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Faculty of Graduate Studies

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Thermal and Magnetic Properties of Exciton in TMD_WS$_2$, WSe$_2$ Monolayer

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201920346

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Dissertation Approval

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Declaration

I declare that, except where explicit reference is made to the contribution of others, this dissertation is substantially my own work and has not been submitted for any other degree at the Arab American University or any other institution.

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Dedication

To My Parents, husband and children.

Reham Reda Yousef Kmail

Acknowledgments

And said, "My Lord, enable me to be grateful for your favor which you have bestowed upon my parents and to do righteousness of which you approve, and admit me by your mercy in to the rank of your good righteous servant".

All thanks go to my god who give me the ability to finish this thesis and Peace and blessings be upon our Prophet Muhammad

I send all thanks for the righteous and mercy heart, to the candle that shine my heart, to the sun that he was like a light for my life and to the mountains of my ideas, to my lovely father.

To the tree in my heart that I bend over in it, to the chrysanthemum flower and the green wheat field, to my spring and my flowers my lovely mother.

Words like racing to make a necklace that no one deserves but you. To you, who worked hard without expecting praise. To you, the best and most special thanks. O you who soar in my sky, like the stars always, never disappearing, we wait for the lightness of your shadow and I feel happy when you shine in my sky every hour, your name deserves to be at the top, for my dear husband Mahmoud.

To my language, to my words that sailings by his support, to my brother Jehad, who gave me power, success and inspiration of my heart.

To whom that build my glory, to the basis of my glory and spikes of happiness of my life, to those who were my sun that shines my darkness, my brothers and sisters.

To the messengers of education, to the lamps of the way of life, to the instructors teachers Prof. Dr. Mohammad Elsaid and Prof. Dr. Muayad Abu Saa .

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To all people who help me for completing this thesis.

Finally, on behalf of myself, thanks for any person believe in rightness and try for the sake of education and life, and for any one call the brotherhood, to Palestine (the name, the identity), to all people I love and I feel that I am one of them and they feel the same.

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Abstract

In this thesis, an exciton present in a sheet of TMD material (WS_2 and WSe_2) was highlighted to conduct studies covering different properties. We solved the Schrödinger equation by shifted 1/N expansion method to obtain the eigen energy for the exciton present in the TMD material.

We talked about energy spectra, as we clarified the energy state values that were obtained mathematically using the 1/N-shift expansion method and compared them with other energy state values that were obtained numerically. After that, we highlighted the ground state energy (average energy) as a function of temperature at different values of the magnetic field (between 0 to 94T for WSe_2 and 0 to 60.16 for WS_2). The thermal and magnetic properties of the exciton contained in a sheet of TMD material were studied based on different values of the magnetic field at different temperatures. Starting with the thermal properties, we talked about the heat capacity, and entropy. In addition, we have displayed the dependence of magnetization and magnetic susceptibility of exciton in QD with various physical parameters (B, T). In addition to the physical description of the effect of each system parameter on the energy spectra, we calculated the density of state of the system. Thermomagnetic properties were also studied under the name Magneto Caloric Effect (MCE) of an exciton found in TMD Material, which represents the difference in randomness (entropy) of the system at two different values of a magnetic field affecting this system. The latest study conducted in this thesis, relates to the magnetism of an exciton found within the TMD material. By knowing the ability of these materials to respond to the applied magnetic field, this was done through studying the so-called diamagnetic shift (σ). Better yet, the results we obtained through 1/N expansion method were matched with results in other important previous studies on the theoretical and experimental levels.

Keywords: Quantum dot · Exciton · 1/N expansion · TMD material · WSe_2·

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List of Definitions of Abbreviations

Abbreviations	Title
TMD	Transition Metal Chalcogenide
DOS	Density of states
QW	Quantum well
$3D$	Three-dimension
$2D$	Two-dimension
$1D$	One-dimensional
$0D$	Zero-dimension
QD	Quantum Dot
M	Magnetization
χ	Magnetic susceptibility
n	Principal quantum number
V_K	Keldysh potential
H_0	zero-order Struve function
Y_0	zero-order Bessel function
m_l	Angular quantum number
r_0	Screening length
B	Magnetic field
ε_0	Vacuum permittivity
k	Average dielectric constant
α	Parameter for characterizing potential
a_0^*	Effective Bohr radius
m^*	Effective mass
m_0	Free electron mass
$\hbar$	Reduced Plank constant
e	Electron charge

ω	Frequency parameter
C_v	Heat capacity
T	Temperature
K_B	Boltzmann constant
E_j	Total energy of the system
S	Entropy
MCE	Magneto-Caloric Effect
Σ	Diamagnetic coefficient
	Partition function
Γ	Broadening factor

Chapter One: Introduction

1.1 Nanotechnology

In the world of speed and accuracy in which we live, there has become an urgent need for the advancement of technological developments to become faster, smaller and more accurate. Therefore, nanoscience has become important for scientific research to study the different properties and characteristics of different types of materials. [1]

Nanotechnology is science, engineering, and technology that is done at the nanoscale. Nanotechnology is the study and application of things that are very small and can be used in all other fields of science, such as chemistry, biology, physics, materials science, and engineering. [2]

Nanotechnology is the use of matter at small, molecular and supramolecular atomic scales for industrial and applied purposes. The first technological goal of nanotechnology is to process atoms with great precision in order to manufacture industrial products with high accuracy. [2] It is also defined as a processing of a material with at least one dimension in a very small size ranging from 1 to 100 nanometers (nm). This definition reflects the fact that the scale, dimensions, and volume of matter are important in quantum mechanical effects.

Thus, we can say that the definition has shifted from a technological goal to a research goal that includes all types of research and techniques that deal with the general properties of matter.

It is therefore common to see the nanotechnology formula used in a wide range of research and applications for which the common feature is size. [3]

It can be said that nanotechnology (defined by size) is naturally broad, as it presents in various fields of science such as surface science, organic chemistry, molecular biology, semiconductor physics, energy storage, engineering, precision manufacturing and molecular engineering. [4,5,6,7]

In addition, there is a great diversity of research and applications associated with this name. It is necessary to talk about the future effects of nanotechnology, which scientists have begun to address and study. It can be said that it is a double-edged sword in terms of being able to create many new materials and devices with a wide range of applications, such as nanomedicine, nanoelectronics, and energy production materials from Vital, consumer products. On the other hand, nanotechnology raises many concerns in terms of the environmental impact of nanomaterials, and its potential impacts on the global economy. [8]

1.2 Exciton– Definition and Types

An exciton is a result of attraction that occurs between an electron and a hole by the electrostatic Coulomb force. It is an electrically neutral quasiparticle found in insulators, semiconductors, and some liquids. An exciton is an elementary excitation of matter through which energy can be transferred without the net transfer of electric charge. [5]

An exciton can form when a particular material absorbs a photon of energy higher than its bandgap. This leads to excitation of an electron from the valence band to the conduction band. Where the electron leaves its place as a positively charged electron hole (ie the place from which the electron moves becomes completely empty). The electron in the conduction band becomes less attracted to this localized hole due to the repulsive Coulomb forces from the large number of electrons surrounding the hole and the excited electron. These repulsive forces provide a stable energy balance. Thus, the exciton has a slightly lower energy than the unbound electron and hole. [10]

Basically, when an electron and a positive hole (an empty electron particle in the valence band) combine and are able to move freely through a non-metallic crystal as a unit, the combination of these two particles is called an exciton. It should be noted that the electron and the positive hole carry opposite charges. Thus, they cancel each other's charges, and there is no electric charge in an exciton because of this feature. Excitons have different properties, and are generally categorized into three types: [11]

1. Frenkel exciton

The Frenkel exciton has a relatively small dielectric constant, and its energy is in the range of 0.1 to 1 eV. The reason it has this is because the Coulomb interaction between the hole and the electron is strong and therefore, it has a lower dielectric constant. Frenkel excitons are found in crystals in general and in particular in organic molecular crystals such as anthracene and tetracene. [12]

2. Wannier - Mott Exciton

The dielectric constant is generally large in semiconductors; The binding energy is very low, generally on the order of 0.01 eV. The reason for this is that the Coulomb interaction between the hole and the electron is relatively weak. These excitons are commonly found in semiconductor crystals and liquids such as xenon. [13] It can be said that there is a special third type which is:

3. Charge Transfer exciton

When the electron and hole are present in neighboring molecules this state is classified as an intermediate state between a Frenkel and a Wannier exciton, and this state has been named as a charge transfer (CT) exciton. They usually occur in molecular and organic crystals. [13]

Excitons play an important key role in transition metal chalcogenide (TMD) monolayers, which is a good and recent example to be discussed later. In particular, excitons in these systems exhibit ambient energy on the order of 0.5 eV with the Coulomb attraction between hole and electrons stronger than in other conventional quantum wells. As a result, photoexcitation peaks are present in these materials even at room temperatures. [14]

1.3 Quantum Confinement

Nanomaterials can be defined as materials that possess, at least, one outer dimension. Nanomaterials are obtained naturally, or created as by-products from combustion reactions, or custom-produced through engineering to perform a specific function. These materials may have different physical and chemical properties than their counterparts [15].

Quantum Confinement is the spatial confinement of electron-hole pairs (excitons) in one or more dimensions within a material and also electronic energy levels are discrete [16].

Nanomaterials are classified based on the number of dimensions in which an electron can move freely without being confinement in the material as the following [16]:

Bulk material, where the electron moves freely in all dimensions (3D). Quantum well material (QW), when electrons move freely in two dimensions but are confined in the third dimension (2D). Quantum Wire material (QW), electrons can move inside the material freely in one dimension, while motion is quantized in the other 2-dimensions (1D). Quantum dot material (QD), the electron cannot move freely and is confined in all three dimensions.

The energy spectra and density of state (DOS) is defined as the number of electron states per unit volume per unit energy. are greatly affected because we can control the direction of the electron movement as shown in Figure (1.1):

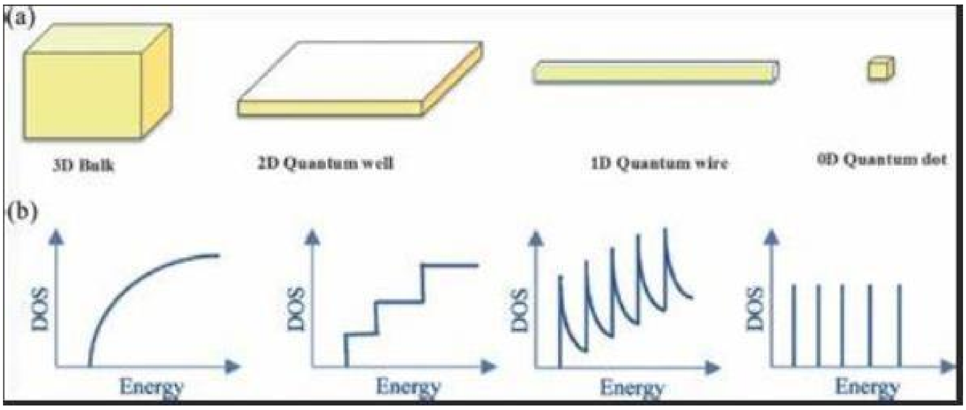

Figure (1.1): Density of states as function of energy for bulk material, quantum well, quantum wire and quantum dot [17]

In QDs, electrons are confined in three dimensions by artificial confining potentials, Where the number of electrons can be controlled by conventional nanofabrication methods, for example in atoms, this is done by ionization, but in QDs it is done by changing the confinement potential [18]

We can control the bandgap of QDs by its size. So we can engineer their Optical and electrical properties. The smallest QDs have large band gaps such as shown in figure (1.2) [19]:

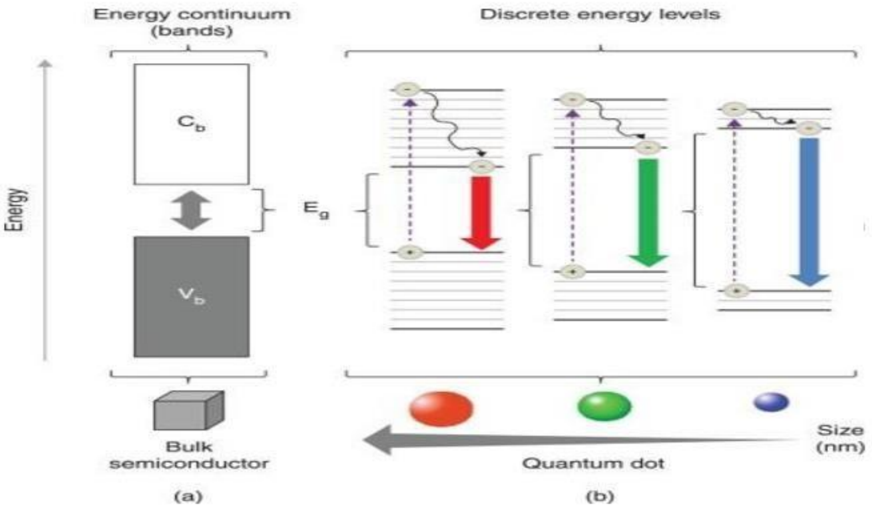

Figure (1.2): The relation between band gap and size in QDs [20]

1.4 Quantum Dots (QDs)

Nanoscience is an interesting field in all fields of research. To support this science in line with the development of modern technology, it is now possible to produce zero dimensional (0d) systems called quantum dots (QDs). Quantum dots (QDs) are important examples of ultra-small systems that areas of electronics and optoelectronics where electrons are trapped in all three dimensions [21].

(QDs) are semiconductor particles that are very small (a few nanometers) in size, and have optical and electronic properties that differ from those of larger particles as a result of quantum confinement. These materials are a central topic in nanotechnology and materials science [21].

QDs with semiconductor nanostructures have become a very hot research topic due to their enormous potential applications in various devices such as: QD lasers, quantum computation, QD solar cell, in addition to biological and medical applications such as photo cancer treatment [22].

The electronic properties of quantum dots are closely dependent on their shape, size, and composition, which makes them highly tunable, as the size distribution of QDs can be controlled during fabrication. For example, the band gap of a QDs, which determines the frequency range of the emitted light, is inversely related to its size [23].

QDs are a topic of research due to their many important applications in various fields, from luminescence, photonic applications, and their use in quantum computing and biological applications. QDs are used for all kinds of applications where controlling colored light is important. The easily tunable bandgap allows QDs to emit relatively pure and saturated monochromatic light. A thin filter made of QDs has been fabricated to be placed over a fluorescent lamp or an LED lamp so as to increase the red emission [24].

1.5 Transition Metal Di-chalcogenides (TMD)

Transition metal chalcogenide dimers (TMD or TMDC) monolayers are an atomically thin MX_2-type semiconductor, with M a transition metal atom (Mo, W, etc.) and X a chalcogen atom (S, Se, or Te). One layer of M atoms sandwiched between two layers of X atoms. They are part of a large family of so-called two-dimensional materials [25].

The main advantage of these materials is the ability of large atoms to interact in the two-dimensional structure, for example, WTe_2 exhibits an anomalous giant magnetoresistance and superconductivity [25].

TMD bulk crystals are formed from monolayers held together by van-der-Waals attraction. TMD monolayers have a set of properties, which are described as follows: TMD: MoS_2, WS_2, $MoSe_2$, WSe_2 and $MoTe_2$ monolayers have a direct bandgap, and can be used in electronics as transistors and in optics as emitters and detectors. [26,27].

The TMD monolayer crystal structure does not have an inversion center, which allows reaching a new degree of freedom of charge carriers and opening up a new field of physics: [28,29]

The strong spin–orbit coupling in TMD monolayers leads to a [30] spin–orbit split of hundreds of meV in the valence band and a few meV in the conduction band, allowing electron spin to be controlled by tuning the photon energy of the excitation laser and by hand [31].

The two-dimensional nature and high spin-orbit coupling in TMD layers can be used as important materials for electronic applications [32].

Work on and use of TMD monolayers is an important research and development area in potential applications in electronics. TMDs are combined with 2D materials such as graphene and hexagonal boron nitride to make van der Waals heterostructures. This is to work on optimizing these heterogeneous structures for use as building blocks for many different devices such as transistors, solar cells, LEDs, photodetectors, fuel cells, photocatalysts, and sensors. We need to use these devices in our daily lives so that they become smaller, cheaper and more efficient by using single layers [33,34].

1.6 Problem Statement

The recent development and rapid advances in the various technologies surrounding us have led to the aspiration to use materials with high efficiency and unique properties, prompting researchers to develop new materials with improved strength.

Transition Metal Di-chalcogenides (TMD). Is a two-dimensional semiconductor material that has distinct electrical, mechanical and optical properties. TMD are a large family of layered materials, many of which exhibit tunable bandgaps and thus enable standard semiconductor fabrication techniques to be used, and thus be utilized in many different fields. [41,42].

This thesis aims to study the structural, magnetic and thermal properties of the exciton system in the TMD material distributed in the following steps:

The first step, required to solve the Schrödinger equation by shifted 1/N expansion method in order to obtain the eigen energy of the exciton in TMD materials in different range of magnetic field strength.

The second step, calculate the partition function (Z), through which all the required characteristics. The magnetic properties like magnetization (M) and magnetic susceptibility (χ) will be studied as function of the physical parameters, in order to complete the magnetic picture, we calculated the diamagnetic shift (σ).

Followed by the third step of calculating the thermal properties like heat capacity ($\boldsymbol{C_v}$) and entropy (S). Thermomagnetic properties were also studied under the name Magneto Caloric Effect (MCE) of an exciton found in TMD Material.

In order for this work to be complete, we will not forget to talk about the density of energy levels, as will be presented later for a system of excitons in TMD materials.

The thesis will follow the sequence which starts with chapter one which displays the introduction taking into account the general features and characteristics of the exciton. Chapter two which displays the literature review. In chapter three, we will explain the basic principle and theoretical background that will guide this study. In chapter four, the results are reported and discussed. Chapter five is the final chapter, where it deals with the summary of this study.

Chapter Two: Literature Review

The study of exciton in transition metal chalcogenide (TMD) monolayers has attracted much attention in recent years, because of the fact that their presence can dramatically affect the performance of semiconductor devices and their electrical, optical and transport properties.

The scientist J Li [1], Y L Zhong, Dong Zhang studied the theory of an exciton consisting of two Dirac massive particles in a monolayer and a double layer of transition metal chalcogenides, in addition to two layers separated by an insulating layer. In low energy limits, in order to obtain the following: separation of the center of mass and relative motion, analytical solutions of the exciton wave function and energy dispersion including the Coulomb interaction between electron and hole, the Bohr exciton radius, and the binding energy and effective mass in monomeric transition metal chalcogenides. Season. In the case of two monolayers separated by a dielectric layer, we find that the effective mass of the exciton can be continuously tuned by separating the interlayer. [35]

The 2D chalcogenide transition metal semiconductors, such as MoS_2, WSe_2, etc., possess very strong properties where they exhibit strong light-matter coupling and possess direct bandgaps in the infrared and visible spectral regimes, which makes them interesting candidates for various applications in optics and Optoelectronics. Here, we review their optical and optoelectronic properties with a focus on exciton physics and devices. Since excitons are tightly bound in these materials and dominate the photoresponse even at room temperature, their properties are investigated in depth, and an overview of progress in applications of optoelectronic devices, such as photoelectronic light emitters, photovoltaic solar cells, and detectors, is also presented. photonics, and opto-optics devices, considering the prominent role of excitonal effects by Thomas Mueller and Ermin Malic. [36]

Because of their strong interaction with optical matter and rich photophysics, twodimensional (2D) transition metal chalcogenides are important candidates for novel photonic devices and phalltronic spin devices [37]. Therefore, scientists Zhonghui Nie, Yongliang Shi, Shuchao Qin, Yuhan Wang and others have used them in order to control the photo-carrier behaviors of single-layer TMD devices to suit the needs of device functionality. Here, by interfacial engineering, that is, by deposition of monolayer MoSe2 on different oxide substrates (SiO_2, Al_2O_3 and HfO_2), we revealed a significant tuning of the exciton relaxation times in monolayer TMDs. Remarkably, the nonradiative recombination of MoSe2 was shortened by almost one order of magnitude, from 160 ± 10 ps (on SiO_2) to 20 ± 4 ps (on HfO_2). Theoretical simulations based on the ab initio non-adiabatic molecular method (NAMD), combined with temperaturedependent photoelectron spectroscopy, identify electron-phonon (e-ph) coupling as the leading mechanism for lifetime tuning. Our results establish interface engineering as an effective parameter for manipulating the excited state dynamics of monolayer TMDs [38].

Transition metal chalcogenides (TMD) have emerged as an ideal material platform for exploring the phenomenon of exciton transfer in the works of Ermin Malic, Raül Perea-Causin, Roberto Rosati, Daniel Erkensten and Samuel Brem. [39]

The wafer-scale supra-axial growth of semiconducting transition metal chalcogenide monolayers such as MoS_2 , WS_2 and WSe_2 , which is of great interest for device applications to circumvent the size limitations associated with the use of exfoliated flakes, has been discussed. Epitaxy is required to achieve single crystal films over large areas via fusion of TMD domains with the same crystal orientation by Joan Redwing. [40]

Elsaid had used 1/N expansion method to calculate the energy states of an electron bound to the donor impurity in the presence of a magnetic field of arbitrary strength [41].

Chapter Three: Methodology

In this chapter, the model and method used in calculations that we have made will be discussed in detail, which is sequenced in successive and sequential steps as follows: The first main point from which it was started is the quantum point Hamiltonian. The Hamiltonian was processed using the 1 / N offset expansion method, in order to obtain many thermal and magnetic properties level in the quantum dot.

3.1 Schrodinger equation for a 2D screened exciton in a monolayer TMD material

Our model consists of a system of exciton with effective mass (m*) and charge (e), moving in a two dimensions (2D) under the effects of constant magnetic field perpendicular to the monolayer plane. The corresponding Schrodinger equation is given as: [43]

$$\hat{H}\psi(x,y) = E\psi(x,y) \qquad 3.1$$

$$\hat{H} = -\frac{1}{2}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right) - \frac{i}{2}\gamma\left(x\frac{d}{dy} - y\frac{d}{dx}\right) + \frac{1}{8}\gamma^2\left(x^2+y^2\right) + V_K(r,\alpha) \qquad 3.2$$

Where:

$r = \sqrt{x^2+y^2}$.

The dimensionless magnetic parameter γ is related to the magnetic field.

$V_K(r,\alpha)$ is the Keldysh potential. This potential is named after the Soviet physicist Leonid Keldysh, which refers to a specific form of effective potential in electron transfer theory in the presence of high electric fields. This potential describes the effect of electrons on the rotational potential of the crystal lattice and its effect on the applied electric field. This effort is important for explaining certain phenomena such as collision ionization, where pairs of electron holes can be produced through collision with the crystal lattice of high-energy electrons in the semiconductor, which leads to an increase in the number of charge carriers. Understanding the nature of this voltage helps in modeling and predicting such complex phenomena in semiconductor devices [43,44,45].

The non-locally screened electron-hole interaction in 2D such as the transition – metal dichalcogenides monolayer (TMDs) is considered by the Keldysh potential that given as: [43]

$$V_K(r) =-\frac{e^2}{8\varepsilon_0 r_0}\left[H_0\left(\frac{kr}{r_0}\right)-Y_0\left(\frac{kr}{r_0}\right)\right] \qquad 3.3$$

Where: H_0 and Y_0 are zero-order Struve and Bessel function, respectively.

r_0 is the screening length related to the 2D polarizability of the monolayer material.

ε_0 is the vacuum permittivity.

k is the average dielectric constant for the surrounding material.

α is the parameter for characterizing potential and equal : $\alpha = r_0/ka_0^*$ where a_0^* is the effective Bohr radius, which will be explained later.

This potential describe tow charges in the electrostatic interaction for thin semiconductor and semi-metal films, predicted by Keldysh , and then discussed in many more works and research. [44,45]

Now the Hamiltonian Eq (3.1) of the system after substitute Keldysh potential is given as:

$$\hat{H}=-\frac{1}{2}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)-\frac{i}{2}\gamma\left(x\frac{d}{dy}-y\frac{d}{dx}\right)+\frac{1}{8}\gamma^2r^2-\frac{e^2}{8\varepsilon_0 r_0}\left[H_0\left(\frac{kr}{r_0}\right)-Y_0\left(\frac{kr}{r_0}\right)\right] \qquad 3.4$$

In this work, we will use the effective Rydberg (R_y^*) as the unit of energy, is given as: [43]

$$2R_y^* = \frac{m^*e^4}{16\pi^2\varepsilon_0^2\hbar^2} \qquad 3.5$$

Where: ħ is the reduced Plank's constant.

Also, we use effective Bohr radius (a_0^*) as the unit of length, given as: [43]

$$a_0^* = \frac{4\pi\varepsilon_0\hbar^2}{m^* e^2} \qquad 3.6$$

The magnetic parameter Υ is related to the magnetic field (B) by equation: [43]

$$B = \frac{2\gamma m^* R_y^*}{e\hbar} \qquad 3.7$$

After talking about these dimensionless effective units and if we try to apply this to the Hamiltonian equation (3.4), we notice that it is difficult to solve this equation manually or analytically, so we want to resort to mathematical programming and use the shifted 1/N expansion method that can solve this Hamiltonian Eq (3.4) to obtain eigen energys. This is so that we can obtain the required thermal and magnetic properties of exciton in TMD monolayer.

3.2 Computational Method (Shifted 1/N Expansion Method)

In order to be able to solve the spherically symmetrical potential Schrödinger equation, we have used a very powerful technique which is the 1 / N shifted expansion method, which gives exact results for the harmonic oscillator and for the Coulomb potential states. Also, one of the most important features that prompted us to use this method is the speed in giving results. Also, this method does not depend on the properties of Hamiltonians, which means that its convergence is guaranteed and thus its accuracy is very high, which encourages its use. The general idea for this method is to transform the Schrödinger equation, which is difficult to deal with in normal ways, into a harmonic oscillator equation.

In this section we will formulate 1 / N shifted expansion for arbitrary potentials and derive the energy correction, this is done by a series of steps starting from the Schrödinger equation and ending with reaching the required energy values as follows [46]:

1st step: we will start from radial Schrodinger equation in N spatial dimensions: [46]

$$\left(-\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dr^2} + \frac{N-1}{r}\frac{d}{dr}\right) + \frac{l(l+N-2)\hbar^2}{2m^* r^2} + V(r)\right)\emptyset(r) = E\emptyset(r) \qquad 3.8$$

The main idea of this model is to rewrite Schrodinger equation Eq (3.8), by using parameters like: $k = N + 2l$ and shifted parameter a. This expansion become more exact with respect to those parameters for Coulomb and harmonica potential. [46]

The eigenvalue of the square of the N dimensional orbital angular momentum and

$l = |m_l|$ where $|m_l|$ is the magnetic quantum number ($m_l = 0, \pm1, \pm2, \pm3, \ldots\ldots$)

which labels the QD energy states, is appear in team: $l(l + N - 2)$.

By using the parameter $k, \bar{k} = k - a = N + 2l - a$ we can rewrite the Eq(3.8) to

become:

$$\left(-\frac{\hbar^2}{2m^*}\frac{d^2}{dr^2} + \bar{k}^2\left(\left(\hbar^2\left(1 - \frac{1-a}{\bar{k}}\right)(1 - 3 - a)/\bar{k}\right)\right)/8m^*r^2 + V(r)/Q\right)\text{Ø}(r) = E\text{Ø}(r) \quad 3.9$$

Where : $Q = \bar{k}^2$, is scaling constant, use to make Eq(3.8) and Eq(3.9) equals.

2nd step: We can get contribution of energy which comes from effective potential (V_{eff}) at large

$\bar{k}$.

$$V_{eff} = \frac{\hbar^2}{8m^*r^2} + \frac{V(r)}{Q} \quad 3.10$$

V_{eff} has a minimum value at r_0, so that we have:

$$\frac{d}{dr}V_{eff}(r_0) = 0 \Rightarrow 4m^*r_0^3V'(r_0) = \hbar^2 Q \quad 3.11$$

A new variable (x) can be defined by shifting the coordinate origin to the position of the minimum (r_0) of the effective potential (V_{eff}):

$$x = \frac{k^{\frac{1}{2}}}{r_0}(r - r_0) \qquad 3.12$$

3rd step: If Eq (3.9) expands around r_0 ($x = 0$) an analytical equation similar to Schrodinger equation of the one dimensional an harmonic oscillator is found. So we can compare the coefficients of two equation easily, to obtain the energy spectra by finding all harmonic oscillator parameters in term of $\bar{k}, Q, r_0$ and the potential derivative.

4th step: we will expand Schrodinger equation in terms of parameter $\bar{k}$ and shifted parameter (a), to complete other steps and to calculate energy eigen values $E(n, l)$. To get QD energy eigen value expression we completed Mathematical steps.

5th step: the energy eigen values, $E(n_r, m_l)$ are given by:

$$E(n_r, m_l) = E_0 + E_1 + E_2 + E_2 + \ldots\ldots\ldots\ldots \qquad 3.13$$

The radial and principle quantum number are related to:

$$n = n_r + l + 1 \qquad 3.14$$

6th step: The shifted parameter a, is chosen to make second order contribution (E_1) vanishes, so:

$$a = 2 - \frac{2(2n_r - 1)m^*\omega}{\hbar} \qquad 3.15$$

ω is anharmonic frequency parameter, which is given by:

$$\omega = \frac{\hbar}{2m^*}(3 + \frac{r_0 V''(r_0)}{V'(r_0)})^{1/2} \qquad 3.16$$

7th step: By using Eq(3.11) and Eq(3.15), we can determine the roots by equation:

$$(\frac{4m_0 r_0^3 V'(r_0)}{\hbar^2})^{\frac{1}{2}} = \mathrm{N}+2\,l-2+(2n_r+1)(3 + \frac{r_0 V''(r_0)}{V'(r_0)})^{1/2} \qquad 3.17$$

All energy eigen values can be computed after determining r_0. The boundary condition for 1/N expansion method related to $r \to \infty$, that's mean the wave function was vanish (goes to zero), from this condition we can find the eigen energy values.

We get a listed of numerical energy values by written a Mathematica computer code. The computed energies are used to study several properties of an exciton in TMD monolayer, in two parts: thermodynamic and magnetic properties, which will be studied in detail in the next sections.

3.3 The thermodynamic Properties of the Quantum Dot.

Thermodynamics, the science of the relationship between heat, work, temperature, and energy. In other words, thermodynamics generally deals with the transfer of energy from one place to another and from one form to another. Considering that heat is a form of energy capable of a doing certain amount of mechanical work is the main concept on which thermodynamics is built. [47]

In thermodynamics, interactions between large groups of things are studied and categorized. The mainstay here is the relationship of a thermodynamic system to its surroundings, and it is important to study this relationship and this connection. A system consists of a collection of particles that have their own motion and properties, and these properties, in turn, are related to each other through equations of state. The internal energy and thermodynamic potential can be expressed by integrating these properties, which are useful in defining equilibrium conditions and spontaneous processes. [48]

Thermodynamics depends in its entirety on heat, as it is the main basis for it. The meaning of heat today is transient energy. Before the laws of thermodynamics were developed, heat was a measure of the calories contained in any substance. Then reference was made to the ability of the material to keep calories in it. The basic definition of heat has changed as a result of developments in thermodynamics and the temperature dependence of heat transfer. [49]

Heat is defined according to modern thermodynamics as a measure of the total internal energy of a system. In order to measure the temperature-dependent thermal energy associated with a substance, two properties have been determined. These properties have been named as heat capacity of system and entropy. [49]

3.3.1 The Heat Capacity (C_v)

One of the most important thermodynamics properties is heat capacity (C_v), which describes the amount of heat stored in a quantum dot system. [50]

Heat capacity is defined as the amount of heat energy required to raise the temperature of a given quantity of a substance by one degree Celsius. [51]

The heat capacity of a particular material is a wide-ranging property because it depends on the size or quantity of the material. The unit of heat capacity is joules per kelvin or joules per degree Celsius. [51]

Mathematically: $Q = C_v \Delta T$, where Q is the heat energy, C_v is the heat capacity of the system under study and ΔT is the change in temperature of the system. Heat energy represents the total internal energy of the system. This includes the total kinetic energy of the system and the potential energy of the particles. The internal energy of a system can be changed either by supplying heat energy to it or by doing work on it. The internal energy of a system increases with increasing temperature. This increase in internal energy depends on the difference in temperature, amount of matter, etc. [52]

In order to be able to calculate the heat capacity of the system we evaluate the mean energy from a statistic energy $(< E >)$ expression, and to find it, we need first to calculate the partition function (Z).

Partition function, represents the number of way that the molecule can reach thermally according to the temperature of the system. At low temperatures, molecules are concentrated in the ground plane with high density. With higher temperatures, molecules can reach higher levels of thermal energy, but with lower densities. [53]

The partition function describes the statistical properties of a system in thermodynamic equilibrium. Partition functions are functions of thermodynamic state variables, such as temperature and volume. Most of the total thermodynamic variables of a system can be obtained and expressed through the partition function or its derivatives, such as total energy, free energy, entropy, and pressure. [53]

So the partition function and mean energy, respectively are: [54]

$$< Z(n_r, m_l, B, T) >= \sum_{j=1}^{i} e^{-E_j/K_B T} \qquad 3.18$$

Where: K_B is the Boltzmann constant.

T is the temperature.

j is the index for the microstates of the system.

E_j is the total energy of the system in the respective microstate.

$$< E(n_r, m_l, B, T) >= \frac{\sum_{j=1}^{i} E_j e^{-\frac{E_j}{K_B T}}}{\sum_{j=1}^{i} e^{-\frac{E_j}{K_B T}}} \qquad 3.19$$

The summation is taken over the sufficient converging energy levels. In the present work, we have ensured the convergence of numerical calculations which was found to be satisfied at $i = 15$. The average thermal energies or partition function are computed for different ranges of temperature.

After we find the partition function and mean energy, we can find heat capacity by taking the temperature derivative of the mean energy: [54]

$$C_v(n_r, m_l, B, T) = \frac{d < E(n_r, m_l, B, T) >}{dT} \qquad 3.20$$

3.3.2 The entropy (*S*)

Entropy is a scientific concept and a measurable physical property commonly associated with the concept of chaos, randomness, or uncertainty. [55]

It is a property of the state of a system, a measure of energy not available in a closed thermodynamic system as well as a measure of the system's disorder, which varies directly with any inverse change in temperature in the system and inversely with the temperature of the system. [56]

To calculate the value of entropy, it is necessary to use the partition function, because it depends on it directly, as shown in the following equation: [54]

$$S(n_r, m_l, B, T) = \frac{d(K_B \mathrm{T} \ln < \mathrm{Z}(n_r, m_l, B, T) >)}{d\mathrm{T}} \qquad 3.21$$

As it appears, the heat capacity (C_v) and entropy (S), are dependent only in physical parameter temperature, and this dependence will be shown in various plot in next chapter.

3.4 The magnetic Properties of the Quantum Dot.

Magnetism is a physical feature associated with the presence of a magnetic field, which allows objects to attract or repel each other. Magnetism is a part of electromagnetism, because electric currents and magnetic moments of elementary particles give rise to a magnetic field. [57]

Every material around us has its own magnetic properties within it. Every material has different properties than others in the presence of a magnetic field. The magnetic properties of a substance arise from the electrons in the atoms or molecules. Each electron in an atom behaves like a small magnet. In addition, electrons are small current loops that retain their magnetic moment. [58]

Magnetic materials are classified into three categories, based on the behavior of materials in the magnetic field. The three types of materials are diamagnetic, paramagnetic and ferromagnetic: [59]

Diamagnetic substances produce negative magnetization when placed in an external magnetic field. Therefore, diamagnetic substances are repelled by magnets.

Paramagnetic substances they are slightly attracted by the magnetic field acquire a small net magnetic moment in the direction of the applied field.

Ferromagnetic materials are strongly attracted by the magnetic field. These materials retain the magnetism even when the magnetic field is removed.

In this chapter, in next section, we will talk about two magnetic properties, namely: magnetization and magnetic susceptibility.

3.4.1 The Magnetization (M)

It is the process through which the material acquires magnetic properties as a result of its exposure to an external magnetic field, which in turn causes the movement of electrons in atoms or the rotation of electrons or the nucleus. The material becomes magnetized and exhibits magnetic properties. [60]

Electrons orbiting around the nucleus have a magnetic moment. When the total magnetic dipole moment reaches zero, the material is no longer magnetized. When the material is placed in an external magnetic field, the magnetic moments are aligned in a certain direction and the material gets a non-zero net dipole moment and thus the material is magnetized. The net dipole moment per unit volume is defined as magnetization. [60]

The Magnetization (M) can be calculated by differentiating the average statistical energy of the 2D QD system with respect to the magnetic field strength. [54]

$$M(n_r, m_l, B, T) =-\frac{d < E(n_r, m_l, B, T) >}{dB} \qquad 3.22$$

Where:

$$< E(n_r, m_l, B, T) >= \frac{\sum_{j=1}^{i} E_j e^{-\frac{E_j(B)}{K_B T}}}{\sum_{j=1}^{i} e^{-\frac{E_j(B)}{K_B T}}} \qquad 3.23$$

By substituting Eq.(3.23) in Eq.(3.22), we can express the magnetization (M) in a common standard form as:

$$M(n_r, m_l, B, T) =-\frac{d}{dB}\left(\frac{\sum_{j=1}^{i} E_j(B) e^{-\frac{E_j(B)}{K_B T}}}{\sum_{j=1}^{i} e^{-\frac{E_j(B)}{K_B T}}}\right) \qquad 3.24$$

3.4.2 The magnetic susceptibility (χ)

Magnetic susceptibility measures the extent to which a material responds to an external magnetic field, as it determines how easy it is to magnetize the material when exposed to a magnetic field. The susceptibility of the material to magnetization can be affected by various factors such as temperature, crystal structure, impurities, and defects in the material. [61]

Magnetic susceptibility is affected by the magnetic field with an increase or decrease, depending on the so-called magnetic saturation phenomenon, which will be discussed later.

The magnetic susceptibility (X) , can be obtained by differentiating the magnetization(M) with respect to the magnetic field strength B, by: [54]

$$\chi(n_r, m_l, B, T) = \frac{dM(n_r, m_l, B, T)}{dB} \tag{3.25}$$

3.5 Density of states (DOS)

Density of states (DOS) can be thought of as the number of different states that electrons are allowed to occupy at a given energy level. The number of electron states per unit volume per unit energy. This function is considered the cornerstone on which bulk properties such as specific heat, magnetism, and other transport phenomena of conductive solids depend. DOS calculations allow determination of the general distribution of states as a function of energy and can also determine the spacing between energy bands in a semiconductor. High DOS for a given energy level indicates that numerous states are open for occupation. [62]

DOS units differ according to their dimensions as follows: DOS in a 3dimensional system is $Volume-1\ Energy-1$, in a 2D system the units of DOS are $Area\ -1\ \ Energy-1$, in a one-dimensional system the units of DOS are $Length-1Energy-1$.[63]

Through the principles of quantum mechanics, the density of states can be said to be the number of electron (or hole) states allowed per volume at a given energy level. It is easy to say that the dependence of the density of states on the energy of the system changes dramatically. Table 3.1 show how DOS changes for combined (3D), 2D, 1D, and 0D systems. [63]

Table 3.1: The DOS as a function of energy in 0D, 1D, 2D and 3D system

System	Dimensionality	DOS vs. E
Bulk	3D	$DOS \propto \sqrt{E}$
Quantum well	2D	$DOS \propto Constant$
Quantum wire	1D	$DOS \propto \frac{1}{\sqrt{E}}$
Quantum dot	0D	$DOS \propto \delta\,(E - E_n)$

The electronic density of states (DOS) in a quantum dot (QD) is another property that can give us important insights into the electronic structure of nanomaterials. It is expressed as the sum of a series of delta functions, given by: [64,65]

$$DOS(E) = \frac{1}{V}\sum_{n=1}^{N} \delta(E - E_n) \qquad 3.26$$

Numerically, DOS can calculate by Gaussian distribution as: [65]

$$DOS(E) = \frac{1}{\sqrt{2\pi\Gamma^2}}\sum\nolimits_n \exp\left[\frac{-(E - E_n)^2}{2\Gamma^2}\right] \qquad 3.27$$

where Γ is the broadening factor, and E_n is the eigen energy of the system, which was shown a result of the 1/N expansion method.

3.6 Magneto-Caloric Effect (MCE)

This phenomenon was discovered in 1881 by the scientist Warburg. It is a thermomagnetic dynamic phenomenon in which a change occurs in the temperature of a certain substance by exposing the substance to a changing magnetic field. In other words, it can be said that it is heating or cooling (The change in temperature of a magnetic material due to the application of a magnetic field). [66]

This effect has been called "adiabatic demagnetization" for many years. In this part of the cooling process, a decrease in the strength of the external magnetic field allows the magnetic fields of the material to be disturbed or to escape from the magnetic field, that is, to become no longer aligned with the magnetic field through the exciting action of thermal energy (phonons) in the material. [67]

In simple terms, when a changing magnetic field is applied to a material, the magnetic moments of the atoms or molecules in the material align in response or not in response to the field. In the process of alignment or misalignment, energy may be required or energy may be released, resulting in a change in the temperature of the material. If heat is absorbed from the surroundings during the transfer or alignment process, the material heats up, this is known as adiabatic magnetization. Conversely, if the system releases energy during the transformation, the material cools. [67,68]

The magnetic caloric effect has many important applications in magnetic refrigeration technology. Magnetic refrigeration systems based on this effect are more environmentally friendly and more energy efficient than traditional refrigeration methods that use compressors and chillers. Researchers are exploring different materials with strong magnetic properties that would be more effective for practical applications in cooling technology. [66]

We can use thermodynamics that relates the magnetic field to entropy and temperature, where the magnetic field changes the magnetic contribution to the entropy.

The intensity of the magnetic field's effect in this phenomenon depends on the properties of each material. So that, we have two basic processes of the magneto caloric effect when a magnetic field is applied or removed in a magnetic system: the first one is isothermal process, which leads to an entropy (S) change, and the second one is adiabatic process, which yields a variation in temperature (T), see figure 2.2. [69]

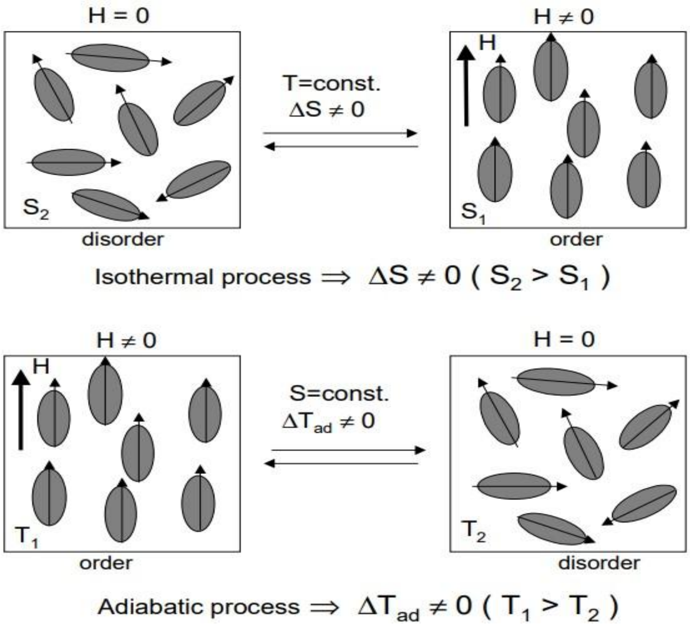

Figure 3.1: The two basic processes of the magneto caloric effect.

Two relevant processes are shown in figure 3.1 to understand the thermodynamics of the MCE:

The first one, when the magnetic field is applied adiabatically (the total entropy remains constant) in a reversible process, the magnetic entropy decreases, but as the total entropy does not change, then, the temperature decreases.

The other one, when the magnetic field is applied isothermally (T remains constant), the total entropy increases due to the increase in the magnetic contribution, and therefore the entropy change in the process is defined as [69,70]:

$$\Delta S_m = S(T_0, B_0) - S(T_0, B_{\neq 0}) \qquad 3.28$$

Where: ΔS_m: magnetic entropy change (eV/ K)

S_m :is the magnetic entropy.

T_0 :is the temperature.

B_0 :is the magnetic field equal zero.

$B_{\neq 0}$:is the magnetic field not equal zero.

Both the adiabatic temperature change, ΔT_{ad}, and the isothermal magnetic entropy change, ΔS_m, are characteristic values of the MCE.

3.7 The Diamagnetic coefficient (σ)

In this section, we will study the magnetic effect of materials as a result of their exposure to an external magnetic field. The magnetic moment of a free atom is the change in the orbital motion of electrons when an external magnetic field is applied.

The change in orbital motion due to the application of an external magnetic field to the material is known as the magnetic effect, and it occurs in all types of atoms, even those in which all electron shells are full. [71]

Diamagnetism is a property of all materials, and always makes a weak contribution to a material's response to a magnetic field. These materials create an internal magnetic field that is opposite to the external magnetic field applied to them. [72,73]

The diamagnetic shift, often denoted by σ (sigma), is an important phenomenon that can be linked to the magnetic susceptibility of a material. Magnetic susceptibility, as previously defined, is a measure of the extent to which a material responds to a magnetic field applied to it. Diamagnetic materials are those that have negative susceptibility, meaning they repel magnetic fields.

Diamagnetism can be defined in another way, which is that it represents the magnetic susceptibility of a material, which is that which creates an opposite magnetic field when exposed to an external magnetic field. This property arises as a result of the orbital movement of the electrons within the atoms of the material, that is, the change in the orbital movement of the electrons when an external magnetic field is applied. [73]

The diamagnetic shift or coefficient, often denoted by (σ), represents the magnetization response of a material to an applied magnetic field. It's typically defined as the second derivative of the average energy (E) with respect to the magnetic field (B). [74]

Mathematically, the diamagnetic shift or coefficient (σ) can be expressed as:[75]

$$\sigma(\mathrm{T},\mathrm{B}) = \frac{1}{2}\frac{d^2E(T,B)}{dB^2} \tag{3.29}$$

Where: σ is the diamagnetic shift or coefficient in unit of eV/Tesla^2.

E is the average energy of the system in unit of eV.

B is the magnetic field in unit of tesla.

It can be expressed in another form [74]

$$E_{dia} = \frac{e^2}{8m^*} < r^2 > B^2 = \sigma B^2 \tag{3.30}$$

That’s mean:

$$\sigma = \frac{E_{dia}}{B^2} \tag{3.31}$$

Where: σ is the diamagnetic shift or coefficient in unit of eV/Tesla^2.

E_{dia} is the average energy of the system in unit of eV.

B is the magnetic field in unit of tesla.

These formula indicates how the average energy of the system changes as the magnetic field strength changes, providing insight into the diamagnetic behavior of the material.

The algorithm of our work can be visualized by the scheme given in Fig. 3.2

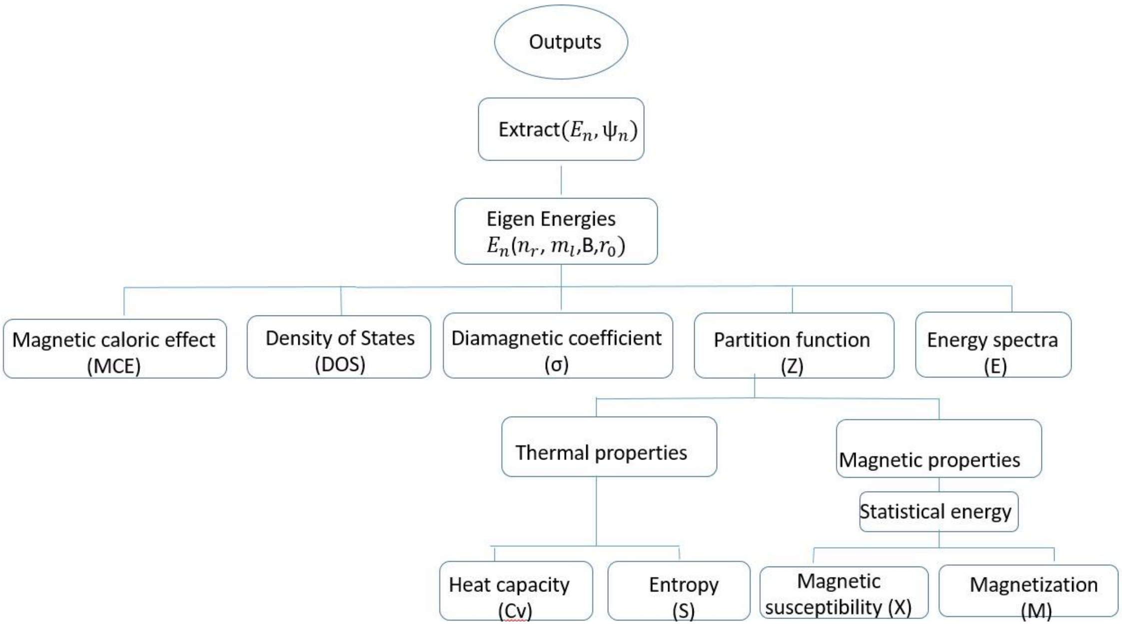

Figure 3.2: Flowchart for the dissertation

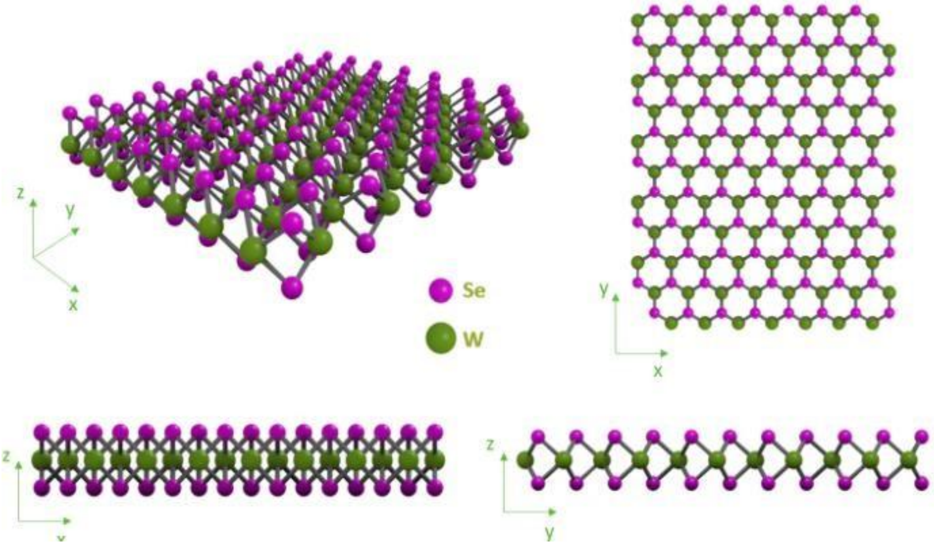

Figure 3.3: Single crystal WSe_2

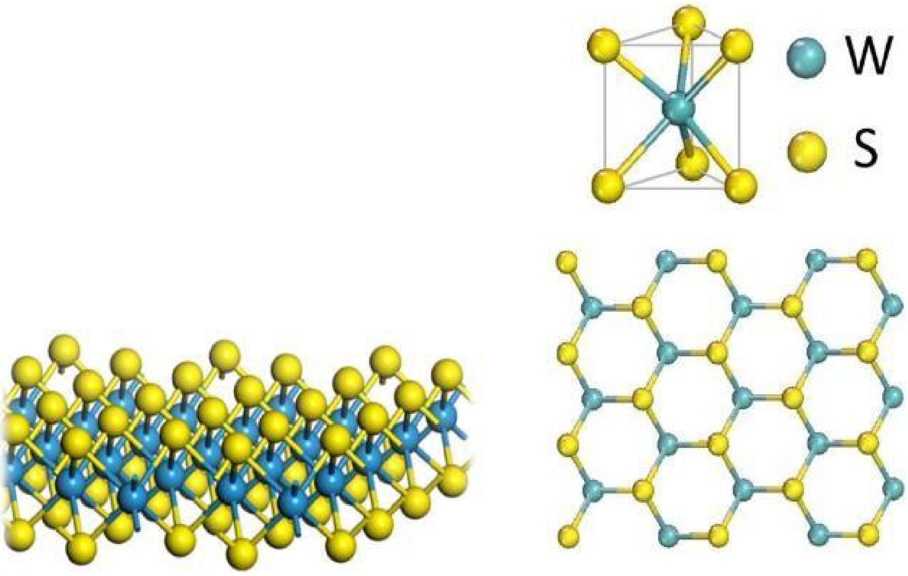

Figure 3.4: Single crystal WS_2

Chapter Four: Results

Broadly speaking, this thesis can be outlined through a series of sequential steps. Initially, an exciton within a TMD material chip was analyzed to investigate its thermal and magnetic characteristics. The analysis involved utilizing the Schrödinger equation and employing the 1/N Expansion technique. This approach was essential for deriving energy values necessary to establish the partition function. Through this process, various properties crucial for this part of the thesis were determined.

In this chapter, the results obtained from mathematical programming will be discussed through two basic steps. The first is to clarify the extent of compatibility between the methodology used in this work and what has been studied in other related works, by presenting the practical and numerical results that indicate its accuracy. The validity of the methodology and method used here will be clarified in the tables and figures in the following lines, since, as we explained previously in this work, we used the 1/N-shift expansions method.

The next step is to show the set of properties that are listed in Chapter three for two types of materials (WSe_2 and WS_2), both of which fall under the name TMD materials.

The physical parameters used for WSe_2 and WS_2 respectively in numerical computations: the effective mass of an electron ($m^* = 0.2m_e, 0.16m_e$), the average dielectric constant of the material ($k = 4.5, 1$), the effective screening length of a monolayer $(r_0 = 45A^o, 75A^o)$, and the parameter related to effective bore radius are $(a = 22.677, 3.779)$. [43]

4.1 Energy Spectra

This section will be an illustrative presentation of the energy state values obtained mathematically using the 1/N-shift expansions method and comparing them with other energy state values obtained numerically for the same materials (WSe_2 and WS_2) and using the same effects (magnetic field specifically).

To complete this work with great accuracy, the first step is to compare our results with the reference results [43]. If we look closely at tables (4.1.(a,b,c) , 4.2.(a,b,c)), we see how close the energy values of the ground state are between the two works.

Table (4.1.a): The ground state energies (1s,2s) (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where γ=0.01 corresponds to the magnetic field B=94T) for WSe_2, calculated by 1/N-shift expansions method, compared with the reported work ref [43], Delta energy = E(present work)- E(Ref [43]).

.WSe_2		1s $< 1\|0 >$		Delta energy	2s $< 2\|0 >$		Delta energy
B(T)	Γ	E(present work) (eV)	E(Ref [43]) (eV)		E(present work) (eV)	E(Ref[43]) (eV)	
0.00	0	-0.1604	-0.1614	0.0010	-0.0371	-0.0373	0.0002
9.4	0.001	-0.1603	-0.1614	0.0011	-0.0366	-0.0364	0.0002
18.8	0.002	-0.1603	-0.1613	0.0010	-0.0357	-0.0355	0.0002
28.2	0.003	-0.1601	-0.1612	0.0011	-0.0336	-0.0334	0.0002
37.6	0.004	-0.1599	-0.1610	0.0011	-0.0313	-0.0308	0.0005
47	0.005	-0.1597	-0.1607	0.0010	-0.0288	-0.0276	0.0012
56.4	0.006	-0.1594	-0.1604	0.0010	-0.0262	-0.0241	0.0021
65.8	0.007	-0.1590	-0.1601	0.0011	-0.0234	-0.0201	0.0033
75.2	0.008	-0.1589	-0.1597	0.0008	-0.0202	-0.0160	0.0042
84.6	0.009	-0.1582	-0.1592	0.0010	-0.0165	-0.0115	0.0050
94.0	0.010	-0.1577	-0.1588	0.0011	-0.0122	-0.0069	0.0053

Table (4.1.b): The ground state energies (3s,4s) (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where γ=0.01 corresponds to the magnetic field B=94T) for WSe_2, calculated by 1/N-shift expansions method, compared with the reported work ref [43], Delta energy = E(present work)- E(Ref [43]).

WSe_2		3s $< 3\|0 >$		Delta energy	4s $< 4\|0 >$		Delta energy
B(T)	γ	E(present work) (eV)	E(Ref [43]) (eV)		E(present work) (eV)	E(Ref[43]) (eV)	
0.00	0	-0.0165	-0.0161	0.0004	-0.0096	-0.0087	0.0009
9.4	0.001	-0.0150	-0.0138	0.0012	-0.0054	-0.0027	0.0027
18.8	0.002	-0.0122	-0.0085	0.0037	0.0072	0.0078	0.0006
28.2	0.003	-0.0056	-0.0015	0.0041	0.0213	0.0206	0.0007
37.6	0.004	0.0032	0.0064	0.0032	0.0361	0.0342	0.0019
47	0.005	0.0128	0.0152	0.0024	0.0514	0.0489	0.0025
56.4	0.006	0.0228	0.0244	0.0016	0.0670	0.0642	0.0028
65.8	0.007	0.0330	0.0337	0.0007	0.0830	0.0762	0.0068
75.2	0.008	0.0435	0.0440	0.0005	0.0991	0.0956	0.0035
84.6	0.009	0.0542	0.0544	0.0002	0.1155	0.1115	0.0040
94.0	0.010	0.0651	0.0647	0.0004	0.1320	0.1279	0.0041

Table (4.1.c): The ground state energies (5s,6s) (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where $\gamma=0.01$ corresponds to the magnetic field B=94T) for WSe_2, calculated by 1/N-shift expansions method, compared with the reported work ref [43], Delta energy = E(present work)- E(Ref [43]).

WSe_2		5s $< 5\|0 >$		Delta energy	6s $< 6\|0 >$		Delta energy
B(T)	γ	E(present work) (eV)	E(Ref [43]) (eV)		E(present work) (eV)	E(Ref[43]) (eV)	
0.00	0	-0.0062	-0.0054	0.0008	-0.0043	-0.0032	0.0011
9.4	0.001	0.0036	0.0048	0.0012	0.0107	0.0114	0.0007
18.8	0.002	0.0419	0.0217	0.0202	0.0264	0.0346	0.0082
28.2	0.003	0.0433	0.0381	0.0052	0.0632	0.0587	0.0045
37.6	0.004	0.0639	0.0603	0.0036	0.0895	0.0843	0.0052
47	0.005	0.0894	0.0598	0.0296	0.1162	0.1104	0.0058
56.4	0.006	0.1062	0.0762	0.6558	0.1432	0.1371	0.0061
65.8	0.007	0.1279	0.0979	0.0300	0.1705	0.1632	0.0073
75.2	0.008	0.1497	0.1197	0.0300	0.1980	0.1915	0.0065
84.6	0.009	0.1717	0.1649	0.0068	0.2256	0.2188	0.0068
94.0	0.010	0.1939	0.1877	0.1683	0.2534	0.2465	0.0069

Table (4.2.a): The ground state energies (1s,2s) (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where γ=0.01 corresponds to the magnetic field B=60.16T) for WS_2, calculated by 1/N-shift expansions method, compared with the reported work ref [43], Delta energy = E(present work)- E(Ref [43]).

WS_2		1s $< 1\|0 >$		Delta energy	2s $< 2\|0 >$		Delta energy
B(T)	γ	E(present work) (eV)	E(Ref [43]) (eV)		E(present work) (eV)	E(Ref[43]) (eV)	
0.00	0.00000	-0.3179	-0.3187	0.0008	-0.1523	-0.1516	0.0007
7.52	0.00125	-0.3179	-0.3184	0.0005	-0.1520	-0.1513	0.0007
15.0	0.00250	-0.3178	-0.3186	0.0008	-0.1514	-0.1507	0.0007
30.0	0.00500	-0.3175	-0.3179	0.0004	-0.1488	-0.1478	0.001
45.1	0.00750	-0.3170	-0.3178	0.0008	-0.1446	-0.1436	0.001
60.1	0.01000	-0.3163	-0.3128	0.0035	-0.1392	-0.1378	0.0014
150	0.02500	-0.3086	-0.3094	0.0008	-0.0888	-0.0853	0.0035
300	0.05000	-0.2854	-0.2862	0.0008	0.0303	0.0339	0.0036
601	0.10000	-0.2188	-0.2188	0	0.3092	0.3106	0.0014
3008	0.50000	0.5246	0.5259	0.0013	2.7905	2.9713	0.1808
4512	0.75000	1.0328	1.0344	0.0016	4.3861	4.3874	0.0013
6016	1.00000	1.5568	1.5525	0.0043	5.9913	5.9938	0.0025

Table (4.2.b): The ground state energies (3s,4s) (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where γ=0.01 corresponds to the magnetic field B=60.16T) for WS_2, calculated by 1/N-shift expansions method, compared with the reported work ref [43], Delta energy = E(present work)- E(Ref [43]).

WS_2		3s $< 3\|0 >$		Delta energy	4s $< 4\|0 >$		Delta energy
B(T)	γ	E(present work) (eV)	E(Ref [43]) (eV)		E(present work) (eV)	E(Ref[43]) (eV)	
0.00	0.00000	-0.0952	-0.0944	0.0008	-0.0657	-0.0648	0.0009
7.52	0.00125	-0.0944	-0.0936	0.0008	-0.0639	-0.0631	0.0008
15.0	0.00250	-0.0922	-0.0909	0.0013	-0.0591	-0.0579	0.0012
30.0	0.00500	-0.0843	-0.0827	0.0016	-0.0439	-0.0404	0.0035
45.1	0.00750	-0.0730	-0.0700	0.003	-0.0227	-0.0178	0.0049
60.1	0.01000	-0.0591	-0.0552	0.0039	0.0027	0.0074	0.0047
150	0.02500	0.0562	0.0596	0.0034	0.1868	0.1872	0.0004
300	0.05000	0.2868	0.2886	0.0018	0.5277	0.5285	0.0008
601	0.10000	0.7839	0.7845	0.0006	1.2436	1.2408	0.0028
3008	0.50000	5.0074	5.0114	0.0040	7.2089	7.2151	0.0062
4512	0.75000	7.6905	7.6978	0.0073	10.979	10.993	0.0140
6016	1.00000	10.383	10.392	0.0090	14.759	14.777	0.0180

Table (4.2.c): The ground state energies (5s,6s) (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where γ=0.01 corresponds to the magnetic field B=60.16T) for WS2, calculated by 1/N-shift expansions method, compared with the reported work ref [43], Delta energy = E(present work)- E(Ref [43]).

WS_2		5s $\langle 5\|0 \rangle$		Delta energy	6s $\langle 6\|0 \rangle$		Delta energy
B(T)	γ	E(present work) (eV)	E(Ref [43]) (eV)		E(present work) (eV)	E(Ref[43]) (eV)	
0.00	0.00000	-0.0481	-0.0474	0.0007	-0.0367	-0.0361	0.0006
7.52	0.00125	-0.0448	-0.0439	0.0009	-0.0312	-0.0300	0.0012
15.0	0.00250	-0.0366	-0.0304	0.0062	-0.0196	-0.0156	0.0040
30.0	0.00500	-0.0119	-0.0069	0.0050	0.0180	0.0226	0.0046
45.1	0.00750	0.0220	0.0261	0.0041	0.0642	0.0674	0.0032
60.1	0.01000	0.0595	0.0631	0.0036	0.1132	0.1158	0.0026
150	0.02500	0.3109	0.3121	0.0012	0.4312	0.4310	0.0002
300	0.05000	0.7616	0.7619	0.0003	0.9917	0.9883	0.0034
601	0.10000	1.6961	1.6937	0.0024	2.1446	2.1421	0.0025
3008	0.50000	9.4029	9.4133	0.0104	11.592	11.581	0.0110
4512	0.75000	14.260	14.276	0.0160	17.537	17.559	0.0220
6016	1.00000	19.127	19.153	0.0260	23.491	23.524	0.0330

In figures (4.1.a and 4.1.b) we have shown the effect of magnetic field confinement on the ground state energies. It also appears in the figures that the first level is not affected by an increase in the magnetic field, as it maintains an almost constant value, while as we rise in the levels, we see a noticeable effect of the magnetic field on the energy values of the levels, as with the increase of the magnetic field the energy values begin to increase. This is completely consistent with the results of reference 43. Looking at and comparing the two figures, we see the extent of the match between the two works.

When an electron is placed in a magnetic field, energy levels may be affected due to the interaction between the electrons magnetic moment and the external magnetic field. This effect is called Zeeman effect. [76]

The Zeeman effect divides energy levels into multiple levels in the presence of a magnetic field. When an electron in its orbit around the nucleus is exposed to a magnetic field, the angular momentum of the electron will interact with the magnetic field, which leads to the energy levels being divided into sublevels. The increase in the energy of the orbitals depends on the direction of the electron's angular momentum vector with respect to the direction of the magnetic field. [76]

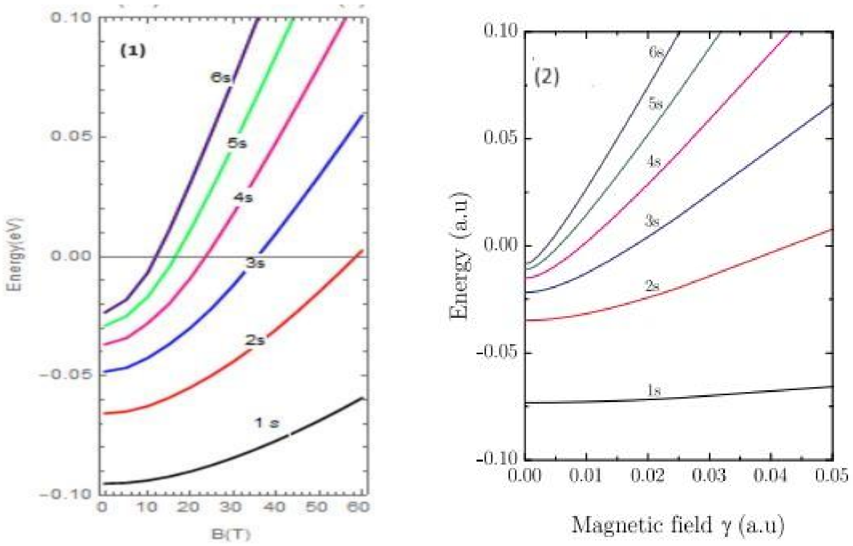

Fig. 4.1.a: The ground state energy as a function of magnetic field for WS_2, note (in figure for ref.43, use Rydberg unit for energy and magnetic field). (1) present work, (2) work ref 43.

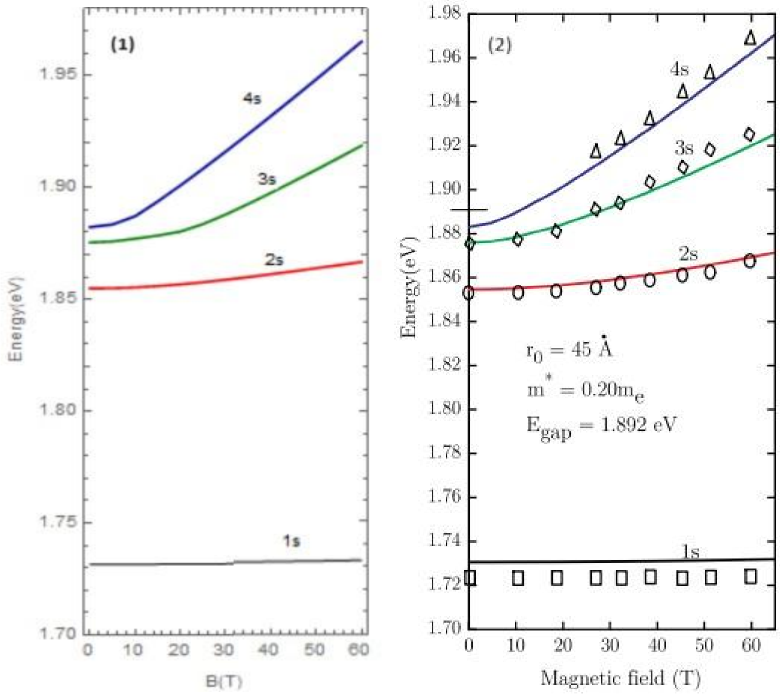

Fig. 4.1.b: The ground state energy as a function of magnetic field for WSe2. (1) present work, (2) work ref 43, where the solid line related to theoretical result and shape line related to experimental result.

Also, we found energy values at different levels for the same field values that were defined in the previous tables in order to make the work more comprehensive. We changed the quantum number from $< s >$ to $< p >$ to see how energy essentially depends on these values and to see the changes that occur in energy at these quantum numbers, see tables (4.3 and 4.4).

Table (4.3): The ground state energies (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where γ=0.01 corresponds to the magnetic field B=94T) for WSe_2, calculated by 1/N-shift expansions method.

WSe_2		1p $< 1 \vert 1 >$	2p $< 2 \vert 1 >$	3p $< 3 \vert 1 >$	4p $< 4 \vert 1 >$	5p $< 5 \vert 1 >$	6p $< 6 \vert 1 >$
B(T)	γ	E(eV)	E(eV)	E(eV)	E(eV)	E(eV)	E(eV)
0.00	0	-0.0483	-0.0191	-0.0102	-0.0064	-0.0043	-0.0031
9.4	0.001	-0.0453	-0.0149	-0.0034	0.0057	0.0598	0.3580
18.8	0.002	-0.0419	-0.0087	0.0088	0.0244	-0.0164	0.8823
28.2	0.003	-0.0382	-0.0010	0.0230	0.0443	0.0638	0.0825
37.6	0.004	-0.0341	0.0076	0.0379	0.0649	0.0902	0.1145
47	0.005	-0.0297	0.0171	0.0532	0.0860	0.1170	0.1469
56.4	0.006	-0.0252	0.0271	0.0690	0.1075	0.1441	0.1796
65.8	0.007	-0.0202	0.0374	0.0850	0.1292	0.1714	0.2126
75.2	0.008	-0.0151	0.0479	0.1013	0.1511	0.1989	0.2457
84.6	0.009	-0.0099	0.0587	0.1177	0.1731	0.2266	0.2789
94.0	0.010	-0.0045	0.0696	0.1343	0.1954	0.2544	0.3123

Table (4.4): The ground state energies (in unit of eV) at different values of magnetic field strength (in unit of T in present work and in unit of γ in ref [43], where γ=0.01 corresponds to the magnetic field B=60.16T) for WS_2, calculated by 1/N-shift expansions method.

WS_2		1p < 1|1 >	2p < 2|1>	3p < 3|1 >	4p < 4|1 >	5p < 5|1 >	6p < 6|1 >
B(T)	γ	E(eV)	E(eV)	E(eV)	E(eV)	E(eV)	E(eV)
0.00	0.00000	-0.1843	-0.1098	-0.0739	-0.0532	-0.0401	-0.0313
7.52	0.00125	-0.1815	-0.1065	-0.0698	-0.0477	-0.0326	-0.0213
15.0	0.00250	-0.1784	-0.1023	-0.0633	-0.0378	-0.0188	-0.0027
30.0	0.00500	-0.1717	-0.0912	-0.0451	-0.0106	0.0195	0.0481
45.1	0.00750	-0.1640	-0.0773	-0.0220	0.0236	0.0657	0.1058
60.1	0.01000	-0.1557	-0.0614	0.0040	0.0611	0.1146	0.1660
150	0.02500	-0.0944	0.0517	0.1883	0.3123	0.4324	0.5502
300	0.05000	0.0299	0.2879	0.5289	0.7627	0.9927	1.2201
601	0.10000	0.3095	0.7848	1.2444	1.6969	2.1453	2.5911
3008	0.50000	2.7907	5.0073	7.2089	9.4030	11.592	13.779
4512	0.75000	4.3861	7.6903	10.979	14.260	17.537	20.811
6016	1.00000	5.9912	10.382	14.759	19.127	23.491	27.852

Also in figures (4.1.c) we have shown the magnetic field confinement on the ground state energies for quantum number (p). It also appears in the figures, we see a noticeable effect of the magnetic field on the energy values of the level, as with the increase of the magnetic field the energy values begin to increase.

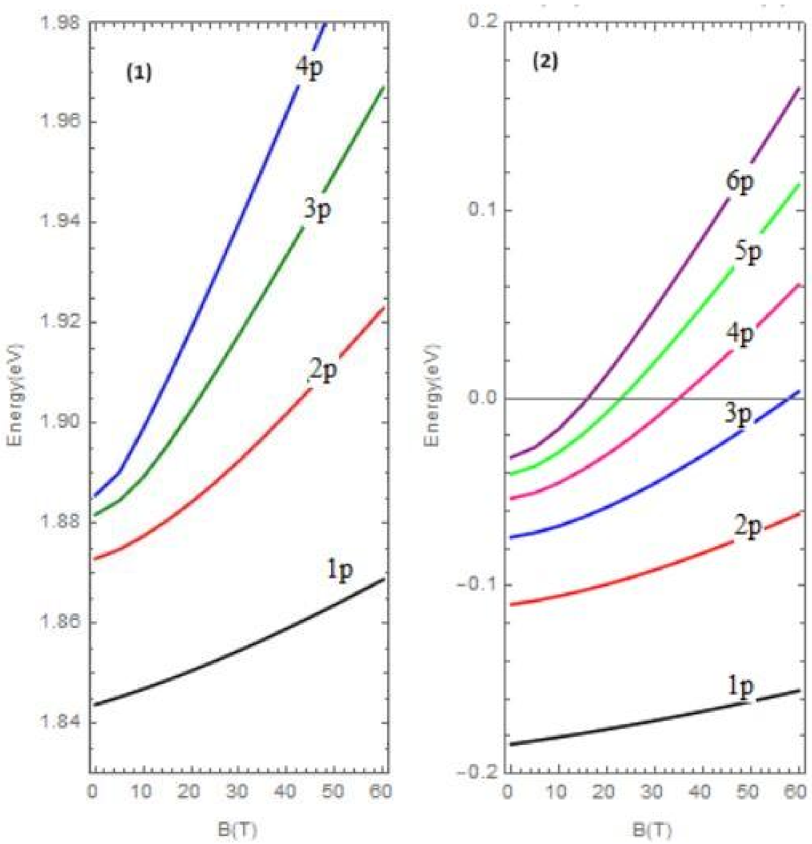

Fig. 4.1.c: The ground state energy as a function of magnetic field, (1) for WSe_2 and (2) for WS_2

Later, we highlighted the ground state energy as a function of temperature at different values of the magnetic field. As shown in figure 4.2 and when we cancel the effect of magnetic field (B=0T), we find that the average energies increase with increasing temperature until they reach 350^0 K and if we look at this figure, we also conclude that the more we move to higher levels (5S, 10S, 15S, 20S), the more convergence limit there is, so that we are running from 15S to 20S.

We used high temperatures (reaching 2000^0 K) because at low temperatures, the thermal energy is low. This does not affect the system or the binding energy.

As we increase the temperature, the thermal energy increases and its effect on the system increases, which leads to an increase in the binding energy. [77]

The relationship between the increase in average energy convergence and the increase in temperature is based on statistical mechanics and the so-called Boltzmann distribution. [78]

Based on the thermal equilibrium in the particle system, with increasing temperature, the average kinetic energy of the particles increases. This is because temperature is a measure of the average kinetic energy of the molecules in the system. As the temperature rises, the molecules tend to move faster and therefore have higher kinetic energies. In this case, through collisions, the convergence of the average energy corresponds to the tendency of molecules to have similar kinetic energies during energy exchange. At higher temperatures, the kinetic energy distribution becomes broader, and the average energy becomes more convergent around the highest average kinetic energy value. [78]

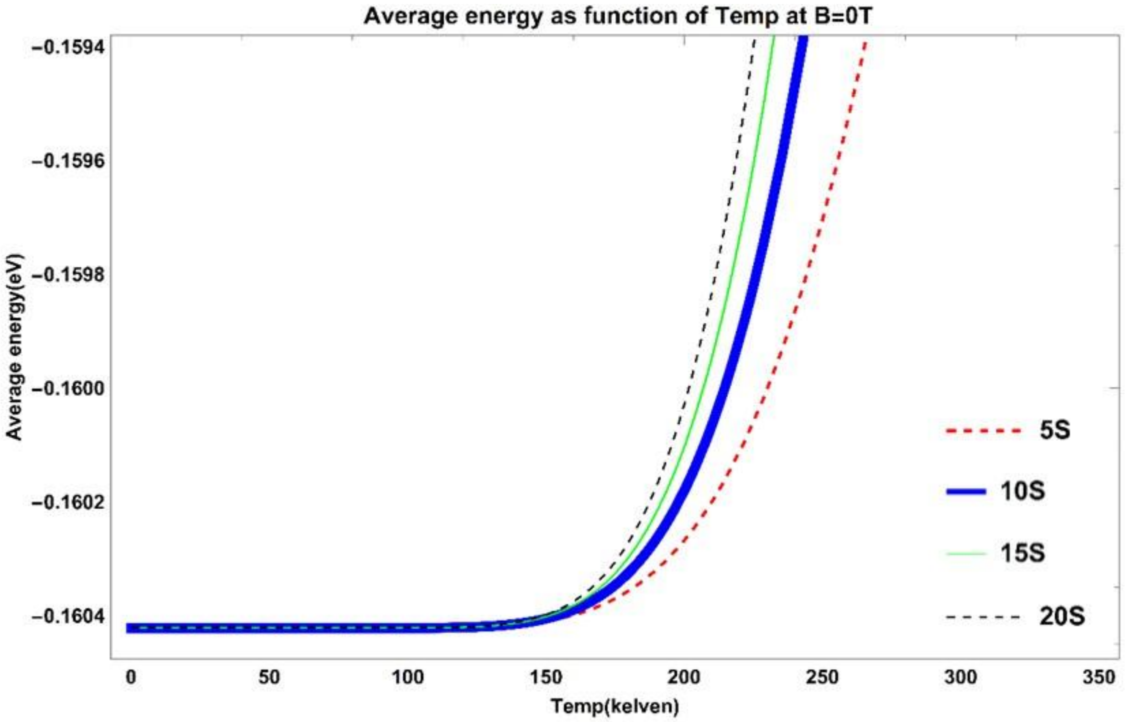

Fig. 4.2: The average energy as a function of temperature at a zero magnetic field for WSe_2

We studied the same relation between average energy and temperature, but now we add the effect of the magnetic field, and we find nearly the same behavior: the average energy will be increase with increasing temperature, and we have more convergences when we move to a higher state (see figure 4.3).

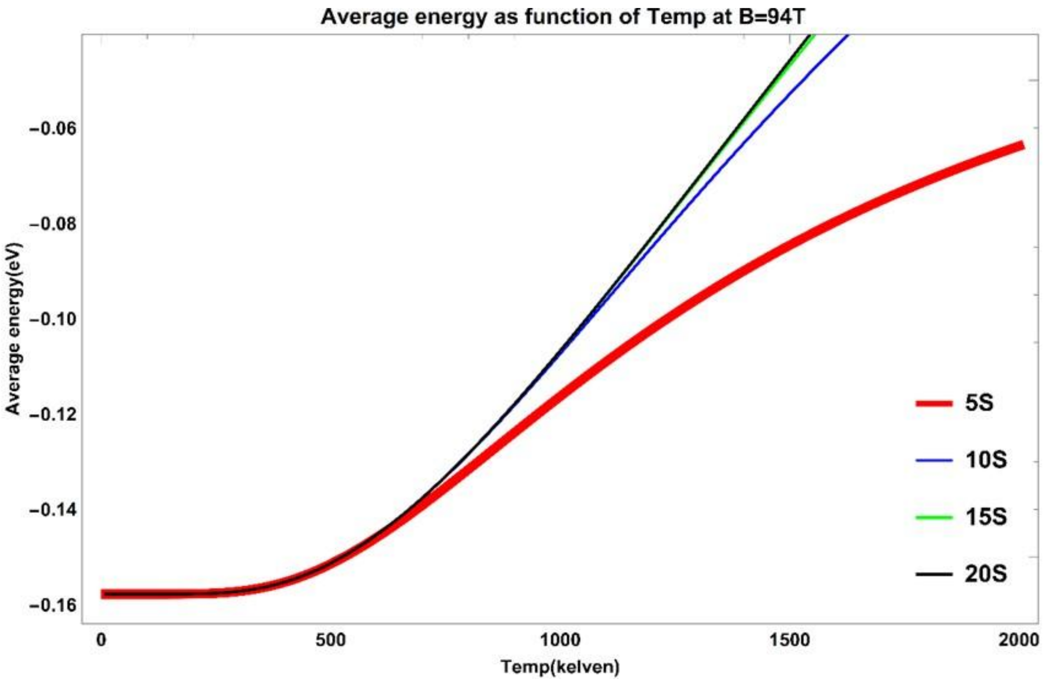

Fig. 4.3: The average energy as a function of temperature with magnetic field for WSe_2

We studied the same relation for WS_2, see figures 4.4 and 4.5. After we looked at the figures, we noted that the average energy state reached the convergences at 15S, so we did not need to run to 20S. This means that the response of molecules inside WS_2 to heat is faster than the response of those in WSe_2.

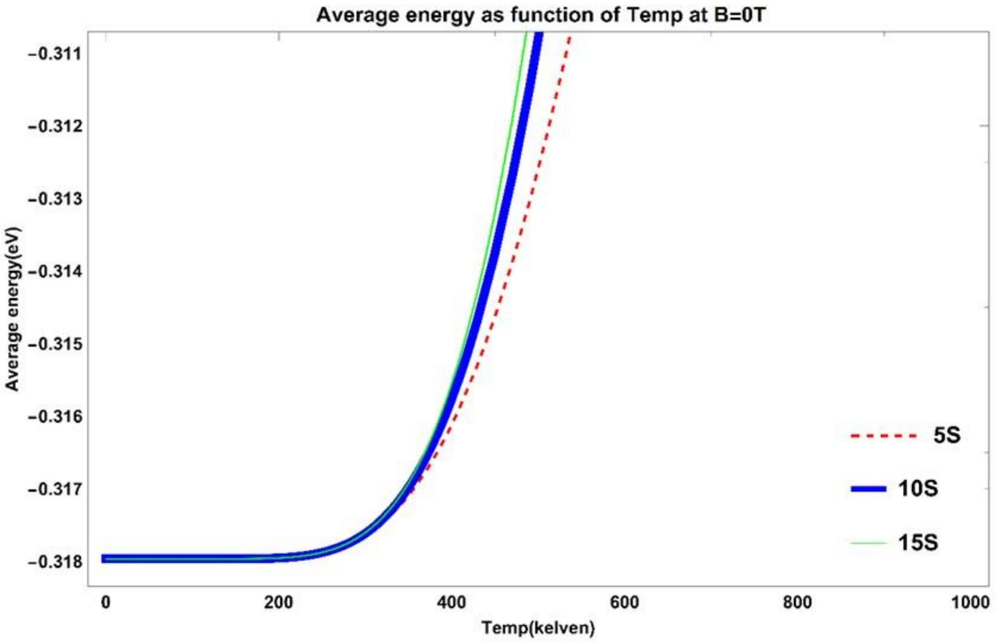

Fig. 4.4: The average energy as a function of temperature at a zero magnetic field for WS_2

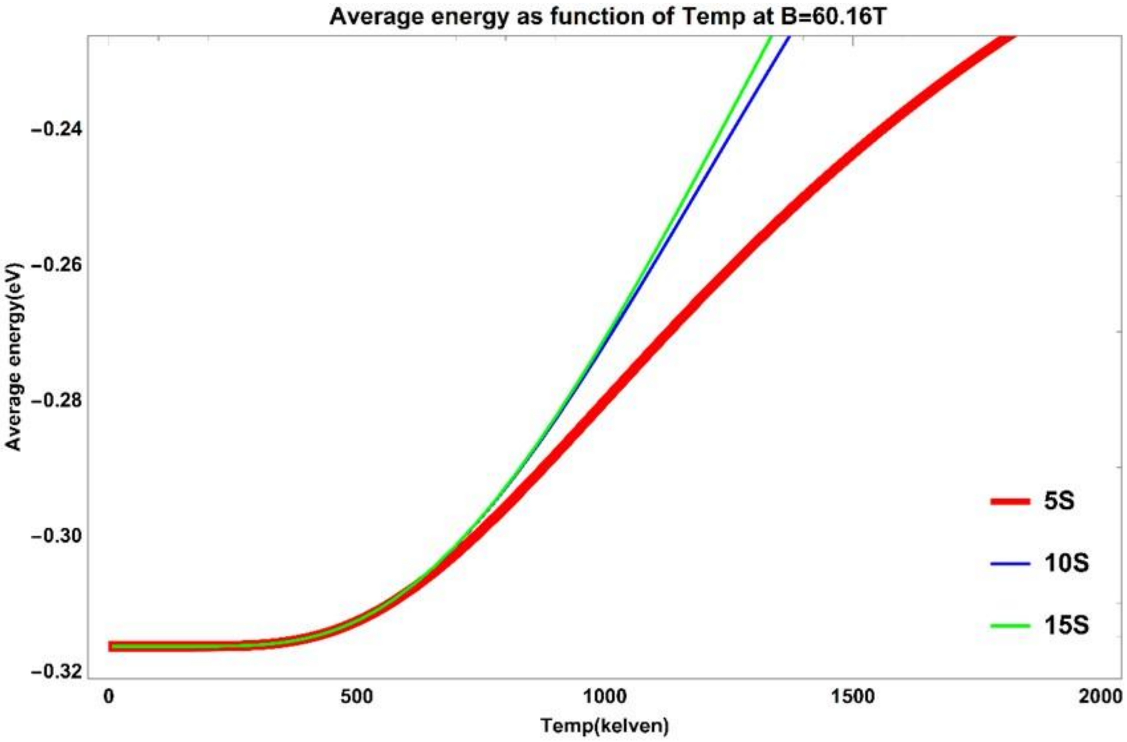

Fig. 4.5: The average energy as a function of temperature with magnetic field for WS_2

4.2 Thermal Properties of the Exciton in Quantum Dot

We can now move to the next step of this work, which is to display the thermal and magnetic properties in terms of different variables, including temperature (T) and magnetic field (B).

Firstly, we will start with the thermal properties of heat capacity (Cv) and entropy (S).

4.2.1 Heat Capacity of the Exciton in Quantum Dot

We study the effect of temperature on heat capacity in two TMD materials (WSe_2 and WS_2).

Figure 4.6, shows the dependence of heat capacity on temperature at zero magnetic field and with magnetic field effect for WSe_2. As we have seen, the heat capacity increases with increasing temperature in two cases, and reaches 2.5 at 500^0 K for zero magnetic effect and 1.4 at near 1000^0 K with magnetic field effect. After this value of temperature, the heat capacity starts decreasing to reach near zero at 2000K at

B = 0T and 8000K at B = 94T. As shown in the figure, we have a peak called the Schottky anomaly known for its heat capacity. This anomaly is considered one of the scientific matters that is still in the process of discussion and research, as they have not found any information about it yet. The increase in heat capacity with temperature (T) can be attributed to the increase in the thermal energy ($E_{th} = K_B T$) of the electrons, which increases the thermal excitation states of the electrons. But with the continuation of the increase in temperature (T), the material reaches a state of saturation, where all energy levels are filled equally, and we have saturation in the heat capacity. Therefore, the material stops responding to the thermal increase, so the heat capacity begins to decrease. [79]

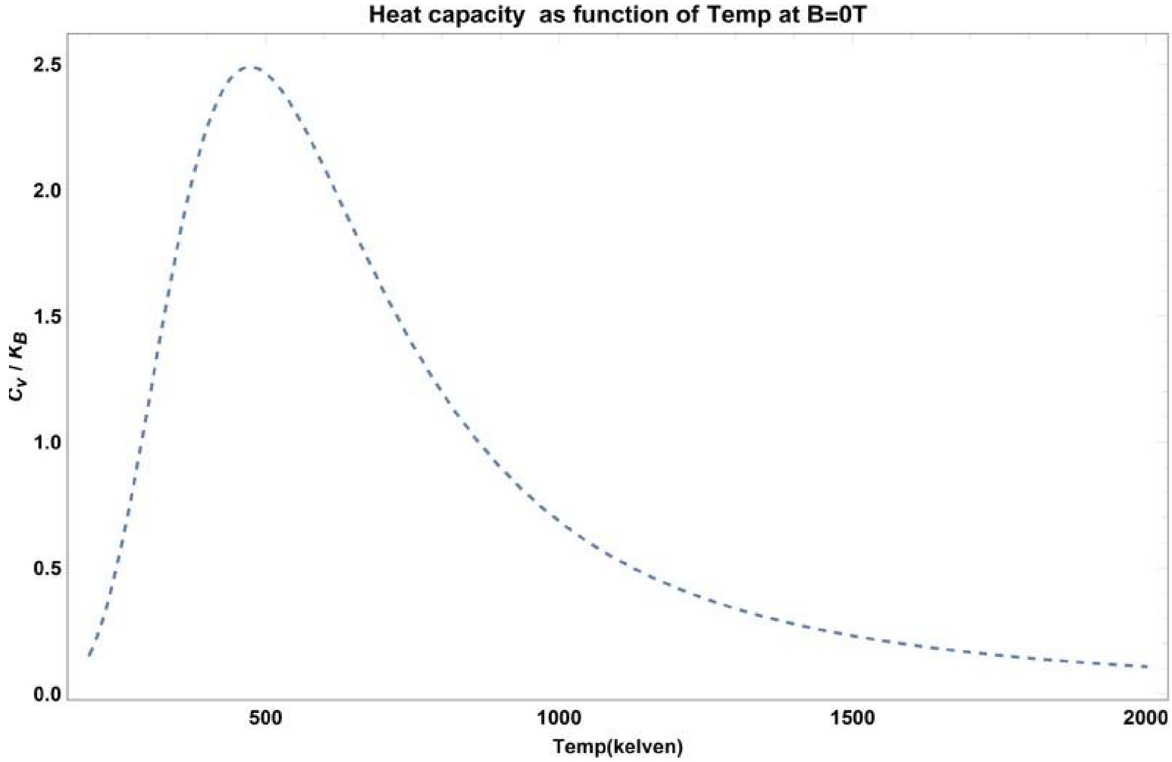

Fig.4.6.a: The heat capacity as a function of temperature for WSe_2 at zero magnetic effect

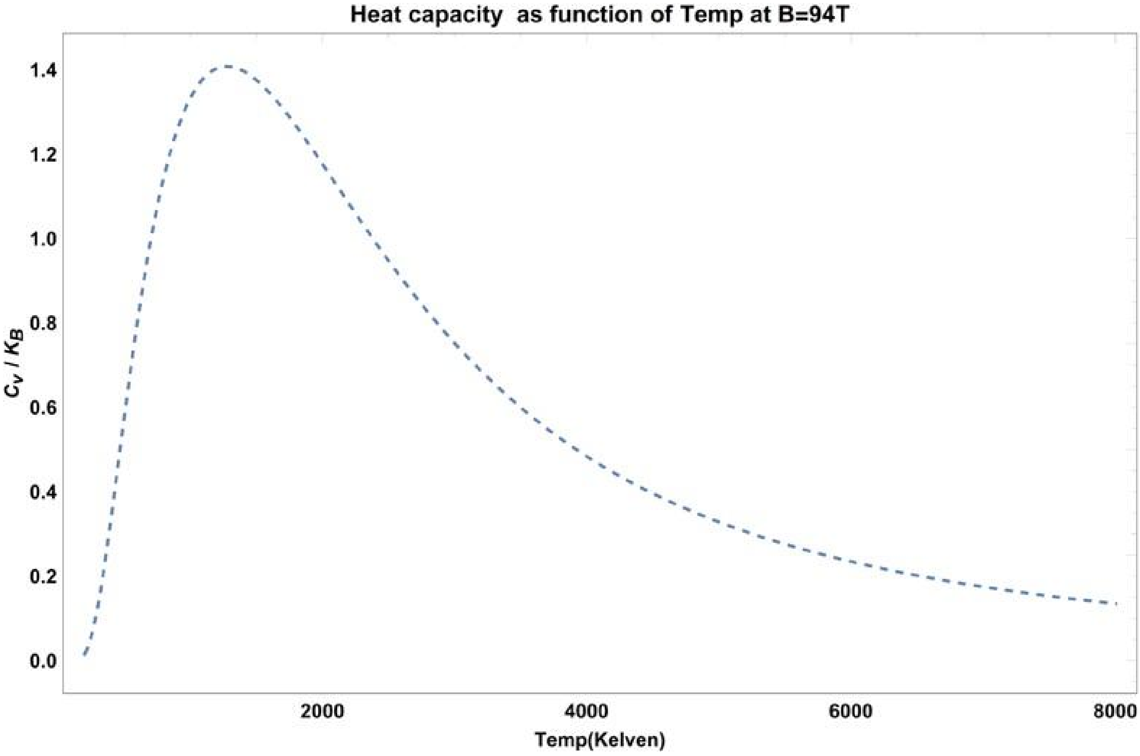

Fig.4.6.b: The heat capacity as a function of temperature for WSe_2 at 94T magnetic effect

The same work was done for WS_2, and we looked at the same behavior. From figure 4.7.a, we find that the heat capacity increases with increasing temperature to reach 2.4 at 1000^0 K at zero effect of the magnetic field, after that, it will decrease to reach near zero at 3000K for WS_2.

In figure 4.7.b, the heat capacity reaches 1.8 at 1200^0 K at 60.16T magnetic effect, after 1800^0 K, it decreases with increasing temperature to reach near zero at 7000^0 K for WS_2.

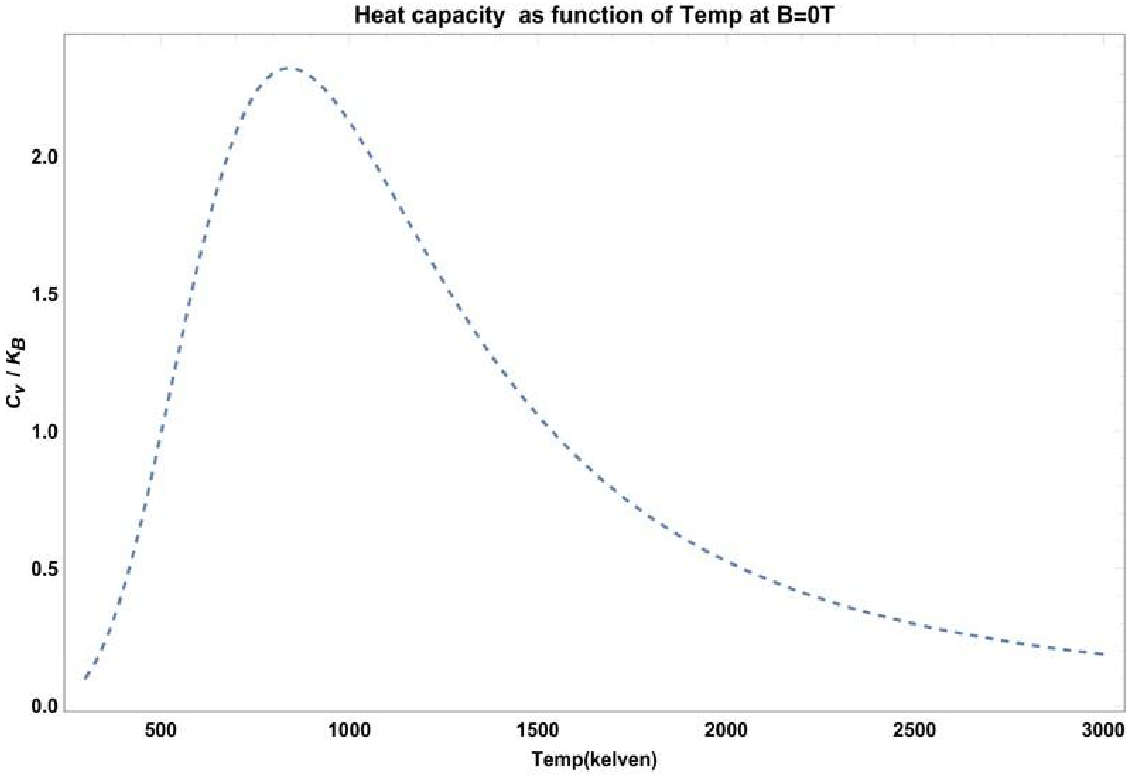

Fig.4.7.a: The heat capacity as a function of temperature for WS_2 at zero magnetic effect.

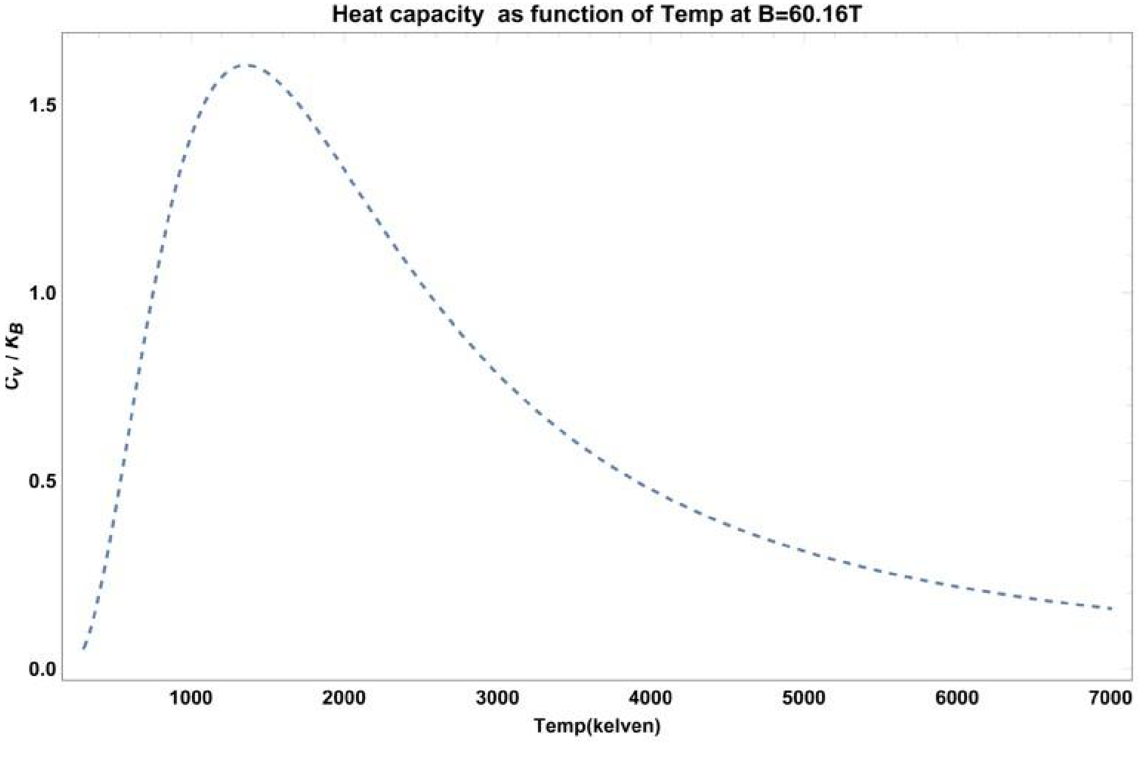

Fig.4.7.b: The heat capacity as a function of temperature for WS_2 at 60.16T magnetic effect.

The apparent behavior of heat capacity at low temperatures is due to lattice vibrations, as when low temperatures increase, the molecules in the substance begin to vibrate, thus triggering more vibration modes and thus increasing the heat capacity. Heat capacity also represents the amount of thermal energy absorbed or released by the molecules of the substance. When the temperature increases, the electrons and molecules have higher energy, and thus they are stimulated and excited to reach more energy levels, which leads to an increase in the heat capacity of the system.

When temperatures increase to a large level, the material reaches a state of energy saturation, or what is called "energy saturation". Then the response of the molecules within the material to heat decreases, leading to a decrease in heat capacity. [79,80]

In many of the studies that talked about TMD materials, they studied the thermal properties of different materials and got results close to those we got in this work. [81]

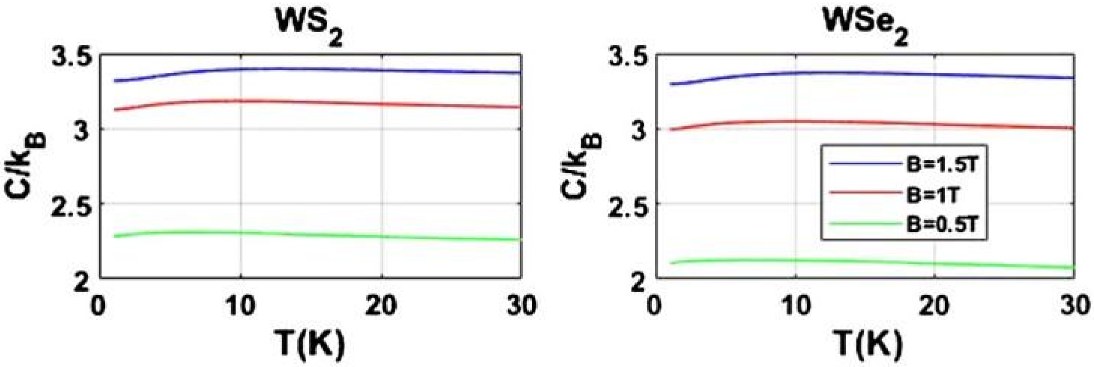

Fig.4.8: The heat capacity as a function of temperature in ref work [81]

In ref [81], T.V. Diffo , et al, studied the effect of temperature on heat capacity at different values of the magnetic field at low temperatures, explaining the general behavior of heat capacity, which increases with increasing temperature, but we note that the increase in heat capacity is very small and almost does not appear due to the low temperature of its use. I think that if they took higher temperatures, a clearer behavior of the heat capacity would appear.

In another work [79], Yahyah, Nehal S., et al, studied the behavior of heat capacity with respect to temperatures, and they had the same behavior and a Schottky anomaly, which means the heat capacity mostly has the same behavior.

4.2.2 Entropy of the Exciton in Quantum Dot

Another important quantity of thermodynamics that we studied and analyzed is entropy. It is a real physical quantity and a specific function of the state of the body. We calculated it based on an important factor, which is the temperature, and we studied the effect of the change in temperature by increasing and decreasing the entropy, as will be shown in the following figures.

As we did previously, we studied entropy in two cases depending on the magnetic field, one without the absence of the field and the other in the presence of the field. This, of course, was done for two materials, WSe_2 and WS_2.

For WSe_2, in figure 4.9 (a, b), we find that entropy is affected by temperature. As temperature increases, entropy increases until it reaches 1.7 at 2000^0 K with zero magnetic field, and at 94T of magnetic field, the entropy reaches 1.6 at 2000^0 K. After that, the entropy begins to stabilize and continues to stabilize as the temperature increases, until it reaches 6000K for both cases with and without the field effect.

As for the second figure (4.9.b), we stopped at a temperature of 2000^0 K in order to show the instability of entropy at this temperature. Therefore, we used a high temperature in the first figure (4.9.a) until we reached a stable state and saw the difference in the entropy behavior with the difference in temperature.

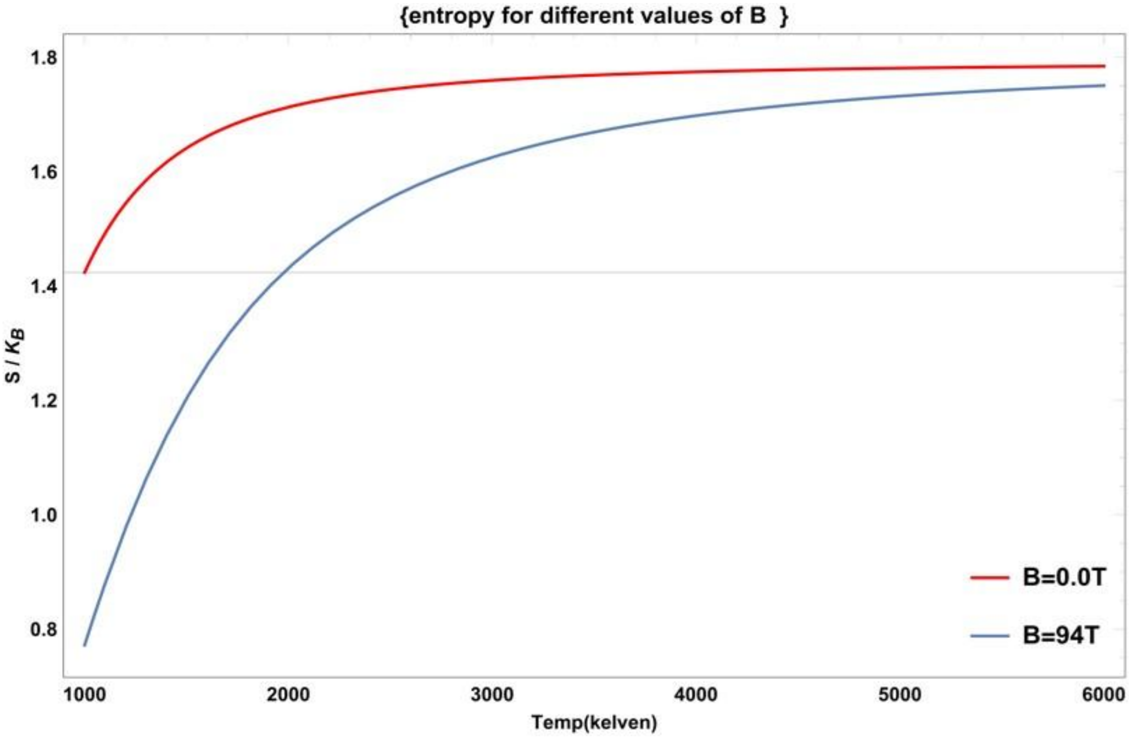

Fig.4.9.a: The entropy as a function of tempreture for WSe_2

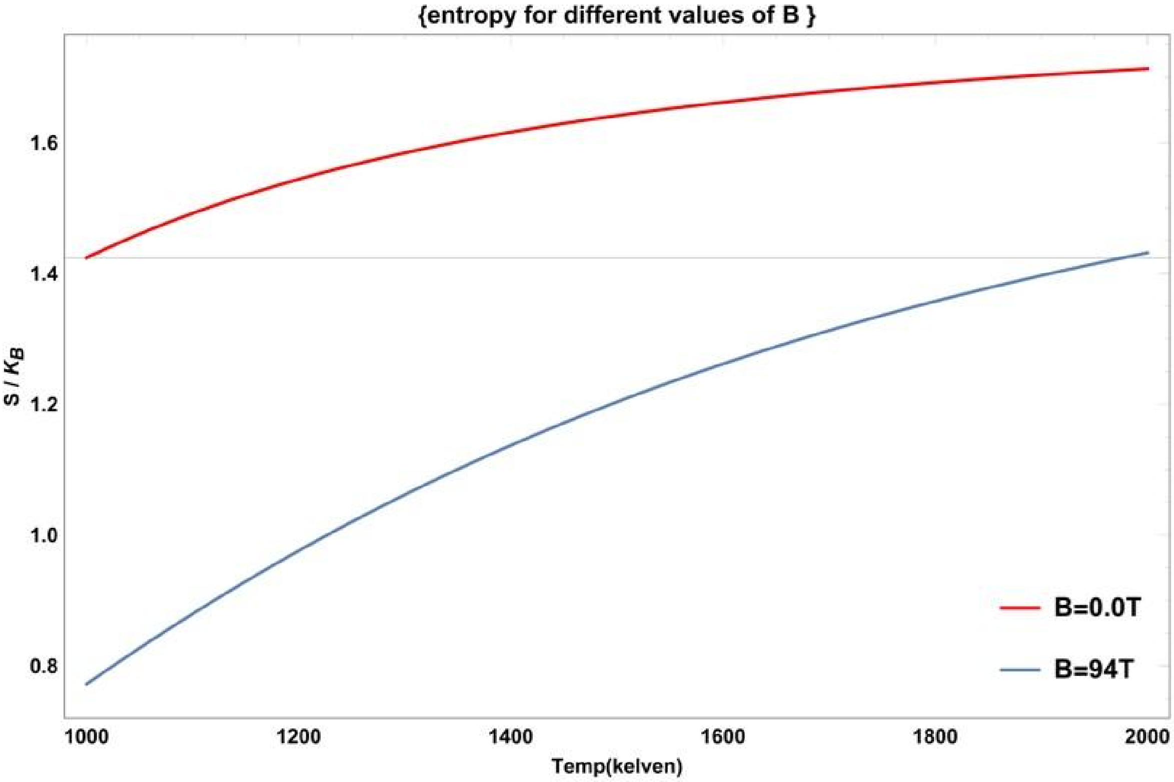

Fig.4.9.b: The entropy as a function of tempreture for WSe_2

The same work was done for WS_2, and when we look at the figures, we have nearly the same behavior. In figure 4.10.a we find that the entropy increases with increasing temperature until it reaches 1.7 for a zero magnetic field at 3000^0 K, and 1.6 at 60.16T at the same temperature. After that, the entropy will be stable and remain constant by increasing temperature until it reaches 7000^0 K.

We reduce the temperature to 3000^0 K to see the instability of entropy in figure 4.10.b for both cases with and without a magnetic field.

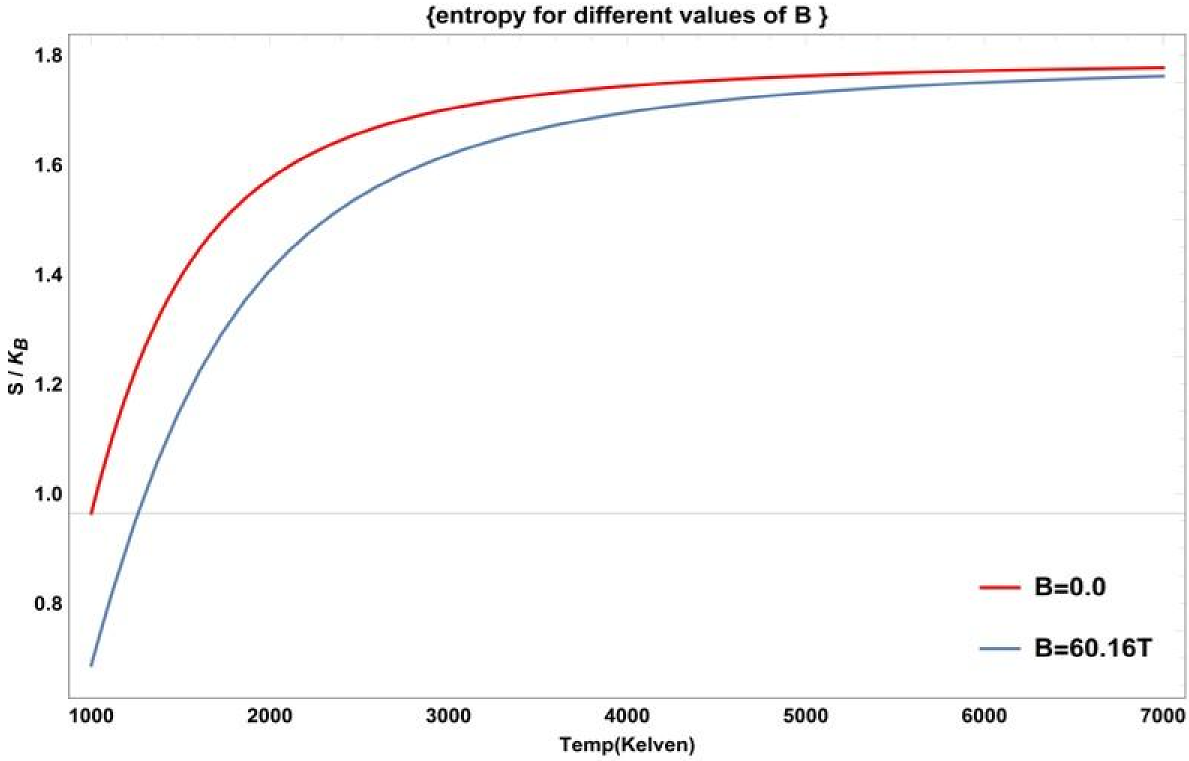

Fig.4.10.a: The entropy as a function of tempreture for WS_2

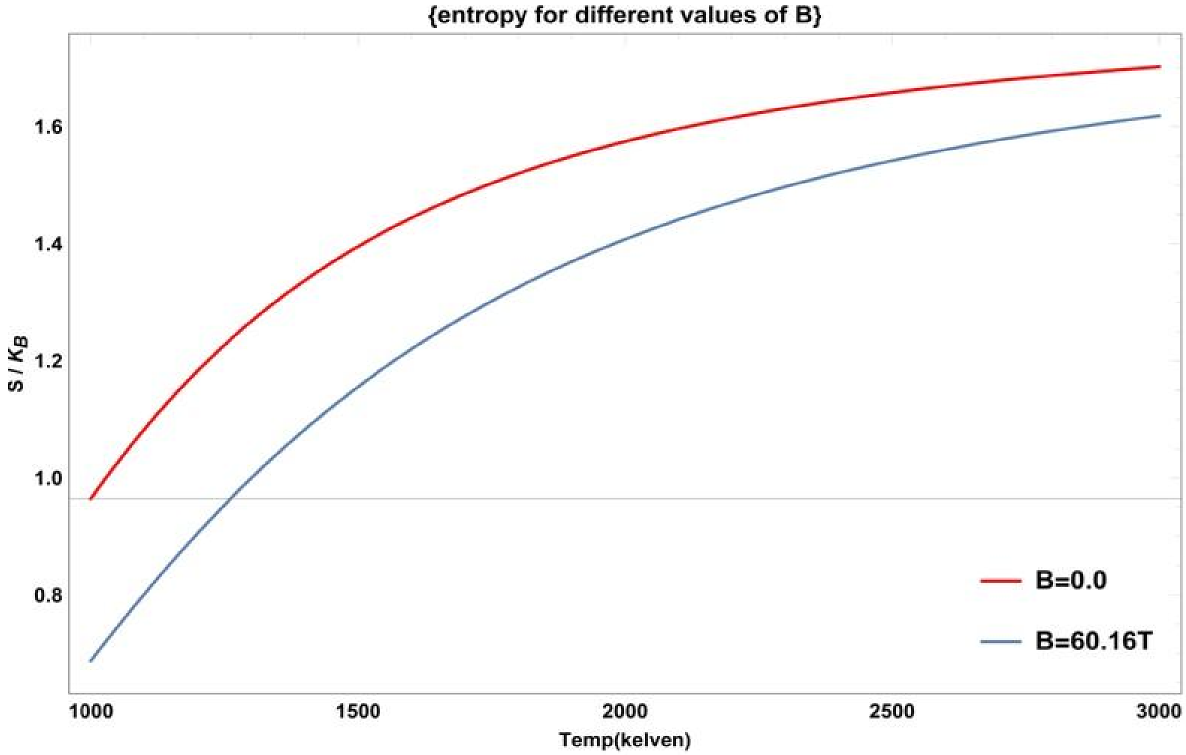

Fig.4.10.b: The entropy as a function of tempreture for WS_2

The relationship between entropy and temperature is a fundamental concept in thermodynamics and statistical mechanics. Entropy tends to increase with increasing temperature due to the statistical nature of the particles in the system, which can be expressed as a set of points:

Kinetic Energy: Temperature is a measure of the average kinetic energy of molecules in a system. When you raise the temperature of a system, the kinetic energy of the particles (atoms or molecules) inside it increases, and they therefore move faster and more randomly.

Chaos: Entropy is often related to the degree of disorder or randomness in a system. When particles move more rapidly and randomly due to increased temperature, the overall disorder of the system, or entropy, tends to increase. [82]

Phase transitions, such as melting. When a solid is heated to its melting point, it turns into a liquid. In the solid phase, the particles are more organized, restricted in their positions, and interconnected with each other. When you raise the temperature to melt the solid, the molecules gain more kinetic energy, break their ordered structure, and become more randomly distributed in the liquid phase. This increased randomness contributes to an increase in the entropy.

In classical thermodynamics and for most common materials, the general trend is that entropy increases with temperature. This is consistent with the second law of thermodynamics, which states that the entropy of an isolated system tends to increase with time. [82]

4.3 Magnetic Properties of the Exciton in Quantum Dot

Magnetic properties refer to the response of a material to an applied magnetic field. Different materials react to the application of a magnetic field differently.

Therefore, it is necessary to talk about this important aspect, which explains the influence of magnetic field on materials, but in order for us to enter into the magnetic properties, we need to calculate the energy in order to study the magnetic properties.

4.3.1 Statistical energy

We have studied statistical energy in terms of several parameters (temperature and magnetic field) for two TMD materials (WSe_2, WS_2) and to show the behavior of statistical energy, you can see figures 4.11.a and 4.11.b. These figures show statistical energy at two different temperatures, and if we look at the two figures for WSe_2, we find that the statistical energy has the same behavior at the same range of magnetic field, where the statistical energy increases with increasing magnetic field to reach 0.16eV at 4T at 100^0 K. In the second figure, we raise the temperature to 300^0 K where the statistical energy reaches -0.15eV at 4T. Mostly, the value of statistical energy does not change with temperature. Also, we studied statistical energy at 10^0 K (at a small magnetic values), but we found the same value and behavior of statistical energy at 100^0 K and 300^0 K.

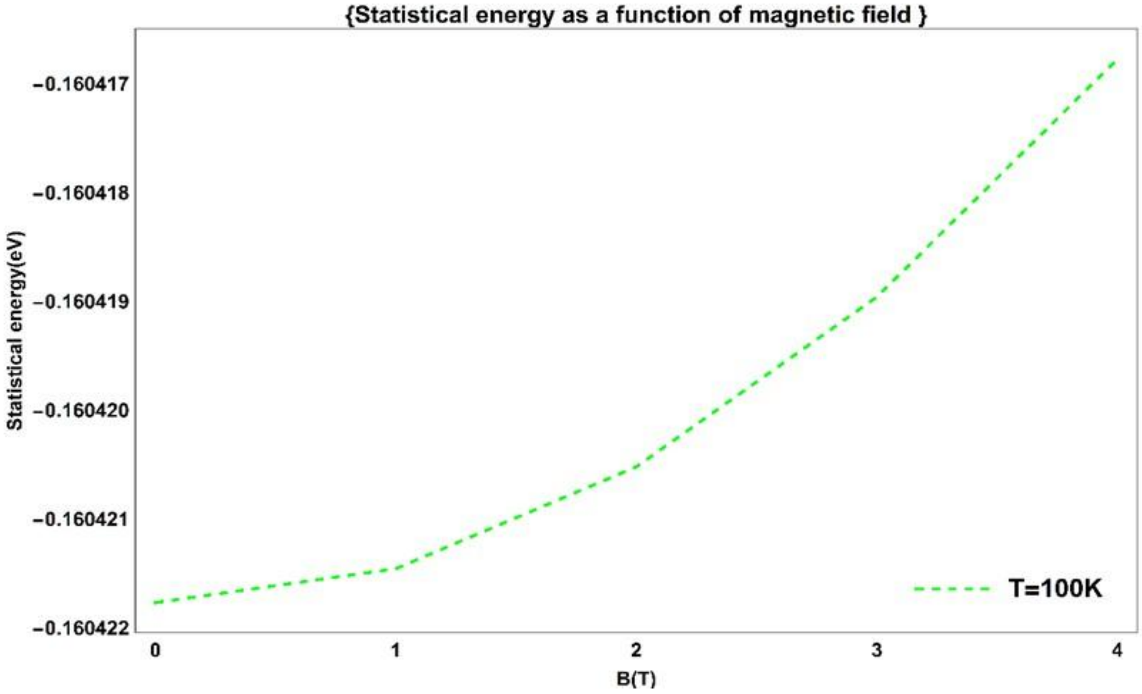

Fig.4.11.a: Statistical energy as a function of magnetic field at 100°K for WSe_2

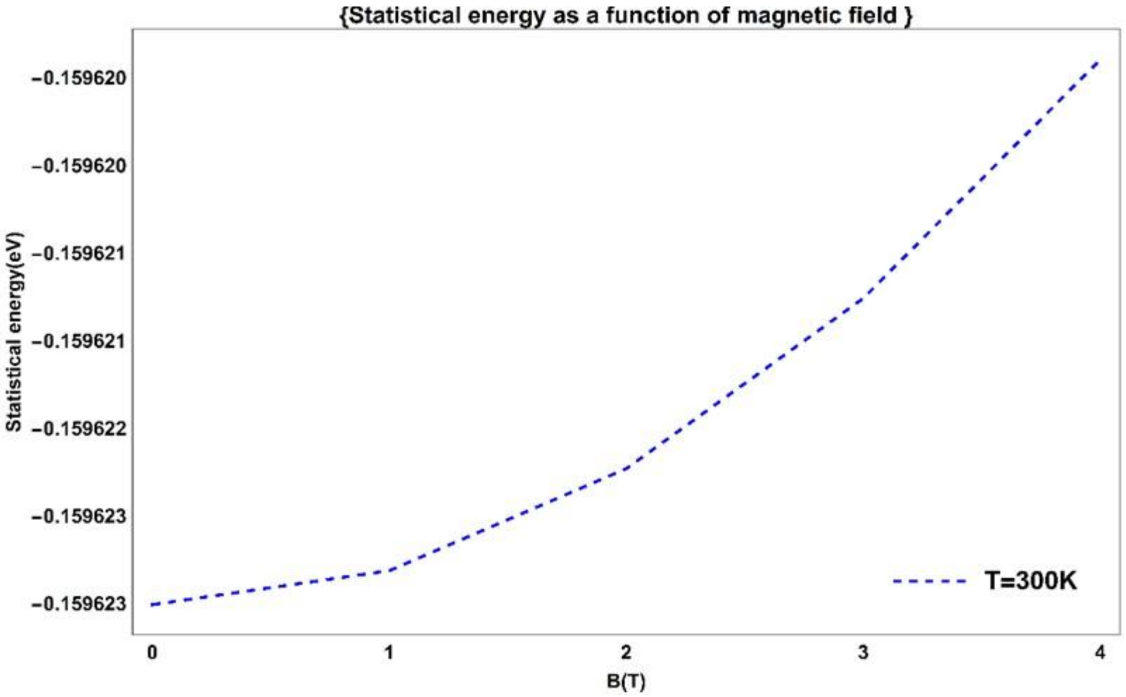

Fig.4.11.b: Statistical energy as a function of magnetic field at 300°K for WSe_2

The same behavior of statistical energy appears in my work for WS_2 at the same temperature in the same range of magnetic field with different values for statistical energy, where the statistical energy reaches -0.318 eV at 100^0 K and -0.317eV at 300^0 K. Figures 4.12.a and 4.12.b.

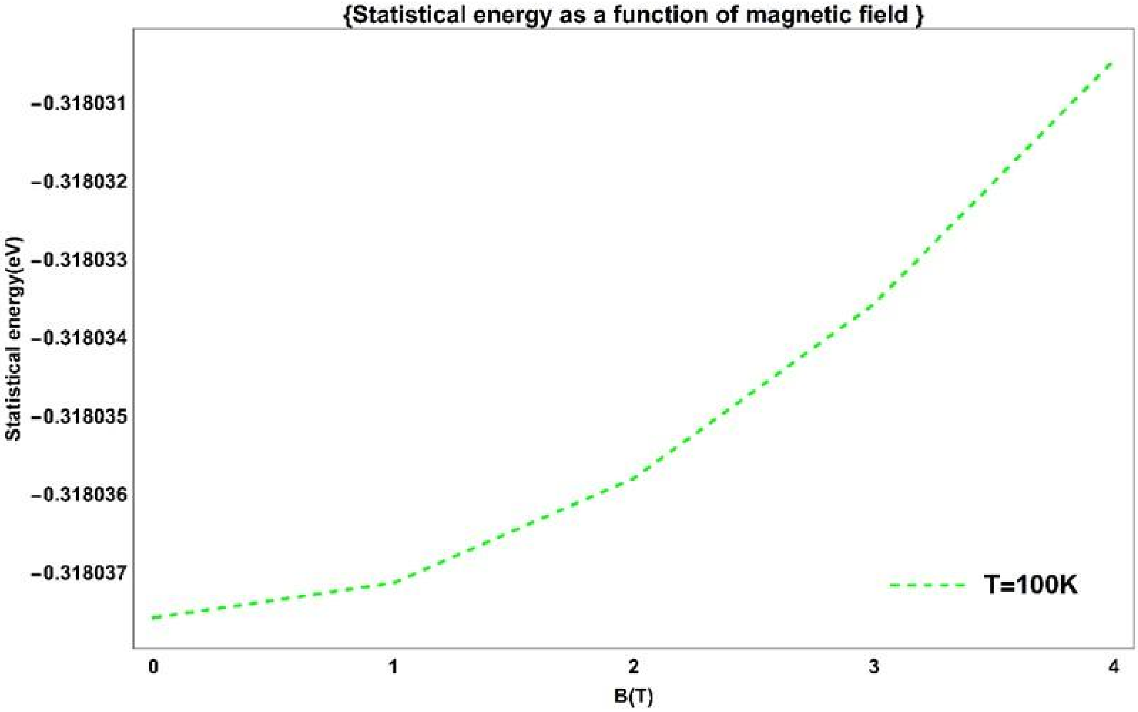

Fig.4.12.a: Statistical energy as a function of magnetic field at 100K for WS_2

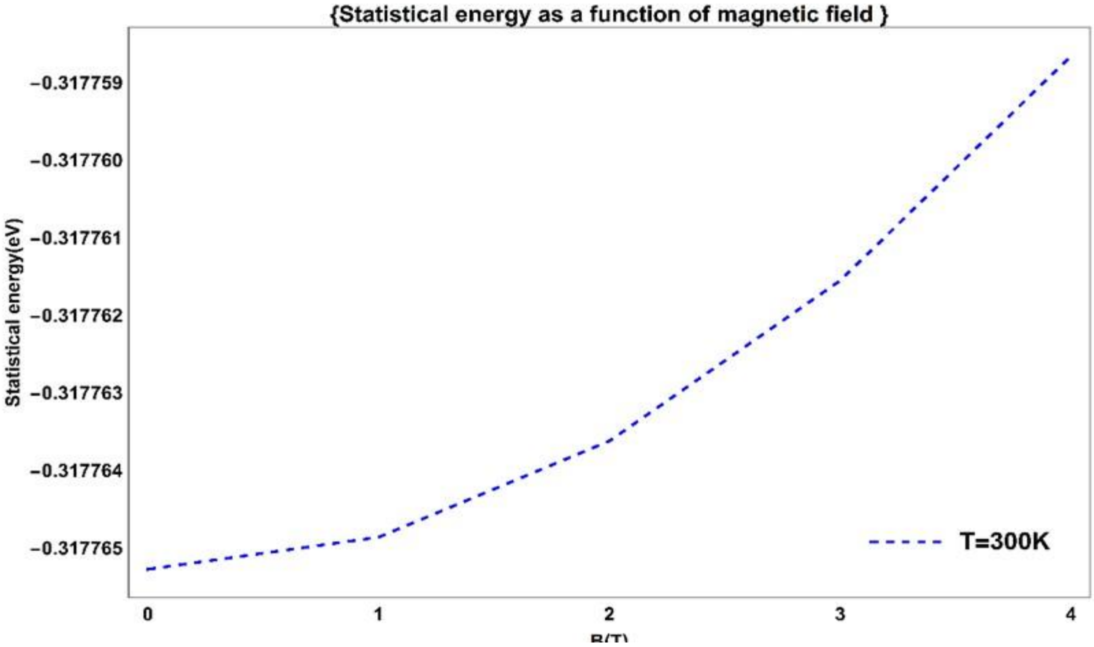

Fig.4.12.b: Statistical energy as a function of magnetic field at 300^oK for WS_2

In general, a magnetic field can have a profound effect on the energy levels and statistical properties of charged particles, especially electrons. It leads to quantization of energy levels, splitting of spectral lines, and changes in the statistical behavior of particles. These effects are described in the field of quantum mechanics and can be summarized as follows: [82,83]

Zeeman Effect: is the splitting of spectral lines in the presence of a magnetic field. When an atom or molecule is placed in a magnetic field, the energy levels of its electrons are affected. Electrons have an intrinsic property called spin, which can interact with a magnetic field. This interaction causes the energy levels to split into multiple sublevels, a phenomenon known as the Zeeman effect. This effect is observed in atomic and molecular spectra and provides important information about the magnetic properties of the system. This division leads to an increase in the value of energy, and this, is the reason for the increase in energy with the increase in the magnetic field, as shown in the previous figures. [82,83]

The statistical properties of a system of charged particles in a magnetic field are described by quantum statistics such as Fermi-Dirac statistics for fermions (such as electrons) and Bose-Einstein statistics for bosons. The presence of a magnetic field can affect the distribution of molecules in energy levels, leading to changes in thermodynamic properties such as specific heat capacity and magnetization. [83]

4.3.2 Magnetization (M)

In this section, we calculate the magnetization (M) of QD as a function of temperature and magnetic field. To study the effect of magnetic field on magnetization, figures (4.13, 4.14.a and 4.14.b). We calculate magnetization in unit of effective Bohr magneton [84] $\mu_B = e\hbar/2m^*$ $=0.289*10^{-3}$ eV/T for WSe_2 and equal $0.3622*10^{-3}$ eV/T for WS_2.

In the first stage, we deal with WSe_2, at 110^0 K in range of zero to four tesla of magnetic field, and we find that the magnetization decreases with increasing magnetic field, it started from -0.001 at 1T to reach -0.008 at 4T. We took another value of temperature of 150^0 K, but we noted the same behavior, the magnetization decreases with increasing temperature, with the same values (starting from -0.001 at 1T to reach 0.008 at 4T).

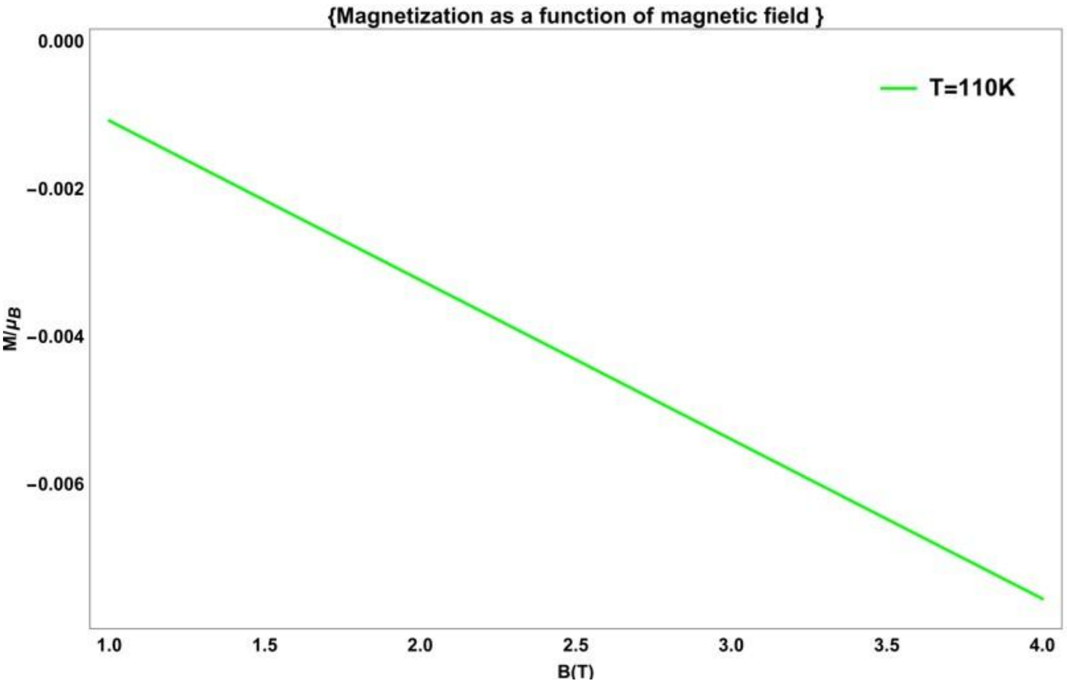

Fig.4.13: Magnetization as a function of magnetic field at 110^0 K for WSe_2

WS_2, figure 4.14.a, show that the magnetization decreased with increasing magnetic field, starting from zero at 0T to reach -0.05 at 60T at 900^0 K.

When we decrease the temperature to 10^0 K, the magnetization reaches -0.14 at 60T, see figure 4.14.b. Means that, when we decrease the temperature, the magnetization decreases at high magnetic fields (60T) but at low magnetic fields (0T) the magnetization takes the same value and starts from zero.

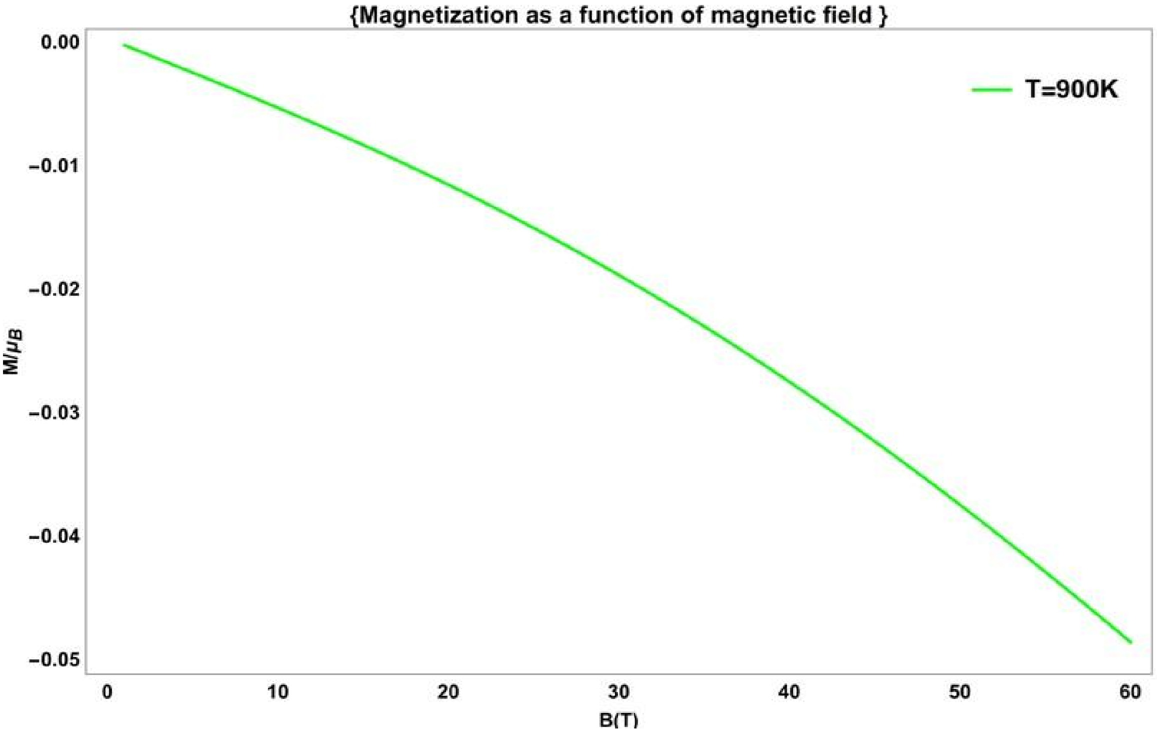

Fig.4.14.a: Magnetization as a function of magnetic field at 900^0 K for WS_2

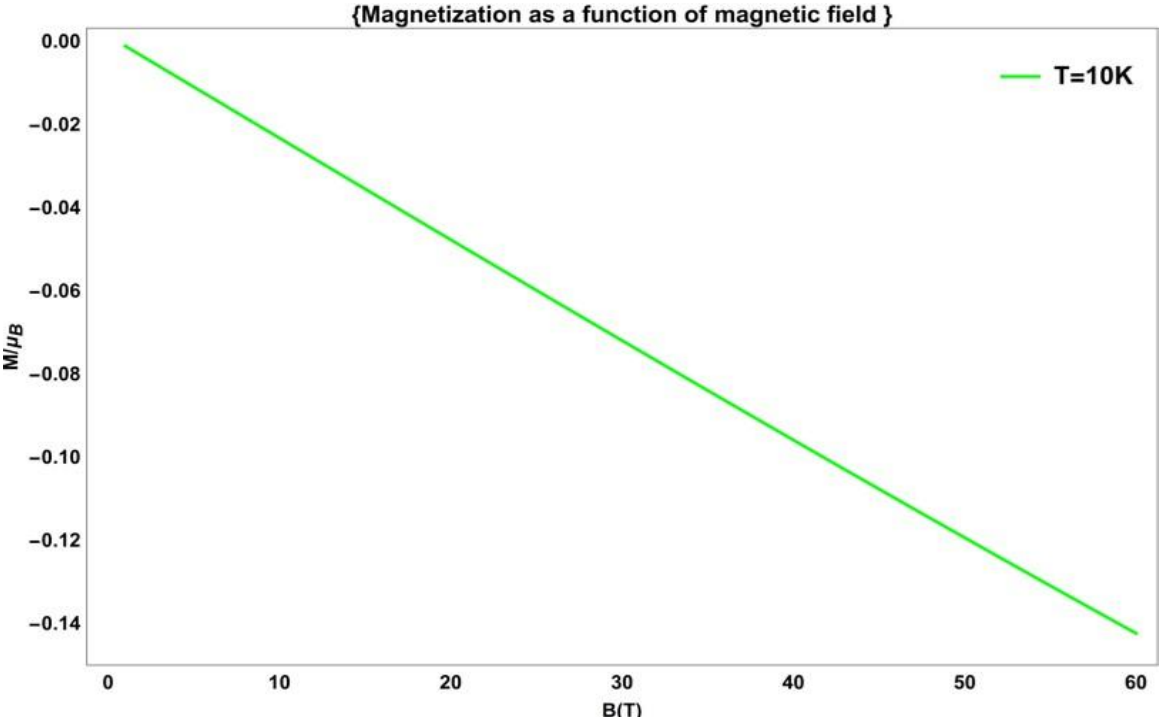

Fig.4.14.b: Magnetization as a function of magnetic field at 10^o K for WS_2

The magnetization of a material can decrease with an increase in the magnetic field under certain conditions, due to the properties of the material and its magnetic behavior. This phenomenon is called "magnetic saturation," and it occurs in ferromagnetic and nonferromagnetic materials. There are various reasons for the decrease in magnetization as the magnetic field increases, including: [85]

Ferromagnetic and nonferromagnetic materials have atomic or molecular magnetic moments that can align with an external magnetic field. When an external field is applied, these moments tend to align with the field, resulting in an increase in magnetization. As the external field strength increases, more and more of these moments align with the direction of the field, resulting in increased magnetization. At this moment, the substance reaches a state called saturation. When all or most of the magnetic moments in a material align with the field, the material becomes “saturated.” At this point, applying a stronger magnetic field does not significantly increase the alignment of the additional moments because most of them are already directed in the direction of the field. At this point, the material begins to lose its magnetism and magnetism begins to decrease as the external field increases.

In short, the magnetization of ferromagnetic materials reaches a maximum value called saturation magnetization when all available magnetic moments are aligned with the external magnetic field. Hence, increasing the magnetic field strength does not lead to a significant increase in the additional alignment moments, which leads to a decrease in the rate of magnetization increase. Understanding this behavior is important in various technological applications, such as the design of magnetic devices and materials.

Many previous studies and research projects have been conducted on the behavior of magnetization and the effect of the magnetic field on matter. The most prominent of these studies were:

Asmaa yaseen, et al, studied the effect of the magnetic field on the impurities present in GaAs, where they studied magnetization as a function of the magnetic field in the presence of impurities or not, and the behavior of magnetization was as it appeared to us, which is a decrease with an increase in the magnetic field in both cases at different temperatures. [86]

Another study by Nouf, Ibrahim, et al showed the effect of a magnetic field on an electron present in a two-dimensional quantum dot. They first studied magnetization as a function of the magnetic field at different temperatures, and the behavior was similar to our result. On the other hand, they studied magnetization as a function of temperature at different values of the magnetic field, and here the behavior of magnetization was different, as it decreased and then increased with increasing temperature until a certain value was reached. [87]

Also, Rehan, Hanaa, et al study the effect of the magnetic field in GaAs semiconductor quantum pseudo-dot systems. Magnetization was studied as a function of the magnetic field at different voltage values, and the behavior of magnetization here was in the form of a sinusoidal curve, decreasing, then increasing, then decreasing, and so on. The study also included the presence or absence of impurities, and based on that, the properties were studied. [88]

4.3.3 Magnetic Susceptibility

In this subsection, we talk about the sensitivity of the exciton to the magnetic field in a two dimensional quantum dot, which is a measurement of the extent to which a material is attracted to or repulsed by a magnetic field. This means that we mean magnetic susceptibility.

Figures 4.15, 4.16.a and 4.16.b show the corresponding magnetic susceptibility as a function of the magnetic field strength at different temperatures for TMD materials (WSe_2 and WS_2). The figures show clearly a great change in the behavior of the magnetic susceptibility curves as we increase the confinement strength from 0 to 4 to 50T. In Figure (4.15) for WSe_2, it is observed that for lower values of temperature (10^0 K and 20^0 K) the magnetic susceptibility of the system is negative and has the same behavior, which means the system is diamagnetic.

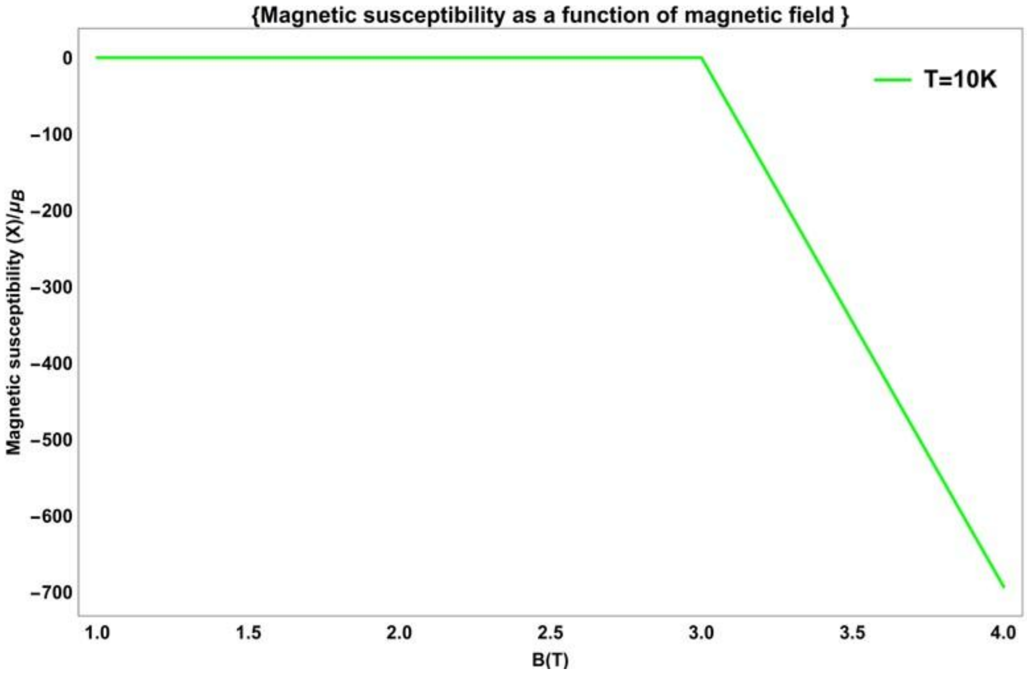

Fig.4.15: The magnetic susceptibility as a function of magnetic field at 10,20° K for WSe_2

On the other hand, for the higher values of the temperature and magnetic field for WS_2, we notice that the behavior of magnetic susceptibility is completely different. In figures 4.16.a and 4.16.b, we observe that for lower and higher values of temperature (10^0 K and 100^0 K), the magnetic susceptibility of the system is positive and has the same behavior, which means that the system is paramagnetic.

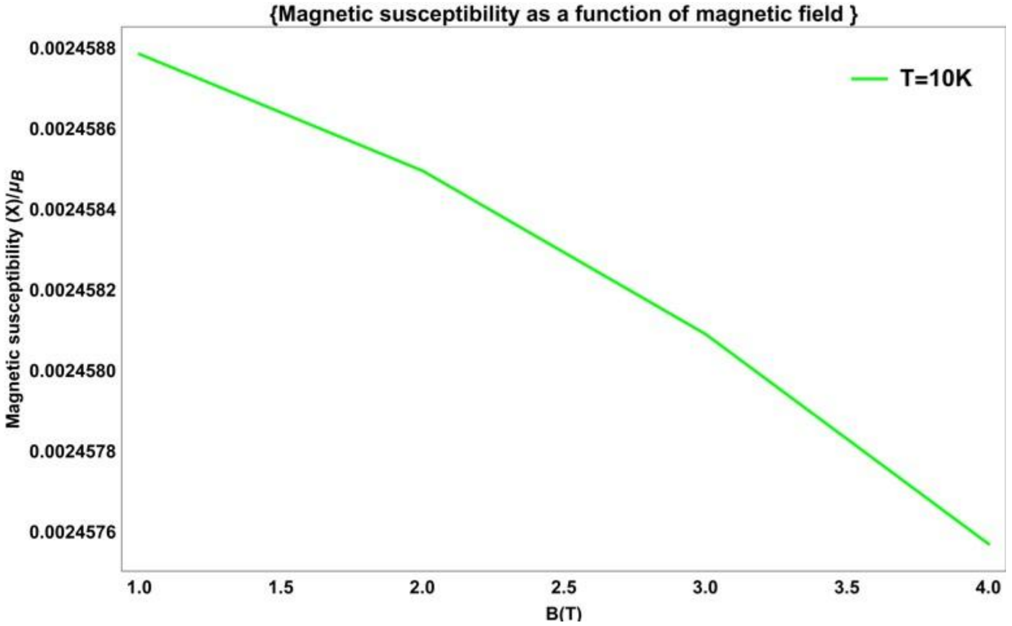

Fig.4.16.a: The magnetic susceptibility as a function of magnetic field at 10° K for WS_2

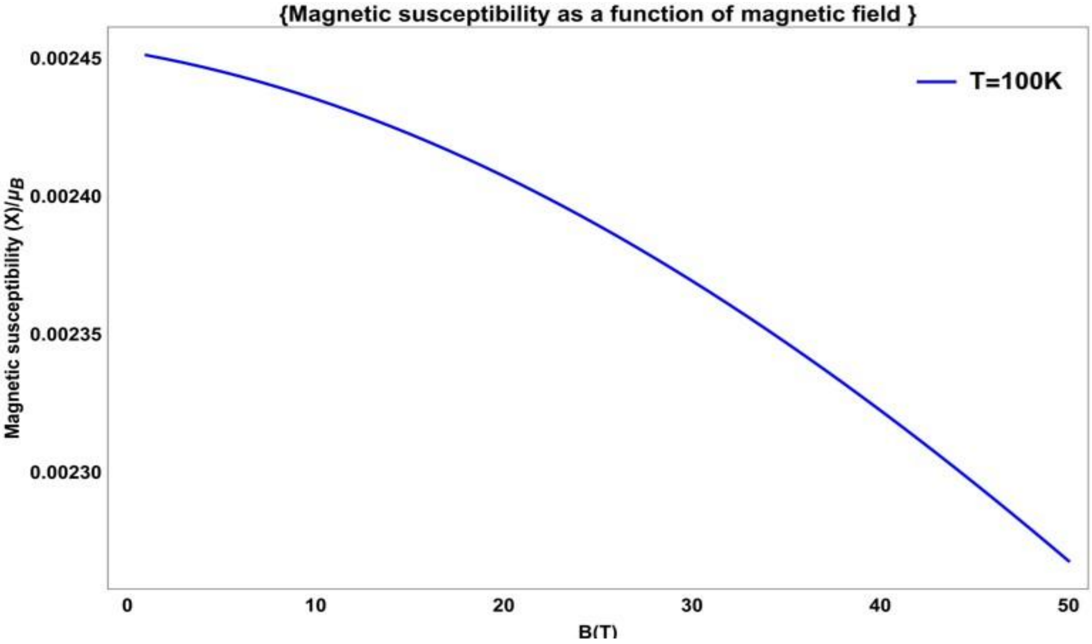

Fig.4.16.b: The magnetic susceptibility as a function of magnetic field at 100° K for WS_2

The behavior of magnetic susceptibility as a function of the magnetic field is a fundamental pillar in the fields of magnetism and condensed matter physics.

There are two main types of magnetic susceptibility: [89]

Paramagnetic: Paramagnetic materials contain atoms or ions with unpaired electrons, which means that their magnetic moment is non-zero. When an external magnetic field is applied, the magnetic moments of these unpaired electrons tend to coincide with the field. This alignment causes the material to become weakly magnetized in the direction of the applied field. Susceptibility is positive for paramagnetic materials and is directly proportional to the strength of the applied field.

Diamagnetic: Magnetic materials have all their electrons spin-paired, resulting in no net magnetic moment in the absence of an external field. When a magnetic field is applied, magnetic materials develop an opposite magnetic moment in the direction of the applied field. This opposition results in negative susceptibility, meaning it is less than zero. The magnetization of magnetic materials weakly opposes the applied field.

In summary, the behavior of the magnetic susceptibility as a function of magnetic field depends on the type of material:

For paramagnetic materials, the sensitivity is positive and increases linearly with the applied field strength.

For diamagnetic materials, the susceptibility is negative, and the magnetization increases linearly in the direction opposite to the applied field.

This relationship between magnetic susceptibility and magnetic field strength is a key factor in understanding how different materials respond to magnetic fields, and is used in various applications, including the design of magnetic materials and devices.

We can compare our results with many previous studies like Asmaa yaseen, , Rehan, Hanaa, et al, studded the most notable of which are: a study conducted on GaAs to study the effect of magnetic field on the impurities of GaAs, and in this work, we studied the relation between magnetic susceptibility and magnetic field at different temperatures, which we observed differently from the behavior seen with us. [86,88] Also, Ibrahim, Nouf, et al, different behaviors are shown in the research he conducted on the effect of rashba and a magnetic field on an electron present in a twodimensional quantum dot. It measured the magnetic susceptibility as a function of temperature at different values of the magnetic field. [87]

4.4 The density of state (DOS)

We study density of States (DOS) to understand the electronic properties of materials, by describing the system's responses to Hamiltonian parameters such as the magnetic field.

In figure 4.17 and 4.18, the DOS was studied as a function of energy at different values of the magnetic field (50T,60.16T and 94T) for both WSe_2 and WS_2, we notice from the figures below that the presence of the external magnetic field eliminates the degeneracy of the states, so the DOS gives one at each value of the energy spectrum. Also, the DOS value is greater when we are affected by a lower magnetic field, as the greater the value of the external magnetic field, the lower the DOS value in general.

Where the DOS value reaches 35 at 50T and 94T for WSe_2 and reaches to 40 at 50T and 35 at 60.16T for WS_2.

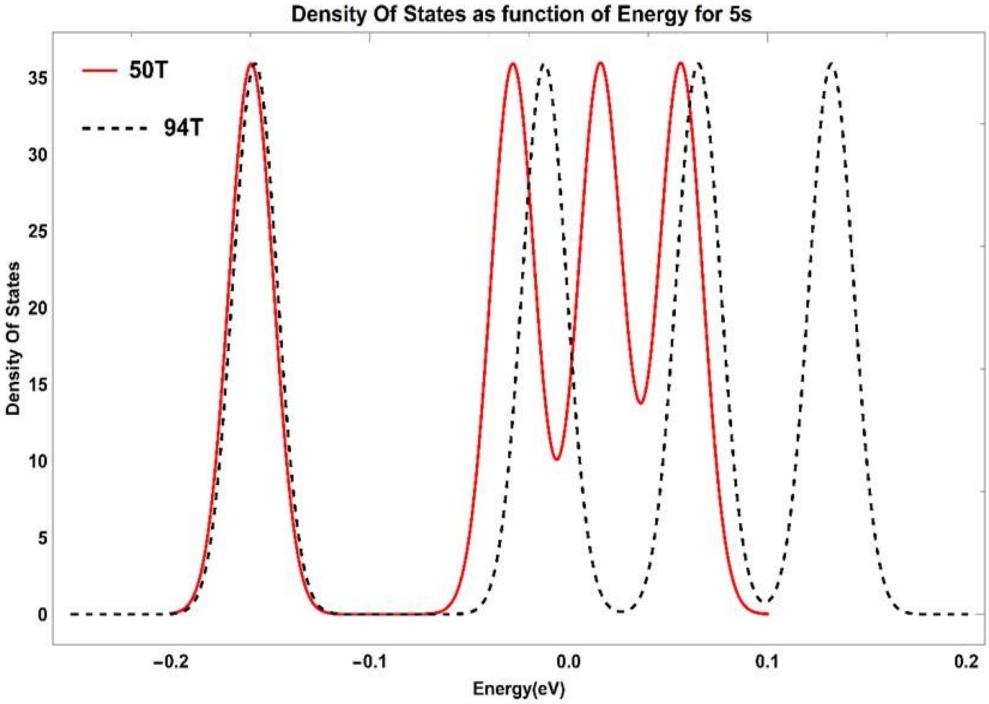

Fig.4.17: DOS vs. Energy for WSe_2 for different magnetic field values

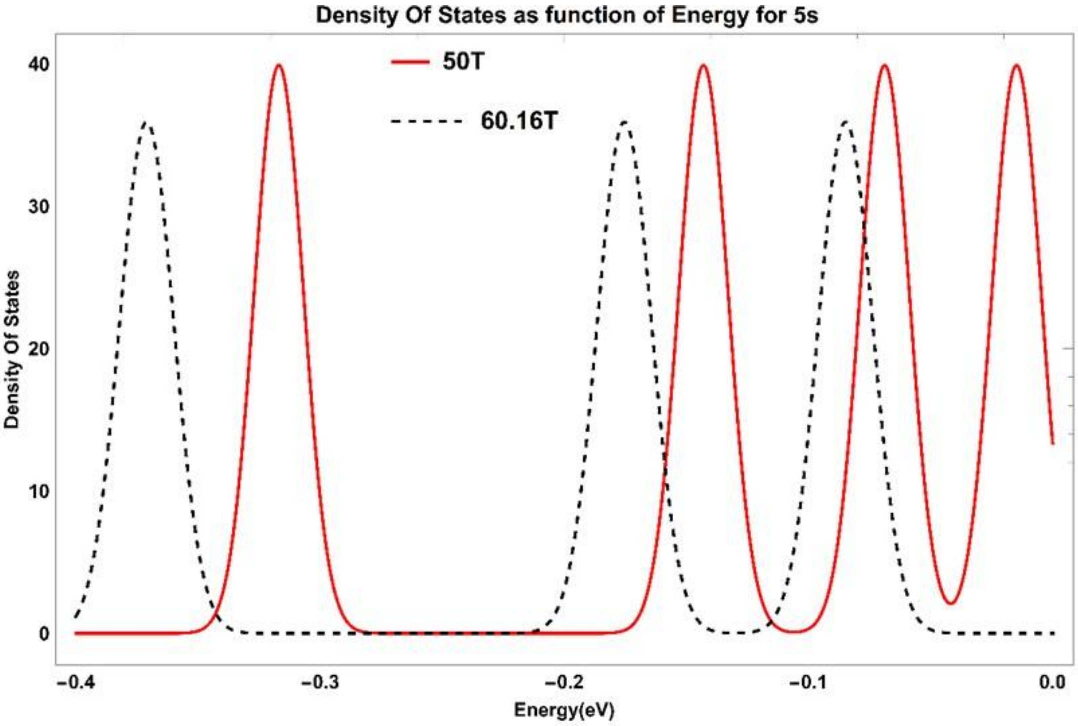

Fig.4.18: DOS vs. Energy for WS_2 for different magnetic field values

The relationship between density of states (DOS) behavior and increasing magnetic field depends on the qualitative properties of the material and the extent of interaction and response between the magnetic field and the electronic structure. In some cases, the DOS system may undergo changes as the magnetic field increases. However, we can say that the relationship between DOS and magnetic field is unpredictable because it can vary based on the general properties of the material.

We can explain why the value of the density of states decreases with the increase of the magnetic field as follows:

Zeeman splitting: When we impact matter with an external magnetic field, the Zeeman effect causes the energy levels of electrons with different spin directions to split, resulting in a change in the distribution of states within the DOS. This partitioning can reduce the available states at certain power levels, resulting in a lower overall DOS in those regions. [90]

It is important to consider specific properties of matter such as magnetic properties, electronic structure, and band structure when we study the effect of a magnetic field on the density of states. We perform experiments and obtain experimental observations as well as theoretical calculations to provide a detailed understanding of how DOS responds to changes in the presence of the magnetic field strength of a given material. The nature of this response may vary greatly depending on the substance and specific conditions of the experiment. [90]

4.5 The magneto-caloric effect (MCE)

Magneto-caloric effect (MCE), was studied in order to identify the thermomagnetic properties by identifying the behavior of the material with the change in temperature when the material is exposed to a changing magnetic field.

In other words, through this property we can study the phenomenon of heating and cooling (the change in temperature of the substance) due to the application of a magnetic field on it. [91]

The study was conducted specifically on TMD materials (WSe_2 and WS_2), in both materials, the behavior was similar, as the behavior took the form of a Gaussian distribution, and the temperature reached a very high value, which is 4000 K. We know that this temperature is not practical, but the reason for it being high is that TMD materials require very high thermal energy and therefore We need high heat in order to increase the kinetic energy of the electron so that it can move from one state to another randomly, so that we obtain randomness in the system and thus obtain the required logical form. (Figures 4.19 and 4.20. [91,92])

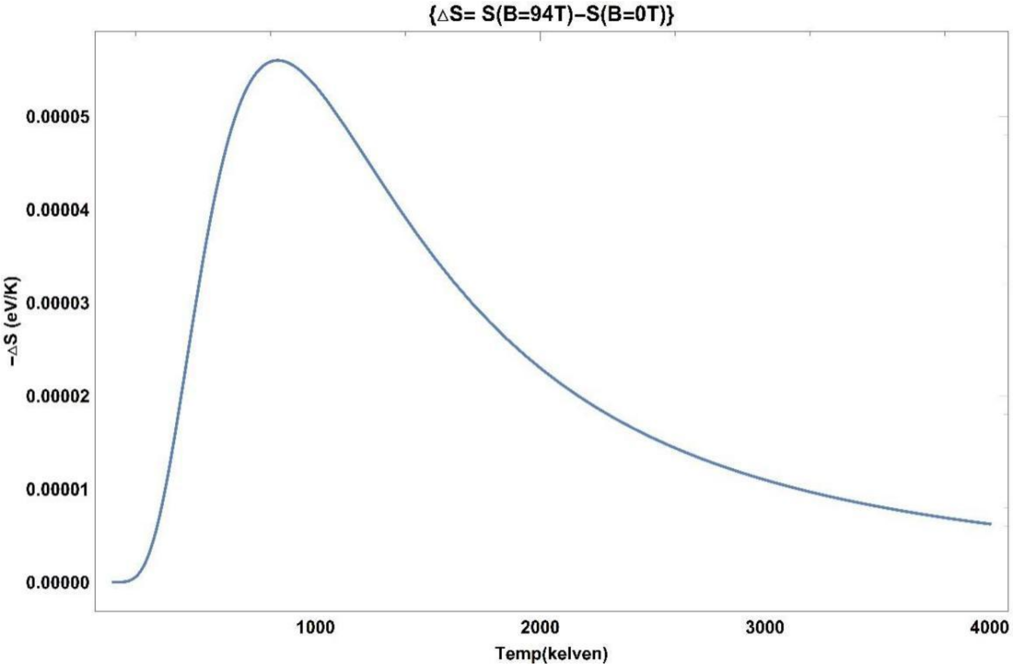

Fig.4.19: MCE vs Temperature for WSe_2 for different magnetic field values

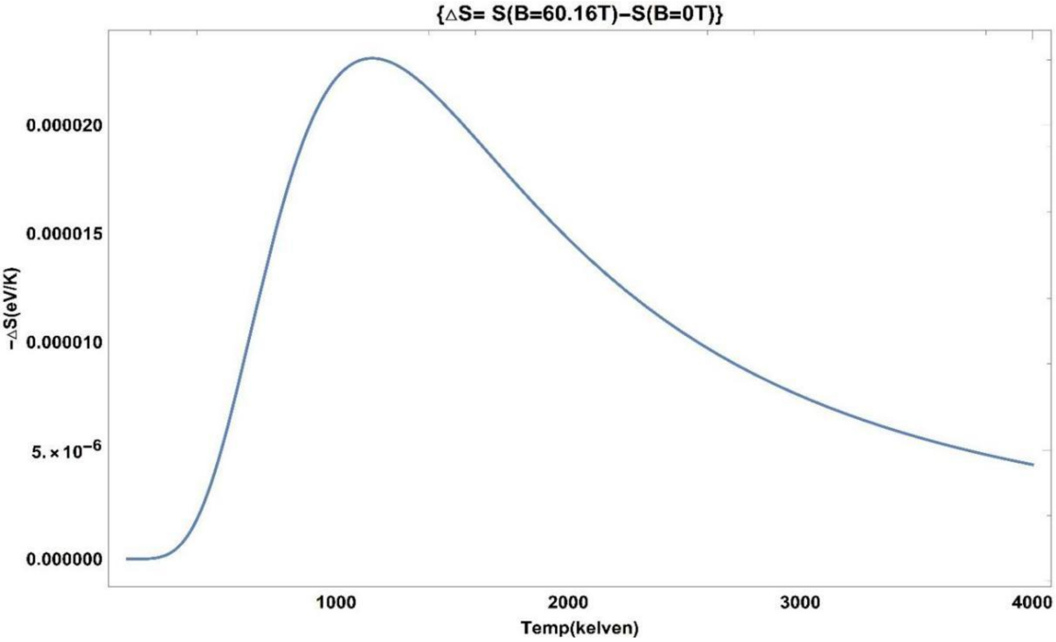

Fig.4.20: MCE vs Temperature for WS_2 for different magnetic field values

4.6 The Diamagnetic coefficient (σ)

In order for the picture to be clearer and more complete, it is necessary to talk about diamagnetic coefficient in terms of studying the relationship between energy and the magnetic field as a derivative and comparing the results that were reached through the 1/N expansion method with previous theoretical and practical results.

The study was conducted as previously on two TMD materials (WSe_2 and WS_2), and the results showed the general behavior between diamagnetic coefficient (σ) in (eV/T^2) and the magnetic field in T, with slight differences between the two materials at different levels (1S,2S and 3S).

For WSe_2, looking at the attached figures (4.21, 4.22and 4.23), which were conducted (without effect of temperature) as magnetic field goes to zero Tesla (small range of magnetic field, at approximately 10 T), we find that diamagnetic coefficient (σ) decreases with the increase in the magnetic field for three levels (1S, 2S and 3S) until it started from $6.24*10^{-7}$(eV/T^2) for 1S, $9.80*10^{-6}$(eV/T^2) for second level (2S) and $0.40*10^{-4}$(eV/T^2) for third level (3S).

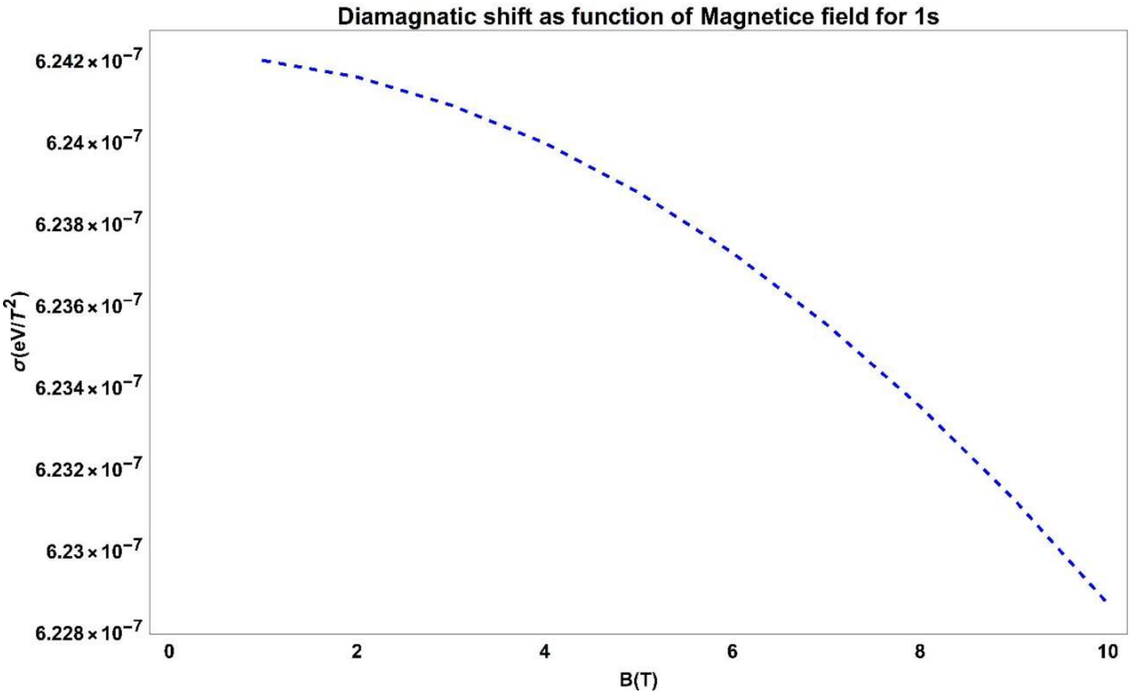

Fig.4.21: The diamagnetic coefficient (σ) vs Magnetic field for WSe_2 for 1S state

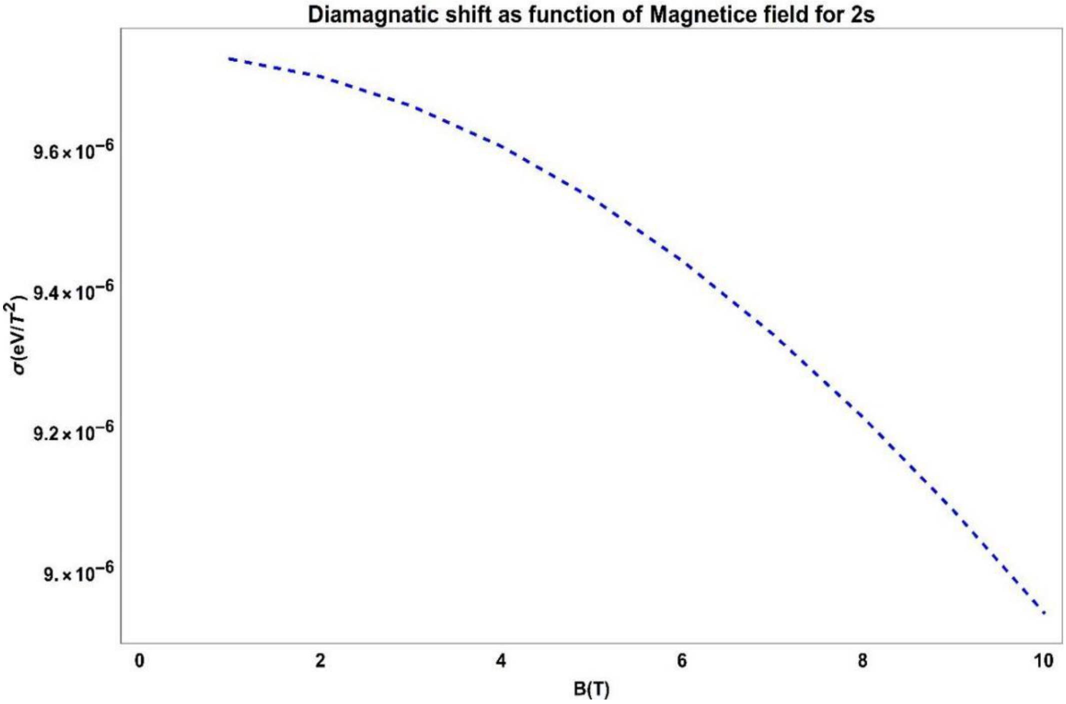

Fig.4.22: The diamagnetic coefficient (σ) vs Magnetic field for WSe_2 for 2S state

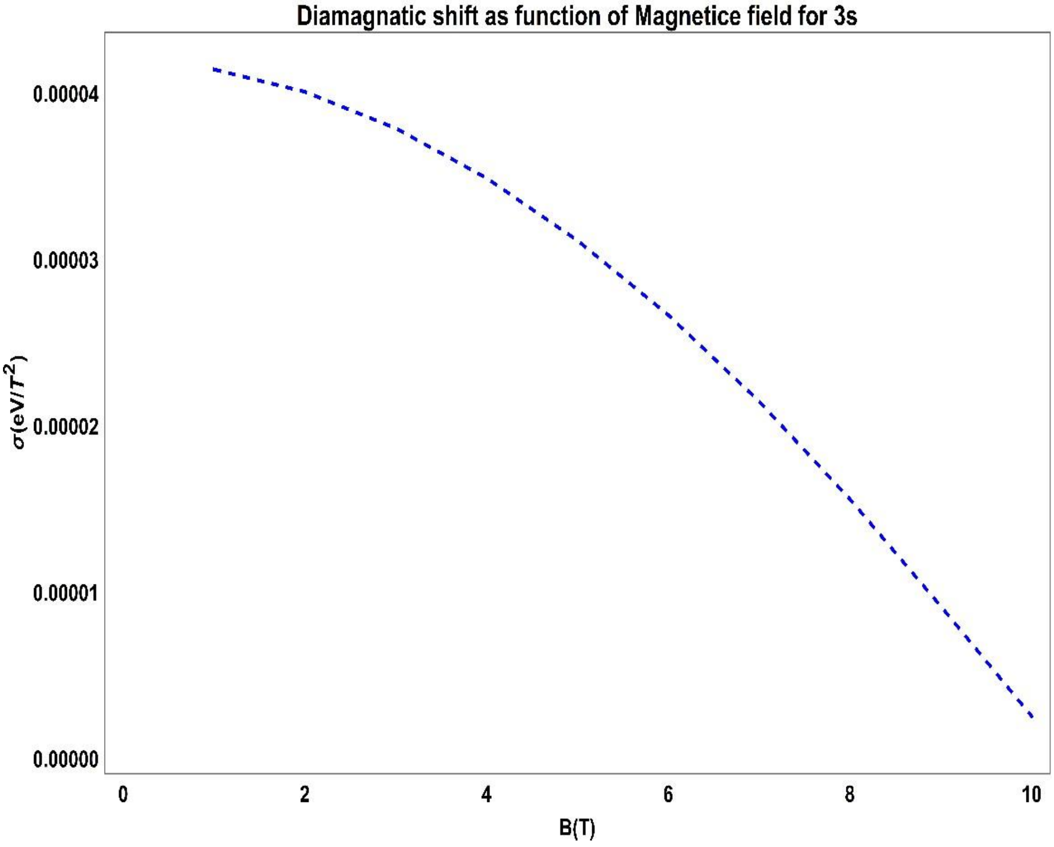

Fig.4.23: The diamagnetic coefficient (σ) vs Magnetic field for WSe_2 for 3S state

Regarding the second material WS_2, we find that the behavior of the diamagnetic coefficient (σ) is similar, as it decreases with the increase of the magnetic field approximately in the three levels (1S, 2S and 3S), with the same value of magnetic field at 10Tesla, as shown in the figures (4.24, 4.25 and 4.26).

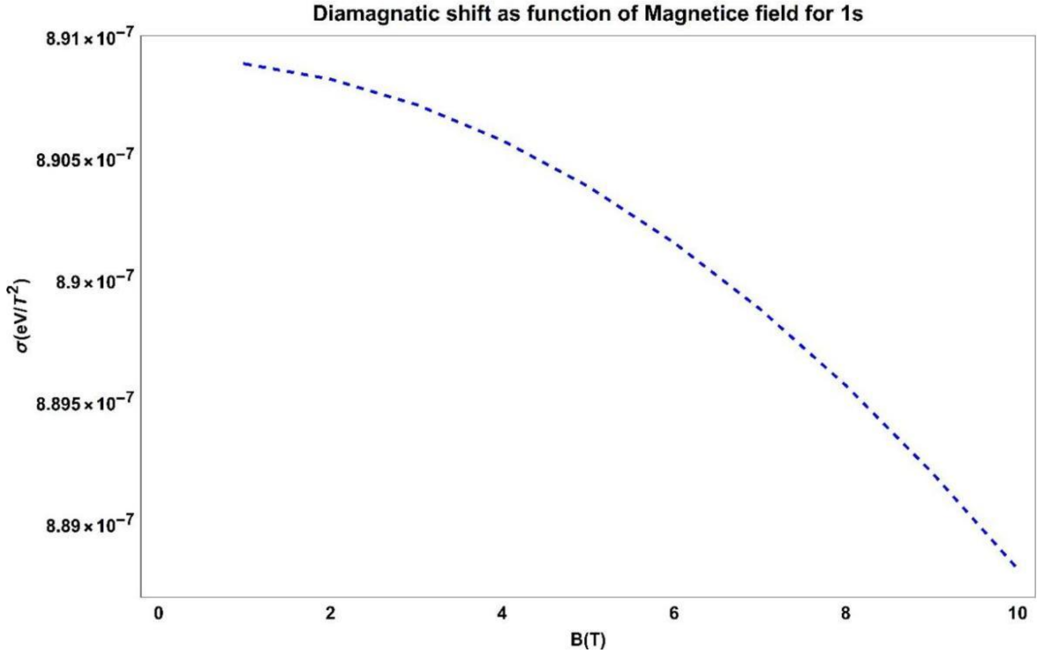

Fig.4.24: The diamagnetic coefficient (σ) vs Magnetic field for WS_2 for 1S state

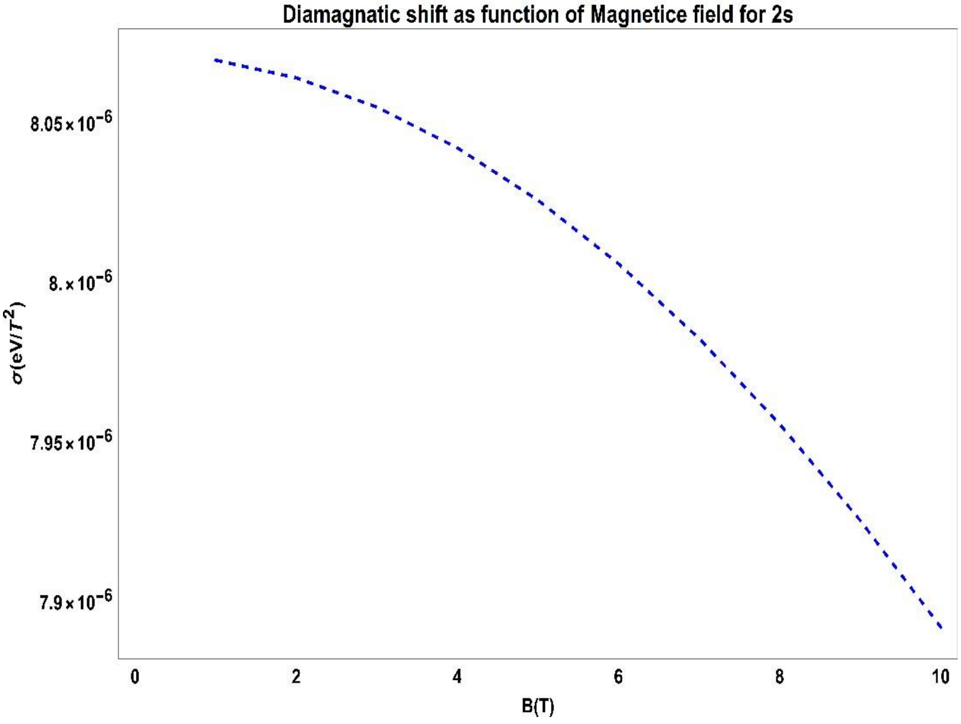

Fig.4.25: The diamagnetic coefficient (σ) vs Magnetic field for WS_2 for 2S state

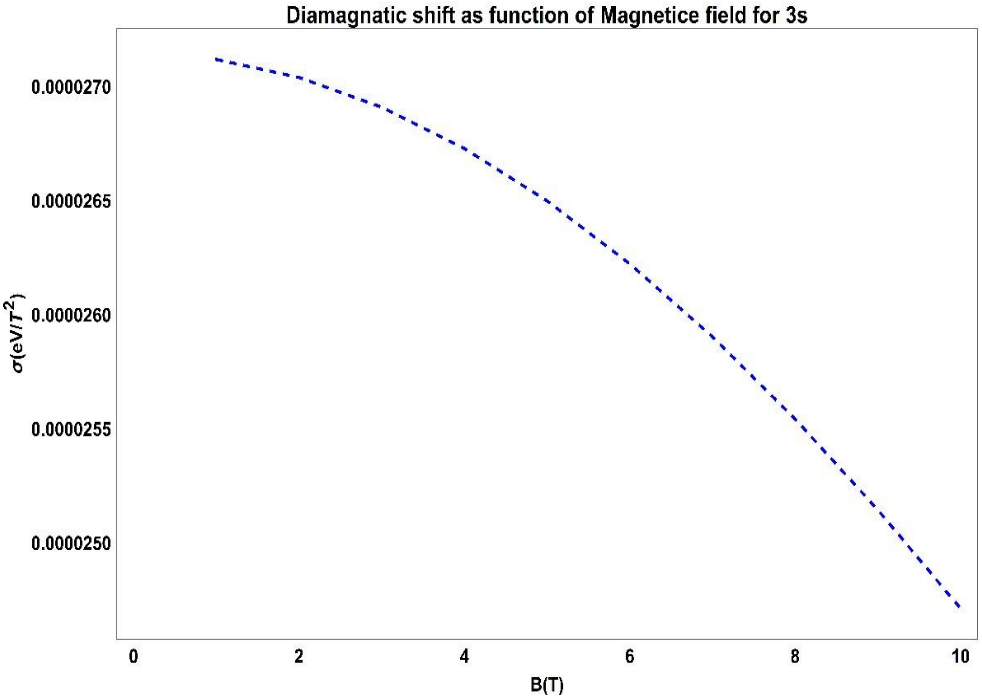

Fig.4.26: The diamagnetic coefficient (σ) vs Magnetic field for WS_2 for 3S state

Diamagnetic coefficient, which is often denoted by the symbol (σ) represents the degree of response of the material to the magnetic field. Magnetic materials produce a magnetic field opposite to the external magnetic field. This leads to a weakening of the total magnetic field within the material. It can be said that the decrease in magnetic coefficient with increasing magnetic field is “saturation”. Initially, when a material is affected by a magnetic field on the material, the diamagnetic material aligns its atomic magnetic moments against the external field, causing the overall magnetic moment of the material to decrease.

However, as the strength of the external magnetic field increases, the magnetic material begins to reach a point where most of its atomic magnetic moments are exactly parallel to the external field. At this point, the material becomes saturated, meaning it cannot increase its induced magnetic moment in response to an increase in the external magnetic field. As a result, the diamagnetic response weakens, and the diamagnetic coefficient decreases with increasing magnetic field strength. In essence, as the magnetic field strengthens, the ability of the material to oppose it becomes limited due to saturation, resulting in a decrease in the magnetic coefficient. [93]

In order for the picture to be complete, the last step must be performed, which is to compare the existing results with other results of different studies. I will compare the different values for diamagnetic coefficient (σ) that I obtained using 1/N expansion method for WSe_2 at zero temperature and magnetic field reach to 90 Tesla, with other results obtained theoretically and other results obtained experimentally, (table 4.5).

Table 4.5. Without effect of temperature and 90 Tesla for WSe_2 diamagnetic coefficients in unit of eV/Tesla^2 compared to the experimental data [94] and theoretical data [75].

WSe_2	1s	2s	3s	2p
σ (eV/T^2) (present work)	$0.520*10^{-6}$	$5.07*10^{-6}$	$2.10*10^{-6}$	$1.03*10^{-6}$
σ (eV/T^2) (Ref [94])	$0.310*10^{-6}$	$4.6*10^{-6}$	$22*10^{-6}$	----
σ (eV/T^2) (Ref [75])	$0.28*10^{-6}$	$5.03*10^{-6}$	$26.5*10^{-6}$	$2.42*10^{-6}$

The results in the table show the extent of convergence between the theoretical results obtained using 1/N expansion method in present work and the experimental results in reference [94] and the theoretical obtained by numerical using the computational method in reference [75].

Chapter Five: Discussion

Recent inventions in the field of two-dimensional transition metal dichalcogenides (2D TMDs) have given rise to several cutting-edge technologies that include nanoelectronics, photonics, sensing, energy storage, and optoelectronics, among other fields. The study focused on the use of transition metal dichalcogenides (TMDs), represented by WS_2 and WSe_2. This material describes applications poised to shape the next electronic and optoelectronic devices.

In this thesis, an exciton present in a sheet of TMD material (WS_2 and WSe_2) was highlighted to conduct studies covering different properties. We solved the Schrödinger equation by shifted 1/N expansion method to obtain the eigen energy for the exciton present in the TMD material as a function of temperature (T) and magnetic field (B).

We talked about energy spectra, as we clarified the energy state values that were obtained mathematically using the 1/N-shift expansion method and compared them with other energy state values that were obtained numerically for the same materials (WSe_2 and WS_2) in other works and using the same effects (especially magnetic field).

After that, we highlighted the ground state energy (average energy) as a function of temperature at different values of the magnetic field (between 0 to 94T for WSe_2 and 0 to 60.16 for WS_2), and the result was that as the temperature increased, the average energy increased at different levels for n.

The thermal and magnetic properties of the exciton contained in a sheet of TMD material were studied based on different values of the magnetic field at different temperatures. Starting with the thermal properties, we talked about the heat capacity as a function of temperature for both materials at the same field values mentioned previously (between 0 to 94T for WSe_2 and 0 to 60.16 for WS_2). We found that the specific heat increases with increasing temperature until a certain value is reached, and then it begins to decrease.

As for the property of entropy, its general behavior was that it increases with increasing temperature until stability and continues to remain stable with increasing temperature.

In addition, we have displayed the dependence of magnetization and magnetic susceptibility of exciton in QD with various physical parameters (B, T).

In summary, the behavior of statistical energy, magnetization and magnetic susceptibility in response to magnetic field and temperature is shown as follows:

we started with statistical energy and studied its behavior with the magnetic field at different temperatures. It increased with the increase in the magnetic field for both materials (WSe_2 and WS_2). A study of magnetization that generally followed a decreasing behavior with increasing magnetic field. Regarding the magnetic susceptibility, it was studied as a function of magnetic field at different temperatures and it also decreased with increasing magnetic field for WSe_2 and WS_2 materials.

In addition to the physical description of the effect of each system parameter on the energy spectra, we calculated the density of state of the system. The plots show that the state density decreases as the magnetic field increases. As a result of the division of energy levels, which may lead to a reduction in the states available for electrons at a certain energy level, and this in turn causes a change in the distribution of states within the system due to the Zeeman splitting.

Thermomagnetic properties were also studied under the name Magneto Caloric Effect (MCE) of an exciton found in TMD Material, which represents the difference in randomness (entropy) of the system at two different values of a magnetic field affecting this system. The general character of this property was the Gaussian distribution.

The latest study conducted in this thesis, relates to the magnetism of an exciton found within the TMD material. By knowing the ability of these materials to respond to the applied magnetic field, this was done through studying the so-called diamagnetic shift (σ). Better yet, the results we obtained through 1/N expansion method were matched with results in other important previous studies on the theoretical and experimental levels, and this is a positive thing that supports and corroborates the results that have been reached.

In the future, we plan to continue our research efforts in studying the effect of these parameters on other interesting QD properties. It is also possible to conduct the same studies, but on other TMD materials like MoS_2, $MoSe_2$, $MoTe_2$, and find out the compatibility of the general behavior of the different properties between these materials, which fall under the name TMD Materials. This is out of our concern for these materials because of their importance in the field of electronics and because they have many specialized applications for the next generation of electronic and optoelectronic devices.

In addition to their unique properties and advantages in technology, the TMD like: MoS_2, WS_2, $MoSe_2$, WSe_2 and $MoTe_2$ monolayers contain a direct band gap, and can be used in electronics as transistors and in optics as emitters and detectors. The singlelayer TMD crystal structure has no reflection center, allowing to reach a new degree of freedom of charge carriers, opening a new field in Valleytronics physics.

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Appendices

Appendix A: Shifted 1/N Expansion Method

The 1/N expansion method is used to solve Eq. (3.8) systematically in terms of the expansion parameter $1/\bar{k}$. At large $\bar{k}$, the contribution of energy comes from the effective potential:

$$V_{eff} = \frac{\hbar^2}{8m^* r^2} + \frac{V(r)}{Q} \qquad (A1)$$

Where : $Q = \bar{k}^2$, is scaling constant. V_{eff} has a minimum value at r_0, so that we have:

$$4m^* r_0^3 V'(r_0) = \hbar^2 Q \qquad (A2)$$

In order to shift the origin of the coordinate to the position of the minimum of the effective potential, it is convenient to define a new variable x:

$$x = \frac{\bar{k}^{\frac{1}{2}}}{r_0}(r - r_0) \qquad (A3)$$

Using Taylor expansion around the effective minimum r0, respectively x = 0, an analytical equation similar to the Schrödinger equation for a one-dimensional solvable nonharmonic oscillator is obtained. The coefficients of both equations were compared to determine all the parameters of the antiharmonic oscillator in terms of $\bar{k}$, Q, r0 and potential derivatives in order to obtain the power spectrum. We will determine the frequency of the oscillator:

$$\omega = \frac{\hbar}{2m^*}\left(3 + \frac{r_0 V''(r_0)}{V'(r_0)}\right)^{1/2} \qquad (A4)$$

To complete other steps, to calculate energy eigen values we will expand Schrodinger equation in power of $1/\bar{k}$ where $\bar{k} = N + 2l - a$, N is the number of spatial dimension and (a) is-so called shifted parameter. The shifted parameter a, is defended as equation:

$$a = 2 - \frac{2(2n_r - 1)m^*\omega}{\hbar} \quad (A5)$$

For any values of radial quantum number n_r or for any value of m_l**,** the energy eigen values, $E(n_r, m_l)$ are given by:

$$E(n_r, m_l) = E_0 + E_1 + E_2 + E_3 \quad \text{(A6)}$$

Where:

$$E_0 = V(r) + (\frac{Q}{8 * m^* * r^2})$$

$$E_1 = \frac{(c_1 * c_3)}{(8 * m^*)}$$

$$E_2 = (E_1 + \alpha_1)/r^2$$

$$E_3 = \frac{\alpha_2}{\bar{k} * r^2}$$

Where:

$Q = (N + 2 * l - a)^2$

$c_1 = (1 - a)$

$c_2 = (2 - a)$

$c_2 = (2 - a)$

$c_3 = (3 - a)$

$\alpha_1 = n_1 * e_2 + 3 * n_2 * e_4 - c_5 * \left({e_1}^2 + 6 * n_1 * e_1 * e_3 + n_4 * e_3^2\right)$

$\alpha_2 = t_7 + t_{12} + t_{16}$

$c_5 = \omega^{-1}$

The forms of previous parameters are given in the following:

$t_7 = t_1 - c_5 * (t_2 + t_3 + t_4 + t_5 + t_6)$

$t_{12} = c_5^2 * (t_8 + t_9 + t_{10} + t_{11})$

$t_{16} =- c_5^3 * (t_{13} + t_{14} + t_{15})$

With:

$t_1 = n_1 * d_2 + 3 * n_2 * d_4 + 5 * n_3 * d_6$

$t_2 = n_1 * {e_2}^2 + 12 * n_2 * e_2 * e_4$

$t_3 = 2 * e_1 * d_1 + 2 * n_5 * {e_4}^2$

$t_4 = 6 * n_1 * e_1 * d_3 + 30 * n_2 * e_1 * d_5$

$t_5 = 6 * n_1 * e_3 * d_1 + 2 * n_4 * e_3 * d_3$

$t_6 = 10 * n_6 * e_3 * d_5$

$t_8 = 4 * {e_1}^2 * e_2 + 36 * n_1 * e_1 * e_2 * e_3$

$t_9 = 8 * n_4 * e_2 * e_3^2$

$t_{10} = 24 * n_1 * e_1^2 * e_4 + 8 * n_7 * e_1 * e_3 * e_4$

$t_{11} = 12 * n_8 * e_3^2 * e_4$

$t_{13} = 8 * e_1^3 * e_3 + 108 * n_1 * e_1^2 * e_3^2$

$t_{14} = 48 * n_4 * e_1 * e_3^3$

$t_{15} = 30 * n_9 * e_3^4$

Where (n’s), (d’s) and (e’s) are parameters given as:

$n_1 = 1 + 2 * n_r$

$n_2 = 1 + 2 * n_r + 2 * n_r{}^2$

$n_3 = 3 + 8 * n_r + 6 * n_r{}^2 + 4 * n_r{}^3$

$n_4 = 11 + 30 * n_r + 30 * n_r{}^2$

$n_5 = 21 + 59 * n_r + 51 * n_r{}^2 + 34 * n_r{}^3$

$n_6 = 13 + 40 * n_r + 42 * n_r{}^2 + 28 * n_r{}^3$

$n_7 = 31 + 78 * n_r + 78 * n_r{}^2$

$n_8 = 57 + 189 * n_r + 225 * n_r{}^2 + 150 * n_r{}^3$

$n_9 = 31 + 109 * n_r + 141 * n_r{}^2 + 94 * n_r{}^3$

$c_4 = 2 * m^* * \omega$

$e_1 = \epsilon_1/\sqrt{c_4}$

$e_2 = \epsilon_2/c_4$

$e_3 = \epsilon_3/c_4{}^{3/2}$

$e_4 = \epsilon_4/c_4{}^2$

$d_1 = \delta_1/\sqrt{c_4}$

$d_2 = \delta_2/c_4$

$d_3 = \delta_3/c_4{}^{3/2}$

$d_4 = \delta_4/c_4{}^2$

$d_5 = \delta_5/c_4{}^{5/2}$

$d_6 = \delta_6/c_4{}^3$

Also:

$\epsilon_1 = c_2/(2 * m^*)$

$\epsilon_2 =- 3 * c_2/(4 * m^*)$

$\epsilon_3 =- 1/(2 * m^*) + \big(r_5 * \mathrm{der}_3\,(r)\big)/(6 * Q)$

$\epsilon_4 = 5/(8 * m^*) + \big(r_6 * \mathrm{der}_4\,(r)\big)/(24 * Q)$

$\delta_1 =- c_1 * c_3/(4 * m^*)$

$\delta_2 = 3 * c_1 * c_3/(8 * m^*)$

$\delta_3 = c_2/m^*$

$\delta_4 =- 5 * c_2/(4 * m^*)$

$\delta_5 =- 3/(4 * m^*) + \big(r_7 * \mathrm{der}_5\,(r)\big)/(120 * Q)$

$\delta_6 = 7/(8 * m^*) + \big(r_8 * \mathrm{der}_6\,(r)\big)/(720 * Q)$

Where:

$\mathrm{der}_1\,(r) = \frac{\mathrm{dV}}{\mathrm{dr}}$

$\mathrm{der}_2\,(r) = \frac{d^2\mathrm{V}}{\mathrm{dr}}$

$\mathrm{der}_3\,(r) = \frac{d^3\mathrm{V}}{\mathrm{dr}}$

$\mathrm{der}_4\,(r) = \frac{d^4\mathrm{V}}{\mathrm{dr}}$

$\mathrm{der}_5\,(r) = \frac{d^5\mathrm{V}}{\mathrm{dr}}$

$\mathrm{der}_6\,(r) = \frac{d^6\mathrm{V}}{\mathrm{dr}}$

الخصائص الحرارية والمغناطيسية ل-اكسيتون داخل طبقة من مادة WS_2، WSe_2

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الملخص

في هذه الأطروحة، تم تسليط الضوء على الإكسيتون الموجود في نقطة كمية من مادة WS2 وWSe2 لإجراء دراسات تغطي خصائص مختلفة. لقد قمنا بحل معادلة شرودنغر (دالة هاملتون) بطريقة مفكوك (1/N) للحصول على قيم الطاقة المختلفة للإكسيتون الموجود في مادة TMD.

قمنا بإيجاد طاقة المستوى الأرضي بالإضافة إلى مستويات علوية رياضيا باستخدام طريقة مفكوك (1/N) ومقارنتها بقيم الطاقة الأخرى التي تم الحصول عليها عدديا في أعمال مختلفة. بعد ذلك، سلطنا الضوء على طاقة الحالة الأرضية (متوسط الطاقة) كدالة لدرجة الحرارة عند قيم مختلفة للمجال المغناطيسي. تمت دراسة الخواص الحرارية والمغناطيسية للإكسيتون الموجود في مادة TMD بناءً على قيم مختلفة للمجال المغناطيسي عند درجات حرارة مختلفة. بدءًا من الخواص الحرارية، تحدثنا عن السعة الحرارية والعشوائية. بالإضافة إلى ذلك، فقد أظهرنا اعتماد المغنطة والقابلية المغناطيسية للإكسيتون في نقطة كمية على العديد من المتغيرات الفيزيائية ممثلة بالمجال المغناطيسي ودرجة الحرارة بالإضافة إلى الوصف الفيزيائي لتأثير كل متغير على قيم الطاقة، قمنا بحساب كثافة حالة النظام. كما تمت دراسة الخواص الحرارية المغناطيسية تحت اسم Magneto Caloric Effect (MCE) للإكسيتون الموجود في مادة TMD، والذي يمثل الفرق في العشوائية (الإنتروبيا) للنظام عند قيمتين مختلفتين للمجال المغناطيسي المؤثر على هذا النظام. ولمعرفة قدرة هذه المواد على الاستجابة للمجال المغناطيسي المطبق، تم دراسة ما يسمى بالتحول المغناطيسي. والأفضل من ذلك، أظهرت المقارنات

المعروضة في الأطروحة تطابقا وانسجاما كبيرا بين النتائج التي حصلنا عليها مع الأعمال المنشورة على المستويين النظري والتجريبي.

كلمات مفتاحية: نقطة كمومية. إكسيتون. مفكوك ١/ن. مواد انتقالية. WSe_2