led scientists to resort to deep learning in the context of solving the Schrödinger equation due to the complexity of physical systems and strong spatial variations. Analytical approximations may not be sufficient and can lead to errors, especially in systems with non-linear or non-perturbative interactions. Accurate solutions to the Schrödinger equation require advanced and precise computational techniques to ensure accurate and reliable results. This necessitates the use of sophisticated computational methods like deep learning to analyze and understand quantum system interactions in a precise and effective manner.

2.3 Deep learning in quantum Sciences

The seamless integration of deep learning and quantum chemistry illustrates the transformative power of interdisciplinary collaboration in scientific research. By combining the strengths of these fields, this research opens up new avenues of exploration and innovation. This integration significantly improves the efficiency and accuracy of molecular property predictions and expands the range of properties that can be reliably determined. Deep neural networks can now predict a variety of molecular properties such as energy levels, bond lengths, and vibrational frequencies, providing insights into complex molecular systems.
In addition to predicting molecular properties, this integration paves the way for a paradigm shift in computational chemistry. Its ability to simulate complex molecular systems efficiently and accurately has the potential to revolutionize fields such as materials science, drug development and energy research[35].

2.3.1 Bridging quantum mechanics and deep learning

The combination of deep learning and quantum mechanics could lead to more efficient and accurate simulations of complex quantum systems, providing deeper insights into the behavior of matter at the fundamental level. The ongoing efforts to bridge the gap between quantum mechanics and deep learning represent a significant milestone in the pursuit of scientific progress and technological innovation. The transformative potential of this interdisciplinary approach is immense, and its impact on various fields is only beginning to unfold. As research continues to advance, we can anticipate groundbreaking discoveries and transformative advancements that will shape the future of science and technology[36].

To bridge quantum mechanics and deep learning, researchers are exploring the fusion of quantum computing and machine learning, leading to the emergence of quantum machine learning (QML). This innovative concept aims to revolutionize computational science, data analytics, and predictive modeling across various fields. Quantum computing provides the computational power to accelerate complex machine learning algorithms, while machine learning offers tools for optimizing quantum circuits and decoding quantum states[37].

The convergence of quantum mechanics and deep learning holds immense promise for shaping the future of science and technology. Their combined power could lead to transformative breakthroughs in various fields.

In the search for common ground and to capture the potential of both domains, scientists are constantly engaged in investigations that result in original constructs, theoretical relationships, and future applications. Such activities can foster novel solutions to problems encountered during research projects and contribute towards major technological advances.

- **Materials Discovery**

  Accurately predicting material properties at the atomic and molecular level could lead to the development of revolutionary materials with enhanced properties, such as superconductors and materials with programmable properties[38].

- **Drug Design and Development**

  Deep learning integrated with quantum chemistry could revolutionize drug discovery by enabling the rapid screening of vast libraries of potential drug candidates, leading to the development of more effective and personalized therapies[39].

- **Precision Medicine**

  Quantum-enhanced deep learning could pave the way for precision medicine, tailoring treatments to individual patients based on their unique genetic and molecular profiles.

- **Quantum Computing Hardware Development**

  Deep learning algorithms could play a crucial role in optimizing quantum algorithms and enhancing the performance of quantum computing hardware, accelerating the development of practical quantum computers.

2.4 Advanced Neural Network Architectures for Quantum Systems

Advanced neural networks offer an innovative solution for understanding and simulating quantum systems, blending artificial intelligence techniques with quantum physics concepts. These networks are a crucial part of recent advancements in quantum computing, unlocking the potential to grasp complex quantum behavior and analyze it efficiently.

2.4.1 Qubit

The name "quantum bit" or qubit, refers to the quantum counterpart of a conventional bit. It was coined by combining the words "bit" and "quantum" It is a "computer description" of a situation that particle, a simple quantum arrangement. A qubit can exist in a superposition of states, in contrast to a traditional bit, which can only take one value at a time[1].

2.4.2 Handling a qubit

It is required to apply some formality before viewing the Bloch sphere. A Hilbert space $\mathcal{H}$ with a dimension of two and an orthogonal basis $\{|0\rangle, |1\rangle\}$ is examined. For the purpose of differentiating the states during the measurement, this basis has to be orthogonal. Because the states are normalized, the basis is also normalized. The fact that 2×2 matrices are used to describe the operations that will be carried out on its members is evident based on the dimension of $\mathcal{H}$[1].

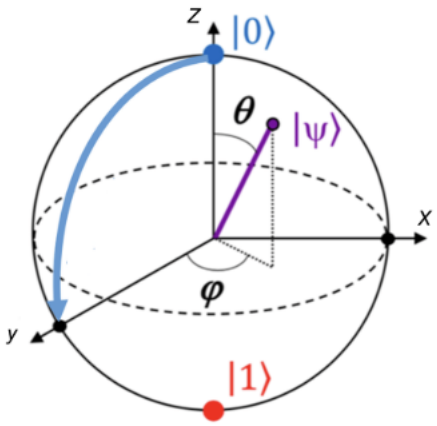

Figure 2.1: Bloch sphere

Using Pauli operators, also known as Pauli gates, we may describe the fundamental rotations around the X, Y, and Z axes in this form.

- **Pauli-X (X)**

  It uses the following operator to rotate around the X axis: $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ [1]

Figure 2.2: X gate

- **Pauli-Y (Y)**

  It uses the operator to rotate around the Y axis: $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ [1]

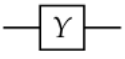

Figure 2.3: Y gate

- **Pauli-Z (Z)**

  It uses the following operator to rotate along the Z axis: $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ [1]

Figure 2.4: Z gate

2.4.3 Quantum circuit

A quantum circuit is a computing process that combines real-time classical computation with coherent quantum operations on quantum states. It consists of sequential quantum gates, resets, and measurements, allowing for the description of any quantum program[1].

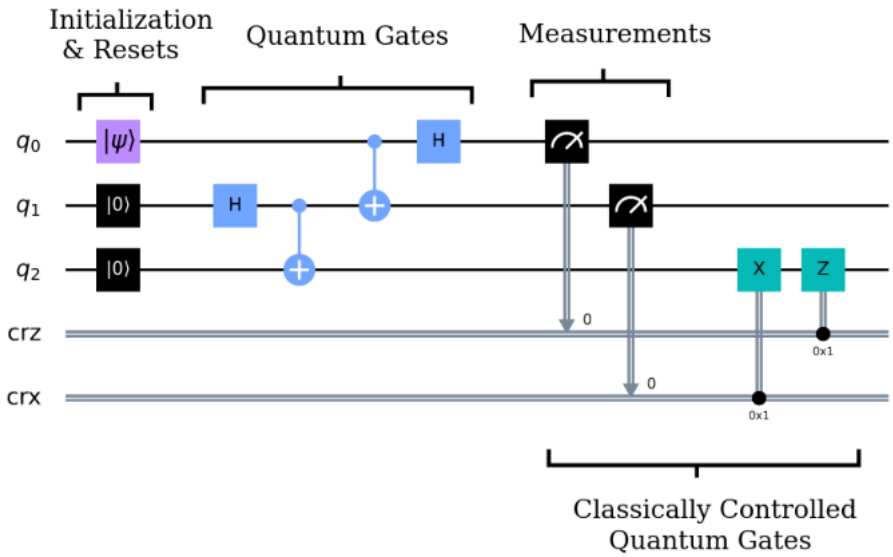

Figure 2.5: Example of a quantum circuit composed of three qubits and two classical bits[1]

2.4.4 Quantum Neural Networks (QNNs)

A sequence of neurons is used to construct a classical neural network, with each layer having a weight matrix that minimizes the objective function. In these networks, inputs and outputs are represented by quantum states, and the objective function is calculated using a unitary transformation[1].

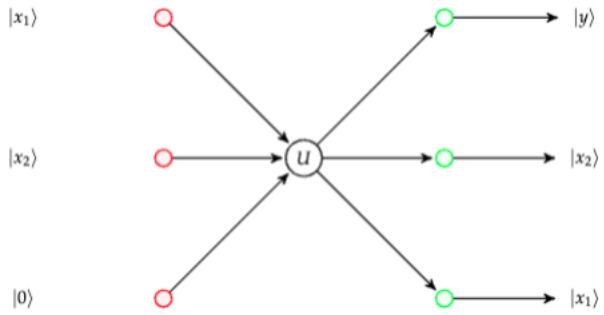

Figure 2.6: Quantum Neural Network[1]

QNN is A subtype of variational quantum algorithms, quantum neural networks are made up of quantum circuits with parameterized gate operations[40]. Models, systems, or gadgets known as Quantum Neural Networks (QNNs) combine elements of quantum theory with neural network characteristics[41]. (QNNs) encode data into one or more read-out qubits after extracting it from the input, which is often a high-dimensional quantum wave function. Typically, QNNs are composed of local unitary quantum gates, and the issue of how to appropriately build QNN architectures should arise in practice[42].A variational model with parameterized gates is applied and optimized for a specific job after information is first encoded into a quantum state using a state preparation procedure or feature map. By applying a classical post-processing function to a measurement, the output of a quantum model can be retrieved, and this is achieved by loss function minimization final result[40].

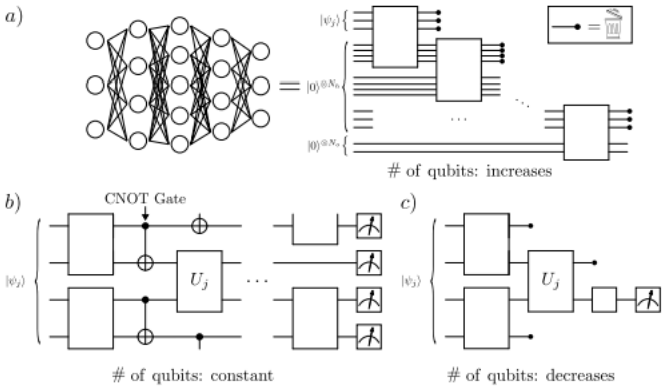

Figure 2.7: Examples of QNN architectures[2]

In figure2.7 there are:

a): three layers make up a typical feed-forward neural network: input, hidden, and output.

b): another possible QNN strategy is to keep the qubits fixed, without discardingor replacing them.

c):shows a convolutional QNN where qubits are measured at each layer to minimize the dimension of the data while keeping its pertinent characteristics[2].

2.4.5 Variational Quantum Circuits (VQCs)

Unitary convolutional layers and pooling layers are used to create the quantum convolutional neural network, a basic variational quantum machine learning . VQCs are quantum circuits having parameters that may be adjusted through iterative optimizations using gradient-free or gradient-based algorithms on a classical computer. Quantum circuits with programmable parameters that are amenable to classical iterative optimizations are known as variational quantum circuits. The word "variational" refers to the ability to update certain circuit components based on a predetermined parameter, known as the "loss".

First, distinguish between a limited and a free architecture before adapting the architecture to the quantum scenario. A variational quantum circuit (VQC) with a free design is characterized by the locations of controlled-not gates (CNOTs) and rotation gates (ROTs). In other words, CNOTs can join any two wires. Instead, a VQC with a restricted design is a circuit in which the ROTs and CNOTs exhibit regular patterns following the first encoding layer. There are numerous architectures available for use, including a basic architecture Ansätze. Typical instances are the architecture that is efficient with hardware or the architecture that is highly entangled[43, 44, 45, 3, 46].

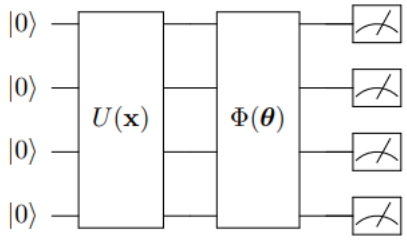

Figure 2.8: Generic circuit architecture for the variational quantum classifier[3].

In Figure 2.8, the data encoding block, represented by $U(x)$, is a crucial part of the architecture, while the learnable portion, $\Phi(\theta)$, is optimized using gradients. These circuits, capable of withstanding quantum noise, are suitable for NISQ device applications[3].

2.4.6 Quantum Convolutional Neural Networks (QCNNs)

Cong's proposed QCNN builds on the main features of current CNN designs for quantum systems. When transferring a quantum physics problem from a many-body Hilbert space to a classical computing environment, the quantity of data needed increases exponentially with system size. The problem stems from the possibility of using qubits in a quantum environment to represent data. These can be avoided by employing a CNN-designed quantum computer.

Tree-like, or hierarchical, structures are used in an intriguing class of quantum neural networks, where the number of qubits in a subsequent layer is reduced by a factor of two. Since these designs contain $O(\log(n))$ layers for n input qubits, they offer shallow circuit depth. They can also ensure trainability by preventing "barren plateau," which is one of the major problems with PQC-based algorithms. Moreover, these structures are naturally related to the tensor

network, offering an invaluable platform to study neural networks, many-body physics, and their interrelationships.

The steady drop in qubit count is analogous to the CNN pooling approach. One of the distinctive features of the QCNN design is its translational invariance [5, 47, 48].

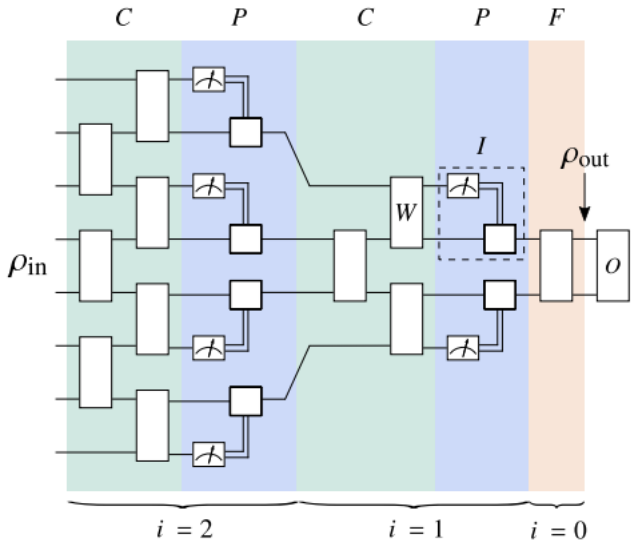

Figure 2.9: Schematic representation of a QCNN [4].

Figure 2.9 shows that an n-qubit quantum state ρ_{in} serves as the QCNN's input. After that, the state ρ_{in} is passed through a series of pooling (P) and L convolutional (C) layers. Two rows of two-qubit unitaries (W) operating on alternate pairs of qubits make up the convolutional layers. The pooling operators (seen in the dashed box) make up the pooling layer. A qubit is measured in each pooling module, and the measurement result governs a unitary applied to a nearby qubit (I). Following the last pooling layer, the remaining qubits are subjected to a fully connected unitary (F), yielding an output state ρ_{out} with a dimension significantly less than ρ_{in}. Lastly, the expectation value of an operator O over the state ρ_{out} is measured [4].

Pooling (red circle), convolutional filters (blue rounded rectangle), and quantum data encoding (green rectangle) are the three elements of the quantum circuit shown in Figure 2.10. The convolutional filter and pooling processes employ parameterized quantum gates, but the quantum data encoding is fixed inside a particular QCNN structure. This example comprises three layers, each of which can have several convolutional filters applied to it. For the ith layer, the number of filters is represented by $\boldsymbol{li}$. The same two-qubit ansatz is applied translationally-invariantly to nearest neighbor qubits via the convolutional filter in each layer. Similarly, the pooling processes of the layer use the same ansatz. In this case, the pooling procedure is represented as a controlled unitary transformation, which activates upon setting the control qubit to 1. However, in general, controlled operations may be used [5].

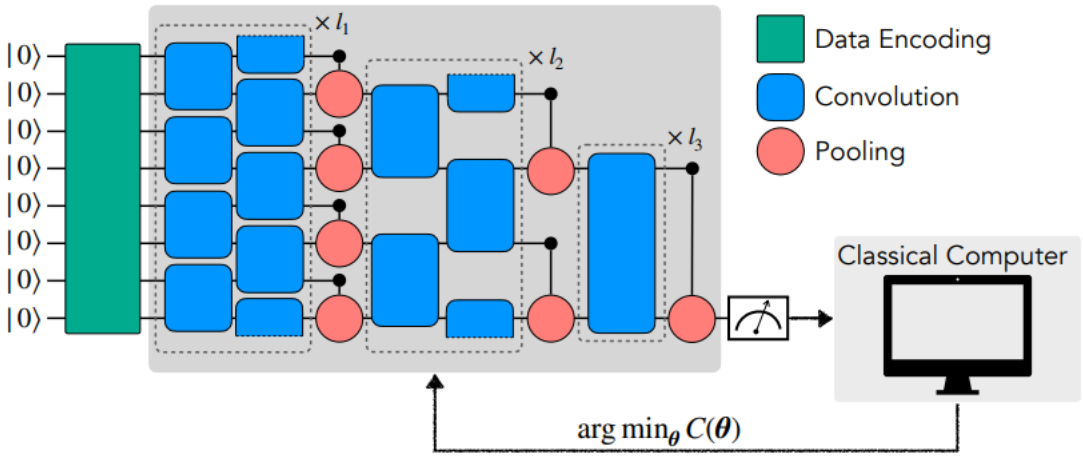

Figure 2.10: A schematic of the QCNN algorithm for an example of 8 input qubits [5].

$$C(\theta) = X \sum_{i=1}^{M} \alpha_i c(y_i, f(x_i, \theta)) \tag{2.1}$$

2.4.7 Quantum Recurrent Neural Networks (QRNNs)

Typically, RNNs are multilayer structures, with each layer containing the basic recurrent block. Depending on the specific design of the recurrent block, an RNN's input layer x_t, hidden layer h_t, and output layer y_{t+1} are all composed of real-valued vectors. In order to improve sequential learning tasks, recurrent neural networks and quantum computing concepts are combined in a new field of study called Quantum Recurrent Neural Networks, or QRNNs. These networks are intended to possibly outperform classical resources in sequential learning applications by utilizing the capabilities of quantum computing devices, specifically near-term noisy intermediate-scale quantum (NISQ) devices. To lessen the algorithm's demands on the coherence time of quantum devices, QRNNs are built using quantum recurrent blocks (QRBs) in a staggered fashion, making them more accessible on NISQ devices. They have outperformed previous quantum neural network models and traditional RNNs in prediction accuracy for sequential learning tasks such as text categorization, stock price prediction, and meteorological indicators. Given their extraordinary ability to generalize from short training sets and their capacity to learn broad causal quantum automata, QRNNs hold great promise for sophisticated quantum processes including memory. The unitary structure of QRNNs improves training efficiency and performance by mitigating the vanishing gradient issue that plagues many quantum classifiers and conventional RNNs currently in use [49, 50, 49, 6, 51, 52, 49].

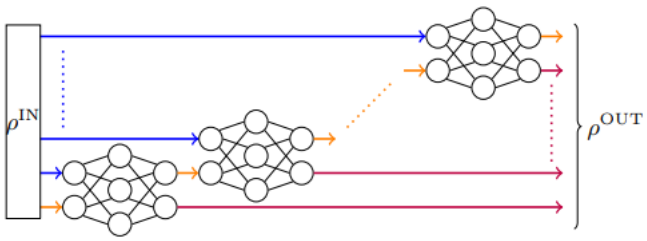

Figure 2.11: A general Quantum Recurrent Neural Network [6].

A QRNN is an iteration over the feed-forward QNN's memory system (orange), where the entire input is divided into an input (blue) and the memory, and the total output is divided into an output (purple) and the memory, as shown in Figure 2.11, with $L = 1$ [6].

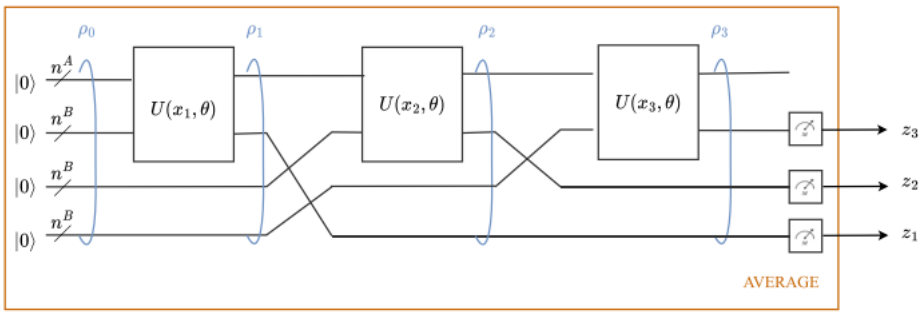

Figure 2.12: The QRNN model [7].

Figure 2.12 may be understood as a variation of a dissipative QRNN, as depicted in the figure with $T = 3$. Here, unitaries $U(x, \theta)$ reuse the same parameter vector θ, and distinct data samples x_t are loaded at each time t [7].

2.4.8 Quantum Graph Neural Networks (QGNNs)

For most GNN models designed for quantum physics calculations, the main output of the model in the energy-centric simulation framework is the energy of the entire atomic system. Rotationally-invariant GNNs are used to forecast the energy [53]. Graph Neural Networks (GNNs) are a powerful class of machine learning models designed to handle graph-organized data. The three main components of a GNN are feature embedding, decoding, and message forwarding. During the feature embedding step, graph nodes and edges are mapped to high-dimensional feature vectors, encapsulating their properties and relationships [54]. A specific family of quantum neural network designs called Quantum Graph Neural Networks (QGNN) is intended to model quantum processes with a graph topology. These networks are very well suited for quantum network execution on dispersed quantum systems. QGNN encompasses specialized designs such as Variational Quantum Circuits (VQC), Quantum Graph Recurrent Neural Networks (QGRNN), and Quantum Graph Convolutional Neural Networks (QGCNN). Applications include learning the Hamiltonian dynamics of quantum systems, generating multipartite entanglement, spectral clustering unsupervised learning, and graph isomorphism classification supervised learning [55, 56, 57, 8].

A circuit including a 6-qubit with angle encoding and two hidden VQC layers is shown graphically in Figure 2.13. Specifically, the ansatz uses R_x rotations for angle encoding and capitalizes on R_x, R_y, and CNOT operations. Pauli-Z expectation is then used as the final step in the circuit measurement process. The result of careful consideration of circuit expressibility and complex node-node interactions embedded within graphical data is this strategic circuit design [8].

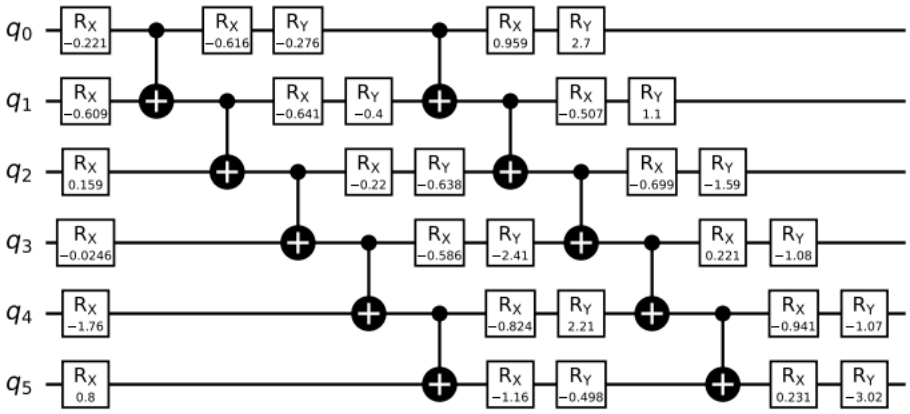

Figure 2.13: Quantum circuit for angle encoding and VQC in the QGNN architecture with R_y, R_x, and CNOT gates [8].

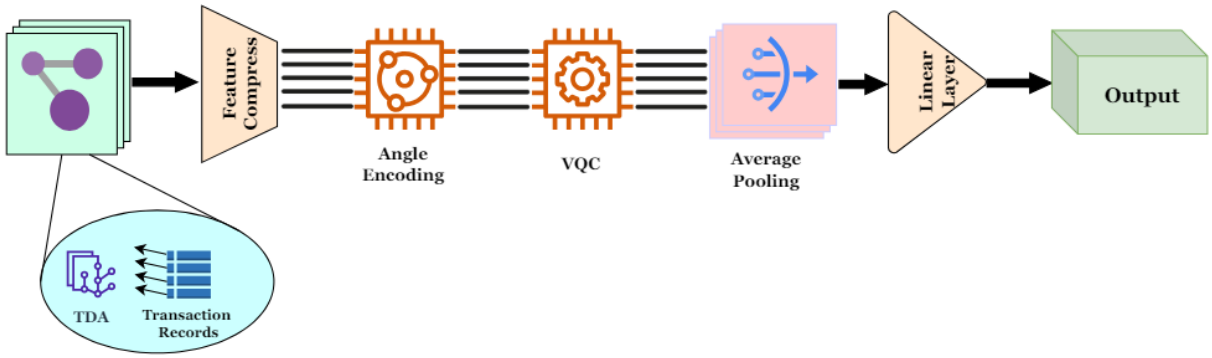

Figure 2.14: Architecture of the quantum graph neural network [8].

Figure 2.14 illustrates that a graph is first fed into the QGNN, and then a feature compression stage is performed. The data is prepared for VQC processing by angle encoding. After passing through a linear layer and average pooling, the VQC's output is delivered into the output layer [8].

Furthermore, for graph-structured data, a brand-new hybrid quantum-classical algorithm known as the Ego-graph based Quantum Graph Neural Network (ego QGNN) has been proposed. It uses tensor product and unity matrix representation to implement the GNN theoretical framework, requiring fewer model parameters while achieving better performance than previous models [55, 58].

2.5 State of the Art of Deep Learning approaches for Solving the Schrödinger Equation

In the ever-evolving landscape of computational physics, the integration of deep learning methodologies has emerged as a transformative force, offering new perspectives and innovative solutions to old challenges. Among these stands the schrödinger equation, a fundamental pillar of quantum mechanics that governs the behavior of particles at the atomic and subatomic levels. Traditionally, solving this equation requires complex mathematical frameworks and computational techniques, often constrained by the complexity of the systems under study.
The advent of deep learning has provoked a paradigm shift in how we approach such problems. By harnessing artificial neural networks and vast datasets, researchers are exploring a new frontier in quantum mechanics: employing deep learning architectures to solve the Schrödinger equation directly. This fusion holds tremendous promise, not only in accelerating the calculation of quantum states but also in revealing deeper insights into the fundamental physics governing quantum phenomena.

Carleo and **Troyer** introduced the concept of using neural networks to represent quantum systems in their groundbreaking **2017** work [59]. Utilizing a neural network called a restricted Boltzmann machine (RBM), researchers successfully represented the wave function of quantum many-body systems, achieving notable success in solving problems related to many-body localization and quantum spin systems. This work showcased the effectiveness of NNQS in capturing the complexity of quantum systems and offering a fresh perspective on understanding quantum many-body systems.
The study delved into the intricacies of many-body quantum systems in Physics, highlighting the non-trivial correlations embedded in the exponential complexity of the multibody wave function. The authors aimed to simplify this complexity into a manageable computational form for specific cases of material significance.
To address this challenge, the authors introduced a variable representation of quantum states based on artificial neural networks with a flexible number of hidden neurons. They employed a reinforcement learning scheme capable of determining the ground state or describing the unitary time evolution of intricate interacting quantum systems. The neural network parameters were optimized using constant variable Monte Carlo (VMC) sampling or time-dependent VMC for dynamic characteristics.
Their approach yielded highly accurate **results** in characterizing the equilibrium and dynamic properties of models representing typical interactive cycles in various dimensions. This method effectively resolved the phase problem commonly encountered in stochastic quantum Monte Carlo methods. Furthermore, the authors explored the potential advantages of artificial intelligence in resolving issues related to multiple quantum entities.
In summary, the researchers successfully demonstrated that systematic machine learning of the wave function through artificial neural networks can significantly simplify the complexity of multibody wave functions, offering a potent tool for addressing the challenges posed by many quantum bodies .

Researchers **Jiequn Han**and colleagues[60], conquered in **2018** the challenge of solving the multi-electron Schrödinger equation, a fundamental problem in computer science. They introduced the Deep Wave Function **(DeepWF)** method, which uses deep neural networks to represent test wave functions and ensure compliance with the Pauli Exclusion Principle. The method was optimized through variational Monte Carlo to accurately represent the ground state energies of a variety of systems, including He, H2, Be, B, LiH, and chains of 10 hydrogen atoms. However, the accuracy of this method decreases as the number of electrons increases.
The future of this approach is promising, as it opens up new possibilities for solving the large-scale multi-electron Schrödinger equation. The authors highlight the simplicity of the method and suggest areas for further improvement, such as: B. Improving the representation of anti-symmetric methods and optimizing variational Monte Carlo processes to achieve more efficient sampling. These prospects demonstrate DeepWF's potential to solve large-scale Schrödinger equations involving many electrons, providing a promising avenue for future research in computational physics and quantum chemistry.

Jan Hermann and colleagues[20], also arrived in **2020** Due to the analytical solvability of the electronic Schrödinger equation only for a hydrogen atom, the approach of numerically complete configuration interaction becomes prohibitively expensive as the number of electrons increases.
This study focuses on the computational hurdles associated with solving the Schrödinger electron equation in quantum chemistry, particularly for systems with a large electron count. The escalating computational complexity with increasing electrons renders achieving high accuracy impractical for most molecules using conventional methods. To tackle this challenge, the research introduces Polynet, a deep-learning wave function trained with variable quantum Monte Carlo. Polynet aims to provide nearly exact solutions to the electronic Schrödinger equation for molecules containing up to 30 electrons by amalgamating valid wave function physics and leveraging the expressive capabilities of neural networks.
The findings demonstrate Polynet's superior performance over modern ansatz resolutions for atoms, diatomic molecules, and linear hydrogen chains. It achieves remarkable accuracy with fewer determinants compared to traditional quantum Monte Carlo methods, showcasing its computational efficiency and scalability. The study emphasizes the significance of trainable reverse flow ansatz in optimizing the nodal surface of the Hartree-Fock baseline to achieve high precision. Furthermore, the successful extension of Polynet to larger molecules with intricate electronic structures underscores its utility for complex systems in quantum chemistry.
In essence, the study addresses the computational constraints of current methods for solving the electronic Schrödinger equation in quantum chemistry by introducing Polynet, a deep learning approach that offers high accuracy with reduced determinants and exhibits scalability for larger systems.

Researchers **Mitsumasa Nakajima** and colleagues[61],in **2022** a new approach to neural networks in their paper "The Neural Schrödinger Equation: A Law of Physics as a Deep Neural Network." They address the challenge of training deep neural networks (DNN) by introducing a new family of neural networks based on the Schrödinger equation (SE-NET). The problem they want to solve is the instability caused by exploding gradients when training deep SE-NET models. In order to solve this problem, they introduced a pure phase optimization method, which only updates the phase of the potential field in the Schrödinger equation, ensuring stable training of the deep SE-NET model while maintaining the uniformity of the system.
The approach they used involved implementing SE-NET on Pytorch using the Crank-Nicolson finite difference method. They demonstrated the deep dependence and stability of SE-NET using a modified National Institute of Standards and Technology (MNIST) database dataset. The results show that the performance of SE-NET improves with increasing width and depth, but the training is unstable due to gradient explosion. However, with the introduction of the pure stage optimization method, the deep SE-NET model also achieves stable training. They also compared the performance of SE-NET and ODE-NET and found that the performance of SE-NET was equivalent to standard ODE-NET but worse than enhanced ODE-NET. Datasets and models become very large.
In addition to solving immediate problems, the researchers also discuss future prospects for their work. They suggested that the performance of SE-NET could be improved by considering the 3D Schrödinger equation and implementing sparse solvers on GPUs. They also highlight the potential of this approach to jointly optimize physical structures and DNNs, as well as the possibility of offloading some digital processing to passive physical structures, thereby reducing energy consumption.

The researchers **Leon Gerard** and colleagues[62],in **2022** from the Johann Radon Institute for Computational and Applied Mathematics at the Austrian Academy of Sciences addressed the challenge of accurately solving the Schrödinger equation in computational chemistry. The Schrödinger equation is crucial for predicting properties of molecules and materials, but its high dimensionality and the need for extreme accuracy make it computationally challenging. Despite decades of research, existing methods struggle to achieve the desired accuracy, leading to a spread of results in energy calculations.
To tackle this issue, the researchers introduced a novel deep-learning architecture that combines deep learning with Monte Carlo methods. Their approach significantly reduced energy errors by 40-70% at 6 times lower computational cost compared to previous methods. By using their method, they established a new benchmark by calculating the most accurate variational ground state energies ever published for various atoms and molecules. The results showed substantial improvements in accuracy across different systems, outperforming existing variational methods, both deep-learning-based and classical ones.
Through systematic analysis, the researchers found that including too much physical prior knowledge in the architecture could actually hinder optimization and decrease accuracy. They highlighted the importance of balancing physical constraints and prior knowledge in achieving

accurate results. Despite the advancements made, challenges remain in terms of computational speed and accuracy for large molecules. Further research is needed to enhance the efficiency and effectiveness of deep-learning-based methods in computational chemistry.
The study demonstrates the potential of deep-learning-based methods as a new gold standard in computational chemistry, offering promising avenues for future research and applications in chemistry and biology. The results pave the way for new discoveries in drug development, material science, and other fields, with implications for advancing scientific knowledge and technological innovations.

The researchers **Kai-Fang Pu** and colleagues[63], in **2023** addressed the challenge of solving Schrodinger equations using physically constrained neural networks. They introduced a method that utilizes a monotonic neural network to represent the Cumulative Distribution Function (CDF) of the ground state wave function, allowing for efficient trial wave functions of Schrodinger equations. By minimizing the violation of the trial function to the Schrodinger equation, they achieved high accuracy in solving quantum many-body problems.
Their method involved using auto-differentiation and stochastic gradient descent to optimize the neural network's parameters, ensuring the trial wave function adhered to physical constraints. Through training on spatial coordinates and minimizing the violation of the wave function to the Schrodinger equation, they obtained ground state wave functions and energies with very low errors for classical quantum mechanical problems like the harmonic oscillator and Woods-Saxon potential.
The results showed that the DNN-based approach provided accurate solutions, with relative errors within 0.06% for the harmonic oscillator problem. The method demonstrated high fidelity in approximating the exact wave function, with performance improving with the number of variational parameters. However, challenges were observed with potentials exhibiting discontinuities, like the infinitely high potential well.
Future prospects include extending the method to solve more complex problems, such as many-nucleon systems, and improving the handling of potentials with discontinuities. The researchers highlighted the efficiency and data effectiveness of their approach, paving the way for advancements in solving nuclear many-body problems and offering a universal solution for problems with unknown exact solutions.

The researchers **Sherif Abdulkader Tawfik** and colleagues [64],in **2024** addressed the challenge of accurately predicting the total energy of materials with imperfections using a novel physics-informed machine learning framework called DIEP.
By integrating the external potential of a structure, DIEP improved the accuracy of predicting total energy per atom for various material imperfections, including diamond defects. The results showed that DIEP outperformed the existing M3GNET model in most cases, demonstrating its effectiveness in predicting the energy of deformed materials. Additionally, the study trained a potential energy surface (PES) model using DIEP, achieving a mean absolute error (MAE) of 61 meV/atom for total energy and 73 meV/ A for atomic forces.
The future prospects of this work include the potential for high-throughput screening in material

discovery processes and the application of DIEP in ab initio molecular dynamics simulations for further advancements in material science research.

In this journey, we aim to provide readers with a comprehensive understanding of deep learning's role in unraveling the mysteries of the quantum world. This review is envisioned as a bridge, connecting the power of deep learning with the complexities of quantum mechanics. By fostering a deeper exploration of this fascinating intersection, we hope to inspire further advancements and discoveries in both fields.

2.6 Advantages and disadvantages of deep learning in quantum mechanics

With the increasing interest in deep learning in quantum mechanics, it has become possible to use these techniques to solve the Schrödinger equation accurately and effectively. However, there are still challenges and weaknesses in using deep learning in this context.

2.6.1 Disadvantages

Among the disadvantages are:

- **Data Requirements:**

  Compared to conventional machine learning models, deep learning models for quantum mechanics require a large quantity of high-quality data and higher processing power[65, 66].

- **Complexity and Interpretability:**

  Unlike typical machine learning algorithms, deep learning models can be difficult for consumers to grasp because of their complicated interpretations and explanations of how they make decisions[65].

- **Bias and Legal Complexities:**

  Deep Learning algorithms have the danger of replicating or escalating preexisting biases in training data, which might produce biased outcomes. Furthermore, there may be legal issues associated with the use of intellectual property and private data in Deep Learning that should be carefully considered[65][66].

2.6.2 Advantages

Among the Advantages are:

- **Enhanced Performance:**

Improved performance in resolving deep-Q learning issues has been demonstrated by hybrid quantum neural networks with deep-Q learning, particularly on larger-scale maze problems[65].

- **Prediction of Chemical Properties:**

  Chemical characteristics may be directly predicted using deep learning algorithms in quantum mechanics, which is a major breakthrough in the discipline[67].

- **Quantum Features Utilization:**

  By utilizing quantum properties like entanglement and superposition, quantum machine learning gives quantum computers special powers[66, 68].

2.7 Conclusion

In this chapter, we tackled the approach of deep learning to solve the Schrödinger equation, illustrating how advanced neural network engineering can revolutionize solving this equation and coming to the conclusion that traditional methods may not offer the same efficiency and accuracy as deep learning when dealing with complex equations like the Schrödinger equation.We started by exploring the limitations and challenges we face when adopting classical and traditional methods in solving such equations, then delved into the role of deep learning in computational quantum mechanics.
Additionally, we analyzed the structures of advanced neural networks designed for quantum systems, and mentioned the latest modern deep learning methods for solving the Schrödinger equation.
Finally, we've highlighted the strengths and weaknesses in these methods.

In the next chapter, we will discuss all the implementation details and the preceding stages, as well as discussing the results obtained.

Chapter 3

Chapter 3

Implementation and Discussion of Results

3.1 Introduction

In this chapter, we applied the proposed approach to calculate the core energy of a physical system using the Schrodinger equation with deep learning and some machine learning techniques in order to highlight the efficiency of deep learning compared to traditional machine learning.
We started by setting up the working environment with programming tools and deep learning libraries, followed by importing and processing the data. Next, we prepared the data for CNN,CNN-LSTM,SVR,Random Forest and XGBoost networks, focusing on representing input data as a periodic table of elements. Then, we designed the architectures models for all networks, and we trained them to solve the Schrödinger equation.
Our principal task was to compare CNN,CNN-LSTM and on top of that, we trained SVR,Random Forest and XGBoost to study the stability of perovskite using the same dataset.The perovskites are a class of materials defined by a specific crystal structure, which is represented by the formula ABX_3.
Finally, we evaluated and analyzed the results obtained, discussed them, and made a comparison between the architectures.

3.2 Environnement

3.2.1 Libraries

During the work we used the following libraries that enabled us to effectively build, train, evaluate, and visualize deep learning models

1. **TensorFlow**

    - It serves as the basis for the construction and implementation of deep learning models. It provides low-level building blocks such as tensors (multidimensional arrays) and their manipulations.

- It offers various backends, including CPU and GPU, allowing efficient execution on different devices[1].

2. **Keras**

   - Built on top of TensorFlow, Keras simplifies the model building process.
   - Provides a high-level API with pre-built layers (like Conv2D, Dense) and activation functions (like relu) for constructing neural networks.
   - Makes the code more concise and readable compared to using TensorFlow directly[2].

3. **Pandas**

   Used for:

   - Loading data from CSV files in the code.
   - Cleaning and pre-processing the data (not explicitly shown in the code snippet).
   - This might involve handling missing values, scaling features, or transforming data into a format suitable for the model[3].

4. **Matplotlib**

   A versatile library for creating various plots and visualizations.
   Used in the code for:

   - Plotting the training loss and R2 score curves to monitor the model's learning process.
   - Visualizing the predicted values against the true values (delta_e) to assess the model's performance[4].

5. **Scikit-learn**

   - Simple and efficient tools for predictive data analysis
   - Accessible to everybody, and reusable in various contexts
   - Built on NumPy, SciPy, and matplotlib
   - Open source, commercially usable - BSD license[5].

[1] https://www.tensorflow.org/?hl=fr
[2] https://keras.io/
[3] https://pandas.pydata.org/
[4] https://matplotlib.org/
[5] https://scikit-learn.org/stable/

6. **NumPy**

   NumPy, short for Numerical Python, is a fundamental package for scientific computing in Python[6].

3.2.2 Configure the computing environment

The hardware environment used for this experiment is a Dell computer. It includes an Intel Core i7-7600U processor operating at a frequency of 2.80 GHz. This device has RAM with a capacity of 8.00 GB (7.64 GB usable). The operating system is Windows 10, a 64-bit architecture, with support for a screen that supports ten-point touch. The Google Colab service was also used in this experiment, as Google Colab offers a web-based integrated development environment in the cloud and provides the possibility of running and developing software using Python and the Jupyter Notebook operating environment for free.

3.3 Import & preprocessing data

3.3.1 Import and description of data

The Open Quantum Materials Database (OQMD) is a database containing density functional theory (DFT) calculated all properties of 1,226,781 materials[7]. This massive database was created by Chris Wolverton's research group at Northwestern University .

- The sheer scale of the database, with over 1.2 million materials computed using accurate density functional theory calculations, is truly remarkable. This vast dataset enables unprecedented opportunities for data-driven materials discovery and design.
- The inclusion of a wide range of computed properties, such as formation energies, densities, elastic constants, and more, makes the OQMD valuable for diverse applications, including thermodynamic modeling, mechanical property prediction, and structure-property relationships.
- The use of consistent computational methods across all entries ensures a high degree of reliability and comparability within the database, which is crucial for developing robust machine learning models and drawing meaningful conclusions from the data.
- The public availability of the OQMD and its integration with various materials science software packages have facilitated its widespread adoption and enabled researchers worldwide to leverage this powerful resource.

[6]https://numpy.org/
[7]https://oqmd.org/

- As the database continues to grow and incorporate more advanced computational methods, it will likely play an increasingly important role in accelerating the development of new materials and driving innovations in fields such as energy storage, catalysis, and advanced manufacturing[69, 70].

Overall, the OQMD represents a significant milestone in the transition towards data-driven materials science, enabling more rapid and efficient exploration of the vast materials space. The dataset is available on: `https://github.com/NU-CUCIS/ElemNet/tree/master/data/`.

3.4 Deep learning architectures

3.4.1 Data preparation for CNN and CNN-LSTM networks

The OQMD provided the dataset that was utilized. It offers thorough information on the characteristics of different materials and is a valuable source for materials science research. Along with electronic characteristics like band structures and electronic band gaps, it also contains formation energies, enthalpy of formation, Gibbs free energies, and other thermodynamic characteristics. The theory of functional density (DFT) is used to create the dataset appropriately, and validation against experimental observations ensures correctness and dependability[69]. After removing the rare-earth elements, the data set used in this work comprises 341450 compounds, of which 90% constitute the training set and 10% the test set. A pre-processing operation was carried out to represent the data in matrix form, equivalent to a periodic table of 86 elements figure3.1. The periodic table is used to determine the location of each element in the matrix, thereby capturing the structure and arrangement of the elements. This representation derives its significance from the element's position in the table and in the compound, as well as its proportional contribution in the compound. A matrix representing the presence and quantity of chemical elements in each chemical compound of the training data set is produced. The chemical composition data can now be transformed into a matrix suitable for model analysis and learning. Next, a certain transformation is applied to the resulting matrices, as shown in Figure 3.1. With this transformation, the values of the elements in the matrices are modified so that empty cases and grey-colored cases take on the value 0, while the rest of the cases take on -1, with the exception of the elements that form the compound, for example in the compound BeScLu2 (Be=Sc=0.25,Lu=0.5), so that the sum of the cases is zero. In fact, there are 86-3=83 elements: 83*(-1)+0.25*83+0.25*83+0.5*83=0 . This can facilitate data normalization and increase the stability of subsequent calculations[71]. This data pre-processing concerns both the training and testing of the two CNN and CNN-LSTM models.

3.4.2 Input data representation as periodic table of elements

The dataset comprises of chemicals with varying stoichiometries organized in a one-dimensional array. This has been pre-processed into a two-dimensional matrix so that our models may utilize it as input.The table in Fig 3.1 has 86 components, which means that there might be

both ternary and quaternary compound in it. The input dataset in reference[72] has been modified by filling the table with the value -1, with the exception of the positions of the compound elements, which are assigned numerical values corresponding to their fractions of the compound. The contents of all cases in the table will sum to zero.

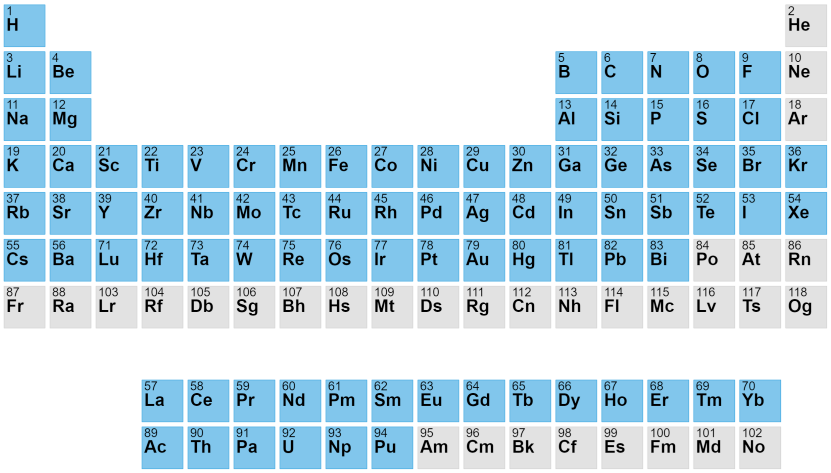

Figure 3.1: Elements included in the dataset in blue according to the compound

3.4.3 Stability trends in perovskites

The stability of perovskites is determined by the minimum of energy. For that, we trained SVR, Random Forest, and XGBoost, and the results are illustrated in the figure 3.2.For position A, elements like Li, Rb, and Cs are the most favorable, with stability decreasing for other elements. Non-metals, transition metals, and light elements form very few stable systems in this position. On the other hand, position B prefers light elements such as B and W. Interestingly, Au and Ru can also stabilize perovskites when placed in this position.

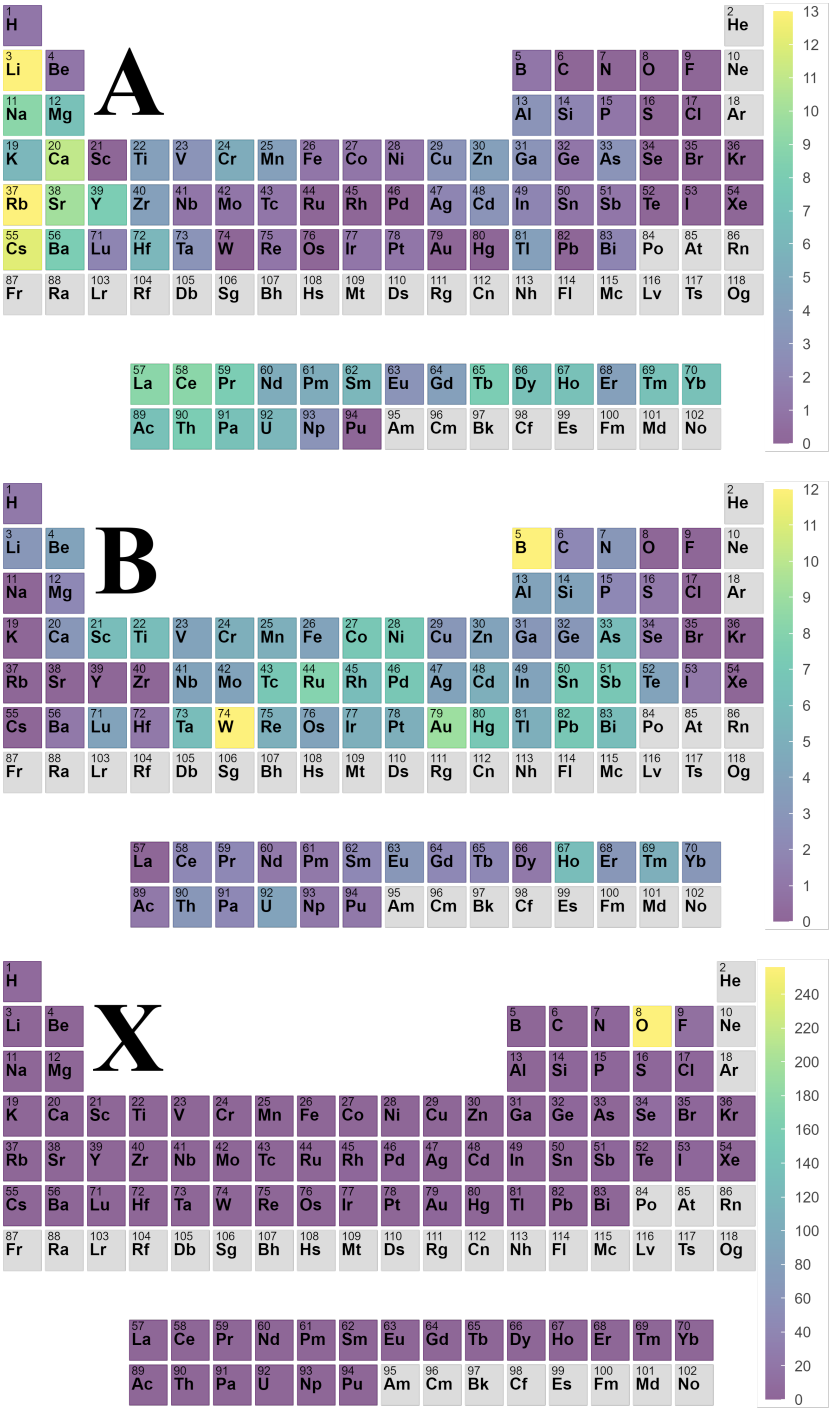

Figure 3.2: Periodic Tables showing the stable structures for possible element A, B and X

3.4.4 Architecture CNN and CNN-LSTM model

Convolutional neural networks (CNN) are one of the most effective models for processing and analyzing visual data, excelling in multiple applications such as image classification and pattern recognition. These networks extract spatial features from the input data through Convolution and filtering layers.

On the other hand, convolutional neural networks integrated with long-and short-term memory modules (CNN-LSTM) combine the ability to extract spatial features of convolutional neural

networks (CNN) and the ability to learn from the temporal dependencies of iterative neural networks (RNN) and especially long-and short-term memory modules (LSTM). This integration makes CNN-LSTM a powerful tool for analyzing sequential data with spatial and temporal dimensions, such as videos and time series of sensory data.

Below, we will give a detailed description of the architecture of the two models adopted in this work:

1. **Architecture CNN model**

   We created a CNN network architecture with aggregation layers and connected layers to reduce dimensions and extract spatial features from the data.

   The following is a description of a Convolutional Neural Network (CNN) architecture implemented using the. `TensorFlow` and `Keras` libraries.

   - **Layer-by-Layer Description**
     - **Input Layer**:
       - *Input Shape*: $(9, 18, 1)$
     - **Convolutional Layer 1**:
       - *Number of Filters*: 32
       - *Filter Size*: 3×3
       - *Padding*: Same
       - *Activation Function*: ReLU
     - **Zero Padding Layer**:
       - *Padding*: 1
     - **Dropout Layer**:
       - *Dropout Rate*: 0.1
     - **Convolutional Layer 2**:
       - *Number of Filters*: 32
       - *Filter Size*: 5×5
       - *Activation Function*: ReLU
     - **Convolutional Layer 3**:
       - *Number of Filters*: 32
       - *Filter Size*: 3×3
       - *Activation Function*: ReLU
     - **Flatten Layer**:
       - This layer flattens the input, converting the 2D matrix into a 1D vector.

- **Dense Layer 1**:
  - *Units*: 192
  - *Activation Function*: ReLU
- **Output Layer**:
  - *Units*: 1

- **Summary** The described CNN architecture is designed for a regression task, with an input shape of $(9, 18, 1)$. It consists of three convolutional layers, followed by a zero padding layer and a dropout layer to prevent overfitting. The network includes two dense layers, with the final layer producing a single output,as in the figure 3.3.

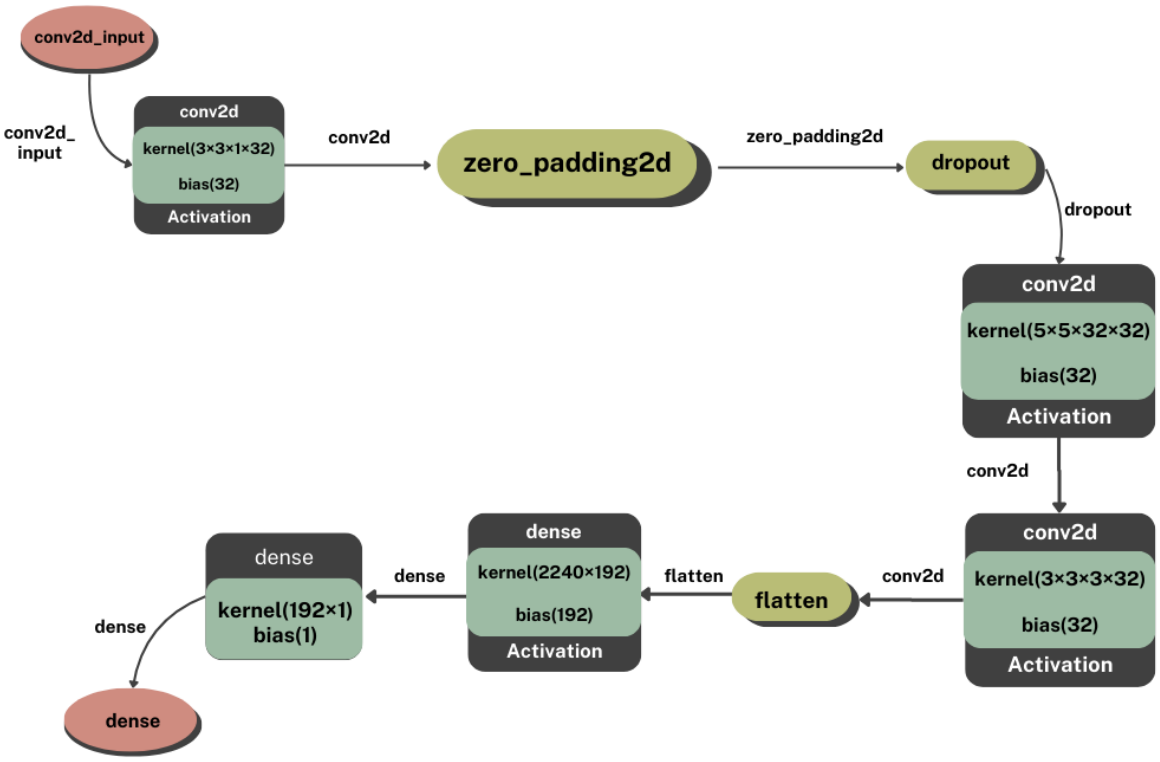

Figure 3.3: CNN architecture

2. **Architecture CNN−LSTM model** We integrated CNN networks with LSTM networks to create a CNN-LSTM network architecture.

- **Layer-by-Layer Description**
  - **Input Layer**:
    - *Input Shape*: $(9, 18, 1)$
  - **Convolutional Layer 1**:
    - *Number of Filters*: 32

    - *Filter Size*: 3×3
    - *Padding*: Same
    - *Activation Function*: ReLU
  - **Zero Padding Layer**:
    - *Padding*: 1
  - **Dropout Layer**:
    - *Dropout Rate*: 0.1
  - **Convolutional Layer 2**:
    - *Number of Filters*: 32
    - *Filter Size*: 5×5
    - *Activation Function*: ReLU
  - **Convolutional Layer 3**:
    - *Number of Filters*: 32
    - *Filter Size*: 3×3
    - *Activation Function*: ReLU
  - **Reshape Layer**:
    - Reshapes the output to a 2D tensor with shape $(-1, 5 \times 14 \times 32)$.
  - **LSTM Layer 1**:
    - *Units*: 256
    - *Activation Function*: ReLU
    - *Return Sequences*: True
  - **LSTM Layer 2**:
    - *Units*: 64
    - *Activation Function*: ReLU
  - **Dense Layer 1**:
    - *Units*: 192
    - *Activation Function*: ReLU
  - **Output Layer**:
    - *Units*: 1

- **Summary** The described CNN-LSTM architecture is designed to handle sequences of spatial data. The network starts with three convolutional layers to extract spatial features, followed by a reshape layer to prepare the data for sequential processing.It includes two LSTM layers to capture temporal dependencies and ends with two dense layers for the final regression output,as in the figure 3.4.

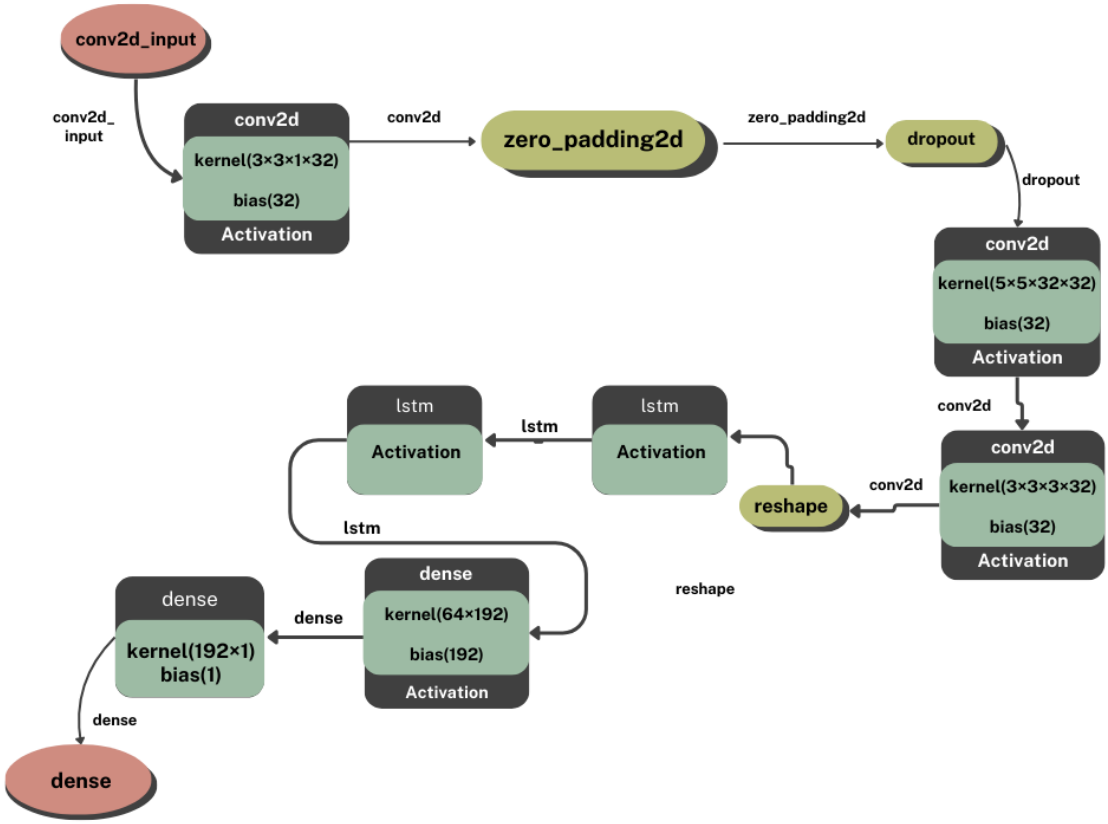

Figure 3.4: CNN-LSTM architecture

3.5 Training CNN and CNN−LSTM models

To train the convolutional neural network model (CNN) and (CNN-LSTM),we used the pre-defined training data ($\mathbf{X}_{\text{train}}, \mathbf{Y}_{\text{train}}$)to train the model for a specified number of epochs.

```
csv_logger = CSVLogger("/content/drive/MyDrive/RES/training_history.csv", append=False)
history = model.fit(X_train, Y_train, epochs=100,validation_data=(X_test, Y_test),callbacks=[csv_logger])
```

Figure 3.5: CNN and CNN−LSTM training

This code in figure 3.5,effectively trains the CNN model by leveraging the training data, incorporating validation for generalization, and logging the training history for later analysis. This structured approach ensures a robust and well-monitored training process.

3.6 Different machine learning algorithms

3.6.1 SVR

Periodic element atomic radii can be predicted by support vector regression (SVR). With a correlation between the experimental and predicted values of over 99 %, a study using SVR to reliably estimate the atomic radii of periodic elements was published in the journal Computational Materials Science[73].

3.6.2 Random forest

The periodic table's elements have been effectively categorized and arranged using random forest algorithms according to their chemical and physical characteristics. To create the predictive models, the random forest models make use of a range of atomic-level characteristics and attributes, such as atomic number, electronic configuration, and other chemical physical descriptors. To get high prediction accuracy with random forest models, hyperparameter tuning such as maximizing the number of trees, leaf nodes, and feature sampling ratios is crucial[74, 75, 72].

3.6.3 XGBoost

The XGBoost architecture's weighted quantile sketch methods, out-of-core processing, and capacity to handle sparse data are particularly pertinent qualities when examining its application to the periodic table. Because of the way it is designed, XGBoost can effectively manage instance weights in approximation tree learning, which makes it appropriate for situations where the data may be weighted or sparse[76].

3.7 Analysis and discussion of the results

We trained two models to compute formation energy, a crucial parameter in forecasting compounds stability, in order to show the suitability of convolutional neural networks for predicting the physical characteristics of materials. The learning curves for the models in terms of accuracy and loss are shown in figure 3.6 .The outcomes demonstrate the good performance of both models, with CNN-LSTM showing a little advantage. In actuality, the former obtained an accuracy of 0.9827, while the latter obtained 0.9807.

The formation energy estimates for CNN and CNN-LSTM, respectively, are revealed by the trained models with an error of 0.0070 ev/atom and 0.0063 ev/atom respectively. The histograms of the real values of the energies compared to the predicted values for the two models are finally displayed in figure 3.7.

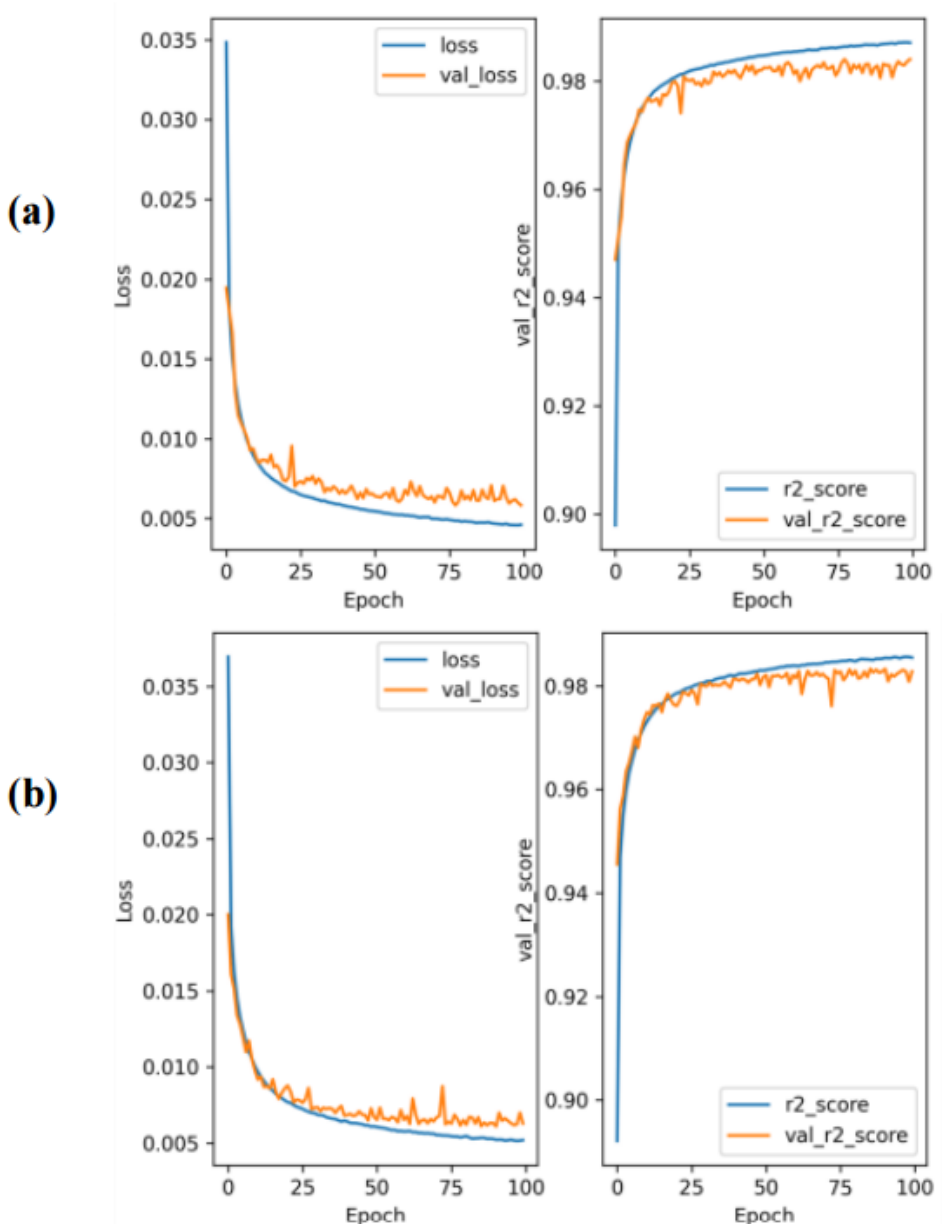

Figure 3.6: Learning curves of the 2 models. (a) CNN. (b) CNN-LSTM

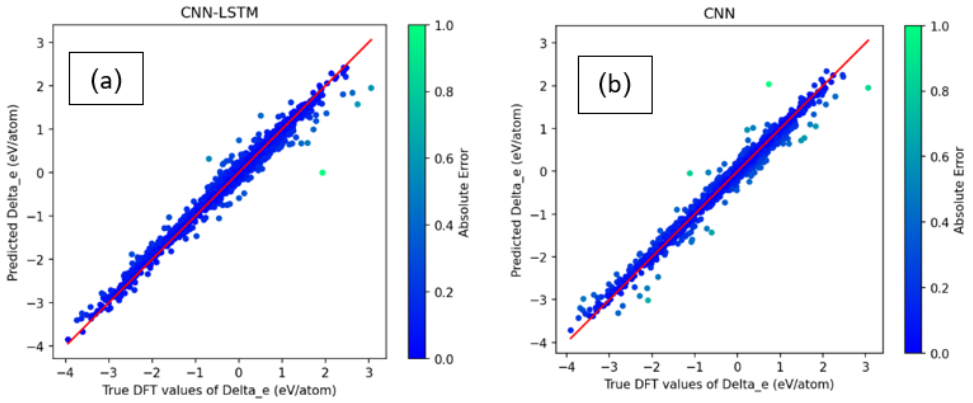

Figure 3.7: Histogram of actual versus predicted energy values. (a) CNN. (b) CNN-LSTM

From figure 3.6, we can note the following:

- during training, both the CNN and CNN-LSTM models show a downward trend in the loss function, indicating that the models learn and improve over time.
- validation loss curves closely follow training loss curves, indicating that both models generalize well to unseen data.
- the curves r2_score (determination coefficient) and val_r2_score (validation r2_score) show an increasing trend, approaching values close to 1, which indicates a good agreement between the expected and real values.

From figure 3.7, we can make the following observations:

- the CNN-list model (left diagram) shows a tighter correlation between the expected and real DFT values of delta_E .
- the CNN model (the right graphic) shows a slightly more scattered distribution of data points, which indicates a higher degree of deviation from the true DFT values.
- the CNN-LSTM model appears to have a smaller absolute error range (Y-axis) compared to the CNN model, indicating better predictive accuracy.

Overall, the CNN-LSTM model seems to outperform the CNN model in predicting the DFT values of the delta_E for the given test dataset. The LSTM component of the CNN-LSTM model is likely to capture temporal dependencies and long-term correlations in the data more effectively, improving predictive performance.

The trained machine learning models reveal formation energy values with n-estimators= 20 and an error of 0.20 ev/atom for SVR and 0.03 for Random forest and error of 0.29 ev/atom for XGBoost. figure 3.8 shows the Histogram of the true vs the predicted values of energies (a)SVR. (b)RF. (c)XGBoost. for the two models.

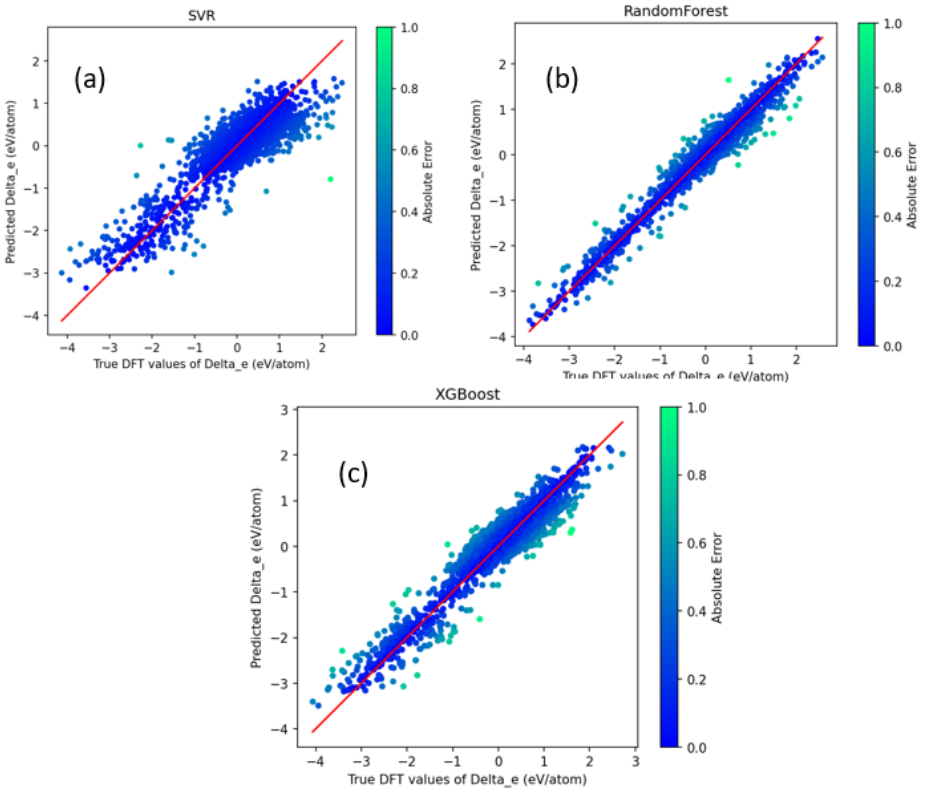

Figure 3.8: Histogram of the true vs the predicted values of energies (a)SVR. (b)RF. (c)XGBoost

3.7.1 Comparisons between Architectures

Figure 3.9 shows a comparative study of the SVR, RF, XGBoost, CNN and CNN-LSTM models, trained on different representations of the input data, with reference to the real OQMD dataset data, which is the formation energy calculated by the DFT. Performance rankings in ascending order were as follows: SVR, XGBoost, RF, CNN and CNN-LSTM.

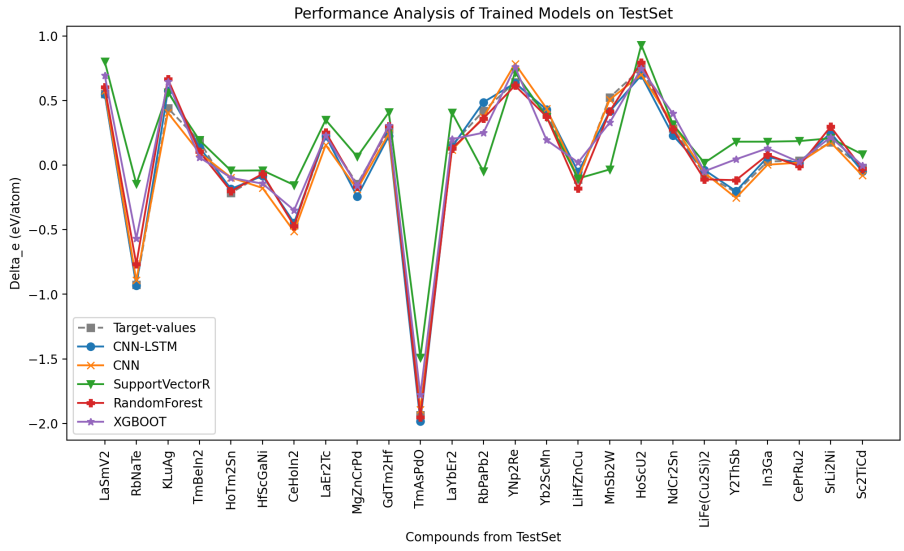

Figure 3.9: Comparison of the performance of the model with respect to the target values

The SVR model, while being a powerful tool for many machine learning tasks, showed the lowest performance in this particular study. This could be due to the high-dimensionality of the data or the presence of non-linear relationships that are not well captured by SVR. The XGBoost and RF models performed better than SVR, demonstrating their ability to handle complex datasets with a mix of numerical and categorical features. However, they were outperformed by the deep learning models, CNN and CNN-LSTM. The CNN model, designed to process grid-like data such as images, showed superior performance, indicating its effectiveness in capturing local dependencies in the data. The CNN-LSTM model, which combines the strengths of CNNs and LSTMs to process sequential data, achieved the highest performance. This suggests that the temporal dependencies in the data were significant and well-captured by the CNN-LSTM model.

3.8 Conclusion

In this chapter, we have implemented the proposed method for determining the fundamental energy of a physical system using the Schrodinger equation through deep learning and some machine learning techniques for comparison. After preparing the environment, construction, and training, we discussed the results in detail.
The results show the effectiveness of using deep learning instead of traditional machine learning techniques to solve the Schrodinger equation. While CNN and CNN-LSTM provide reasonably accurate predictions compared to other machine learning algorithms SVR, RF and XGBoost. This comparative analysis sheds light on the potential of deep learning and encourages further investigation of its promotion and application in similar areas.

General Conclusion

General Conclusion

Our thesis focuses on the use of deep learning to solve the Schrödinger equation and prove its efficiency in solving by making a comparison between it and traditional machine learning techniques.

We first looked into the principles of this equation and its basic concepts, then discussed the challenges facing traditional methods and how deep learning can offer effective solutions.
After that, we applied the deep learning approach to calculate the fundamental energy of a physical system, where we prepared the working environment, processed the data, designed the neural network models (CNN),(CNN-LSTM),(SVR),(RF) and (XGBoost), Then train them, evaluate the results and make a comparison.

The results showed that deep learning can be effective in solving the Schrodinger equation, hitting high accuracy with an error margin of around 0.0063 ev/atom,opening up new horizons for improving and developing models.

To move forward, we aim to build a new framework for predicting the bandgap and the energy. This requires developing more complex models to handle multidimensional data, enhancing prediction accuracy, understanding the physical properties of quantum systems, and opening the door to new scientific and technological discoveries.

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بصفتي رئيس والمسؤول عن تصحيح مذكرة تخرج ماستر الموسومة بـــــــ

.....

A deep learning approach to solve the Schrodinger equation

.....

من انجاز

الطالب(ة): .....Fatima Zohra BENSALEMـ

والطالب(ة): .....Kheira LAIOURATE

الكلية: العلوم والتكنولوجيا.

القسم: الرياضيات والاعلام الالي.

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التخصص: الأنظمة الذكية لاستخراج المعارف.

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أشهد ان الطالب (الطلبة) قد قـام (قـاموا) بالتعـديلات والتصـحيحات المطلوبـة من طـرف لجنـة المناقشة وان المطابقة بين النسخة الورقية والالكترونية استوفت جميع شروطها.

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