Thermodynamical Properties for Some Position-dependent Mass (PDM) Quantum Systems

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We certify that we have read this thesis and that in our opinion it is fully adequate in scope and quality as a thesis for the degree of Master of Science in Physics.

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ABSTRACT

This thesis studies thermodynamical properties for position-dependent effective mass (PDM) in pseudoharmonic potential. We use a PDM Hamiltonian obtained by the creation $\hat{A}$ and annihilation $\hat{A}^{+}$ operators approach. The PDM Hamiltonian operator is utilized to reach a PDM radial Schrödinger equation. Which is separated into a z-dependent and a radial-dependent parts. Eigenenergies and eigenfunctions are determined for PDM model, $M(\vec{r}) = m_0 g(r)$; $g(r) = -\xi/r^2$. We obtain the partition function, which is utilized to obtain thermodynamical properties like mean energy U, mean free energy F, entropy S and specific heat capacity C. We show a graphical representation of the pseudoharmonic potential for different values of parameters.

Keywords: position-dependent mass (PDM) Hamiltonian, posedoharmonic potential, thermodynamical properties, PDM creation and annihilation operators.

ÖZ

Bu tez, psödoharmonik potansiyelde pozisyona bağlı etkin kütle (PDM) için termodinamik özellikleri inceler. $\hat{A}$ oluşturma ve yok etme $\hat{A}^{+}$ operatörleri yaklaşımıyla elde edilen en basitleştirilmiş kullanıcı dostu PDM Hamiltonian'ı kullanıyoruz. PDM Hamiltonian operatörü, bir PDM radyal Schrödinger denklemine ulaşmak için kullanılır. Hangisi z bağımlı ve radyal bağımlı parçalara ayrılır. PDM modeli için özenerjiler ve özfonksiyonlar belirlenir, $M(\vec{r}) = m_0 g(r); g(r) = -\xi/r^2$. Ortalama enerji U, ortalama serbest enerji F, entropi S ve özgül ısı kapasitesi C gibi termodinamik özellikleri elde etmek için kullanılan bölme fonksiyonunu elde ederiz. Farklı parametre değerleri için psödoharmonik potansiyelin grafiksel bir temsilini gösteririz.

Anahtar Kelimeler: pozisyona bağlı kütle (PDM) Hamiltoniyen, pozdoharmonik potansiyel, termodinamik özellikler, PDM oluşturma ve yok etme operatörleri.

DEDICATION

To my family

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TABLE OF CONTENTS

LIST OF FIGURES

Chapter 1

INTRODUCTION

Physical models for position - dependent mass (PDM) have received a lot of attention in recent years [1-7]. Schrödinger equations with position dependent mass recently achieved extensive analysis in semiconductor electrical characteristics , inhomogeneous crystals [8], quantum dots [9], quantum liquids [10] and nuclear many body problem [11] . It is evident that research on the PDM Schrödinger equation has a significant influence on condensed matter physics and associated disciplines of physics . Similarly , some accurately solvable models have been generated using supersymmetric quantum mechanical techniques [12-14] . Particles having position - dependent effective mass would be a more accurate and enlightening term . That is, a distortion in the coordinate system may make the mass position - dependent. A moving point mass in curved space becomes an effective position - dependent mass in Euclidean space [15-17] .

1.1 Position-dependent Mass (PDM) Hamiltonians

We begin with, the von Roos PDM Hamiltonian proposal [18] (with $\hbar = 2m_0 = 1$)

$$H = -\frac{1}{2}\left\{m(\vec{r})^{\alpha}\vec{\nabla}\, m(\vec{r})^{\beta}\vec{\nabla}\, m(\vec{r})^{\gamma} + m(\vec{r})^{\gamma}\vec{\nabla}\, m(\vec{r})^{\beta}\vec{\nabla}\, m(\vec{r})^{\alpha}\right\} + V(\vec{r}), \qquad (1.1)$$

with the von Roos condition

$$\alpha + \beta + \gamma = -1;\ \alpha, \beta, \gamma \in \mathbb{R} \qquad (1.2)$$

By using equation (1.1) and equation (1.2), and considering cylindrical symmetric settings, it can easily be recast in a straightforward manner as follows [49, 50]

$$H = -\vec{\nabla}\left(\frac{1}{m(\vec{r})}\right)\vec{\nabla} + V_{PDM}(\vec{r}), \tag{1.3}$$

and

$$V_{PDM}(\vec{r}) = \frac{1}{2}(1+\beta)\frac{\vec{\nabla}^2 m(\vec{r})}{m(\vec{r})^2} - [\alpha(\alpha+\beta+1)+\beta+1]\frac{\left(\vec{\nabla} m(\vec{r})\right)^2}{m(\vec{r})^3} + V(\vec{r}), \tag{1.4}$$

where the first two terms represent an additional potential produced by the structure of the PDM kinetic-energy operator. Equation (1.4) shows that, an ordering ambiguity is introduced as the kinetic energy operator changes when $\alpha, \beta \; and \; \gamma$ change. Moreover, α , β , γ are called the von Roos ambiguity parameters. In contrast to the quantum mechanical, the classical mechanical Hamiltonian does not have such ordering ambiguities. Nevertheless, it has been proposed that the quantum and classical mechanical correspondence may resolve this ordering ambiguity issue [45].

In the literature there are several suggestions for the kinetic energy operator. Among them; the Gora and Williams $(\beta = \gamma = 0, \alpha = -1)$[19], Ben Danial and Duke $(\alpha = \gamma = 0, \beta = -1)$ [20], Zhu and Kroemer $(\alpha = \gamma = -1/2\,, \beta = 0)$ [21], and Li and Kuhm $(\beta = \gamma = -1/2\,, \alpha = 0)$[22]. However, the Hermiticity of the Hamiltonian, current density conservation, experimental studies of Brezini et al [23], and condensed matter theories (Burt [24] and Geller and Kolm [25]) may, provide some insight into the identity of the von Roos parameters ambiguity. The application of Hamiltonian (1.1) at the heterojunction between two crystals (see, for example, Burt [24], Geller and Kohn [25] Einevoll [26],), suggested that for $\alpha \neq \gamma$ the wavefunction disappears. Hence, the only feasible case is due $\alpha = \gamma$ to ensure the continuity of the wavefunction and of $m(x)^{\alpha}\psi(x)$ and $m(x)^{\alpha+\beta}[\partial_x \psi(x)]$ at the hetrojunction boundary.

Conversely, Dutra and Almeida [27] recently conducted a test on the reliability orderings. They utilized a perfectly solvable Morse model to establish that Gora and Williams' orderings are correct: $(\beta = \gamma = 0, \alpha = -1)$[19], and, that of Ben Danial and Duke $(\alpha = \gamma = 0, \beta = -1)$[20] should be discarded as their results given complex energies. They classified the ordering of Zhu and Kroemer $(\alpha = \gamma = -1/2,\ \beta = 0)$[21], and Li and Kuhn $(\alpha = 0, \beta = \gamma = -1/2)$[22] as good ones. Eventually, following Mustafa and Mazharimousavi [45] at the prompt heterojunction the conditions, on the parameters setting, $(\alpha = \gamma = k, \beta = 2j)$ is found to yield $\alpha = \gamma = -1/4$ and $\beta = -1/2$ and is found to be good ordering. This ordering motivates our present methodological approach.

Furthermore, the harmonic oscillator model is essential in quantum mechanics. Within quantum physics, rather than simply calculating the Schrödinger equation, this model is handled utilizing the creation $\hat{A}^{+}$ and annihilation $\hat{A}$ operators. Therefore, the PDM harmonic oscillator is applied and PDM creation $\hat{A}^{+}$ and annihilation $\hat{A}$ operators are introduced. However, the commutation relation for the harmonic oscillator is shown and fulfilled.

Moreover, a number of theoretical articles exist on the quantum antidot structure in the context and exclusion of repulsive antidot possibility, parabolic confinement prospect, magnetic, and Aharonov-Bohm (AB) flux fields. Bogachek and Landman [29] represented an antidot by a repulsive potential $V(\vec{r}) \sim 1/r^2$ and obtained a precise solution of the Schrödinger equation. They proved that edge states at the antidotes' boundaries produce magnetization oscillations as a consequence of magnetic flux through the inside opening. In presence of magnetic fields, Aquino et al. [31] described

a quantum antidot as an electron travelling beyond a cylinder of radius R. Reijniers et al. [32] investigated a setup in which electrons were restricted to move in 2-dimensions by a nonhomogeneous magnetic field. Their own quantum dot model was distinct from other quantum dot models. Because electrons are magnetically bound in their domain, this is known as magnetic antidot.

Furthermore, the so called pseudoharmonic potential was first discussed by Gol'dman et al. [33]. Various researchers have studied this potential because of its relevance in Chemical Physics, Molecular Physics, and many fields of Physics [34-39] .Sage and Goodisman [40] emphasized the merits of such a potential possibility and straightforward building of the potential energy curve over the standard presentation.

The mean purpose of studying thermodynamic properties is to find its partition function. The temperature dependent of partition function, helps us in obtaining additional thermodynamic properties. The partition function for pseudoharmonic potential models may be easily calculated by computing the energies of the quantum antidot potential and harmonic quantum dot potential [29-30] .Various scholars have used complex numerical ways to evaluate partition functions, including the Poisson summation technique [41], the commulant expansion methodology [42], the standard method [43], and the Wigner-Kirkwood formulation [44]. Moreover, to investigate the thermodynamical properties, one starts with the radially dependent part of Schrödinger equation with pseudoharmonic potential. The energies and related wave functions are then calculated. In the current study, we use the pseudoharmonic model, and study the thermodynamical properties like internal energy U, free energy F, entropy S and specific heat C.

The plan of the current study is as follows. Chapter 2, describes the position-dependent mass (PDM) for Schrödinger equation, using PDM creation and annihilation operators approach [28]. Moreover, working with the PDM creation and annihilation operators for the harmonic oscillator potential that satisfy the commutation relation $\left[\hat{A}\,,\hat{A}^{+}\right] = 1$. Then, the corresponding PDM Hamiltonian $\widehat{H} = \omega\left(\hat{A}^{+}\hat{A} + \frac{1}{2}\right) = \omega\left(\hat{A}\,\hat{A}^{+} - \frac{1}{2}\right)$ determines the exact values for $\alpha\,,\ \beta\,, and\ \gamma$. The PDM momentum operator is utilized [15] to solve the corresponding PDM Schrödinger equation, which is separated into a z-dependent and a radial-dependent parts. In chapter 3, we use the pseudoharmonic potential, and find its exact energy eigenvalues and eigenfunctions for a PDM model, $M(\vec{r}) = m_0 g(r)$; $g(r) = -\xi/r^2$. In the same chapter, we evaluate the thermodynamical properties for such PDM-particles in a pseudoharmonic potential. The partition function $Z(\beta)$ of the system at a specified temperature T is determined. Thermodynamical properties like mean energy U, mean free energy F, entropy S and specific heat capacity C are obtained. Our results are reported graphical for each of the thermodynamical properties for different parameters. Our conclusion is found in Chapter 4.

Chapter 2

PDM- SCHRÖDINGER EQUATION

In this chapter, the position-dependent mass (PDM) required for Schrödinger equation is developed following the PDM creation and annihilation operators' approach. In quantum mechanics, it is imperative to start with the PDM Hamiltonian von Roos [18]

$$\widehat{H} = -\frac{\hbar^2}{4}\left\{M(\vec{r})^{\alpha}\vec{\nabla}\, M(\vec{r})^{\beta}\vec{\nabla}\, M(\vec{r})^{\gamma} + M(\vec{r})^{\gamma}\vec{\nabla}\, M(\vec{r})^{\beta}\vec{\nabla}\, M(\vec{r})^{\alpha}\right\} + V(\vec{r}), \tag{2.1}$$

where the PDM is $M(\vec{r}) = m_0\, m(\vec{r})$. Which, m_0 is the rest mass, $m(\vec{r})$ is position-dependent mass dimensionless scalar multiplies that forms the position-dependent mass $M(\vec{r})$, and the parameters $\alpha, \beta,$ and γ are the von Roos ambiguity parameters. This ambiguity is attributed to the infinite kinetic energy operators which fulfil the constraint ($\alpha + \beta + \gamma = -1$). Notably, the kinetic energy operators' profile as well as the effective potential will differ as the values of $\alpha, \beta,$ and γ are changed within the allowable constraint limits. Moreover, according to Mustafa and Mazharimousavi [45] at the prompt heterojunction the conditions, on the parameters setting, $\beta = 2j$ and $\alpha = \gamma = k$ where $\alpha, \beta, \gamma \in \mathbb{R}$, rewritten in one-dimension and using $m_0 = \hbar = c = 1$ units, as

$$\widehat{H} = -\frac{1}{2}\, m(x)^k \partial_x\, m(x)^{2j} \partial_x\, m(x)^k + V(x). \tag{2.2}$$

It should be noted that a PDM particle moving in $V(x) = 0$, is considered to be a quasi-free particle. Thus, the assumption of a deformed harmonic oscillator is valid under PDM-settings leading to the constant mass harmonic oscillator potential ($\omega^2 q^2/2$) to

$$V(x) = \frac{1}{2}\,\omega^2 x^2 Q(x) = \frac{1}{2}\,\omega^2 q(x)^2 \;; q(x) = \sqrt{Q(x)}\,x. \tag{2.3}$$

This assumption remains valid as long as $q(x)$ is found during the construction of the PDM creation $\hat{A}^+$and annihilation $\hat{A}$ operators. Consequently, substituting equation (2.3) into Hamiltonian (2.2) yields

$$\hat{H} = -\frac{1}{2}\,m(x)^k \partial_x\, m(x)^{2j} \partial_x\, m(x)^k + \frac{1}{2}\,\omega^2 q(x)^2, \tag{2.4}$$

Where

$$k + j = -\frac{1}{2}\,, q(x) = \sqrt{Q(x)}\,x, \tag{2.5}$$

$Q(x)$ represents a deformation function of the coordinate x to be calculated in the sequel, and $V\big(q(x)\big) = \frac{1}{2}\,\omega^2 q(x)^2$ is a deformed harmonic oscillator. As for the PDM creation $\hat{A}^+$ and annihilation $\hat{A}$ operators, they can be, respectively, constructed in the following forms

$$\hat{A}^+ = -\frac{1}{\sqrt{2\omega}} m(x)^k \partial_x\, m(x)^j + \sqrt{\frac{\omega}{2}}\, q(x), \tag{2.6}$$

$$\hat{A} = \frac{1}{\sqrt{2\omega}} m(x)^j \partial_x\, m(x)^k + \sqrt{\frac{\omega}{2}}\, q(x). \tag{2.7}$$

Then, the commutation relation

$$\big[\hat{A}\,, \hat{A}^+\big] = 1 \Leftrightarrow \hat{A}^+\hat{A} + \frac{1}{2} = \hat{A}\,\hat{A}^+ - \frac{1}{2}\,, \tag{2.8}$$

must be satisfied. Clearly, it is similar to the case of the textbook one. Therefore, given the nature of the commutation relationship for the PDM Hamiltonian, we obtained

$$\hat{A}^+\hat{A} = -\frac{1}{2\omega} m(x)^k \partial_x\, m(x)^{2j} \partial_x\, m(x)^k - 2kq(x)\left(\frac{1}{\sqrt{m(x)}}\right)' -$$

$$\left(\frac{q(x)}{2\sqrt{m(x)}}\right)' + \frac{\omega}{2} q(x)^2 \tag{2.9}$$

and

$$\hat{A}\ \hat{A}^{+} = -\frac{1}{2\omega} m(x)^{j} \partial_x\, m(x)^{2k} \partial_x\, m(x)^{j} - 2kq(x)\left(\frac{1}{\sqrt{m(x)}}\right)' -$$

$$\left(\frac{q(x)}{2\sqrt{m(x)}}\right)' + \frac{\omega}{2} q(x)^2 + \frac{q'(x)}{\sqrt{m(x)}}. \tag{2.10}$$

Furthermore, substituting (2.9) and (2.10) in (2.8) we get

$$-\frac{1}{2} m(x)^{k} \partial_x\, m(x)^{2j} \partial_x\, m(x)^{k} = -\frac{1}{2} m(x)^{j} \partial_x\, m(x)^{2k} \partial_x\, m(x)^{j} + \frac{q'(x)}{\sqrt{m(x)}} - 1. \tag{2.11}$$

Consequently, we get

$$\frac{q'(x)}{\sqrt{m(x)}} - 1 = 0 \Leftrightarrow q(x) = \int \sqrt{m(x)}\, dx = \sqrt{Q(x)}\text{x}, \tag{2.12}$$

and the kinetic energy terms in the equation (2.11) are equal, that is

$$-\frac{1}{2} m(x)^{k} \partial_x\, m(x)^{2j} \partial_x\, m(x)^{k} = -\frac{1}{2} m(x)^{j} \partial_x\, m(x)^{2k} \partial_x\, m(x)^{j}\,. \tag{2.13}$$

As a result, two essential findings are obtained. The first establishes the composition of $q(x)$ in equation (2.12), while the second limits the ambiguity parameters to the identity $k = j$ in equation (2.13). However, the substitution of this into von Roos constraint $k + j = -1/2$ yields $k = j = -1/4$. Thus, the creation $\hat{A}^{+}$(2.7) and annihilation $\hat{A}$ (2.8) operators for the PDM settings are determined as

$$\hat{A}^{+} = -\frac{1}{\sqrt{2\omega}} \frac{1}{\sqrt[4]{m(x)}} \partial_x \frac{1}{\sqrt[4]{m(x)}} + \sqrt{\frac{\omega}{2}} q(x) \Leftrightarrow \hat{A}^{+} = -i\left(\frac{\hat{p}(x)}{\sqrt{2\omega\, m(x)}}\right) + \sqrt{\frac{\omega}{2}} q(x), \tag{2.14}$$

and

$$\hat{A} = \frac{1}{\sqrt{2\omega}} \frac{1}{\sqrt[4]{m(x)}} \partial_x \frac{1}{\sqrt[4]{m(x)}} + \sqrt{\frac{\omega}{2}} q(x) \Leftrightarrow \hat{A}^{+} = i\left(\frac{\hat{p}(x)}{\sqrt{2\omega m(x)}}\right) + \sqrt{\frac{\omega}{2}} q(x), \tag{2.15}$$

where

$$\hat{p}(x) = -i\left(\partial_x - \frac{1}{4}\frac{m'(x)}{m(x)}\right), \tag{2.16}$$

is the momentum operator for the PDM as per the recent work of Mustafa and Algadhi [15]. Hence, the PDM Hamiltonian $\widehat{H}$ of equation (2.4) takes its operator form

$$\widehat{H} = \omega\left(\hat{A}^{+}\hat{A} + \frac{1}{2}\right) = \omega\left(\hat{A}\,\hat{A}^{+} - \frac{1}{2}\right), \tag{2.17}$$

and a differential form

$$\widehat{H} = -\frac{1}{2}\frac{1}{\sqrt[4]{m(x)}}\partial_x \frac{1}{\sqrt{m(x)}}\partial_x \frac{1}{\sqrt[4]{m(x)}} + \frac{1}{2}\,\omega^2 q(x)^2. \tag{2.18}$$

As a consequence, the ambiguity in the PDM kinetic energy operator of equation (2.2) is now removed, the PDM kinetic energy operator is now given by

$$\hat{T} = -\frac{1}{2}\frac{1}{\sqrt[4]{m(\vec{r})}}\vec{\nabla}\frac{1}{\sqrt{m(\vec{r})}}\vec{\nabla}\frac{1}{\sqrt[4]{m(\vec{r})}} = \left(\frac{\hat{\boldsymbol{p}}(\vec{r})}{\sqrt{2m(\vec{r})}}\right)^2. \tag{2.19}$$

Which essentially resembles the kinetic energy operator for constant mass, when $m(x) = 1$. Ultimately, the PDM harmonic oscillator Hamiltonian can be conveniently simplified and rewritten as

$$\widehat{H} = \left(\frac{\hat{\boldsymbol{p}}(\vec{r})}{\sqrt{2m(\vec{r})}}\right)^2 + \frac{1}{2}\,\omega^2 q(\vec{r})^2. \tag{2.20}$$

In the next section, we work on the PDM Schrödinger equation to obtain the z-dependent part and the one-dimensional radial-dependent part.

2.1 The radially-dependent part of the PDM Schrödinger equation

Upon obtaining the kinetic energy operator (2.19), which contains the PDM momentum operator $\widehat{\boldsymbol{P}}\,(\vec{\boldsymbol{r}})$, and the simplified Hamiltonian (2.20), now we consider the PDM Schrödinger equation (using $2m_0 = \hbar = c = 1$ units)

$$\left[\left(\frac{\widehat{\boldsymbol{P}}\,(\vec{r})}{\sqrt{m(\vec{r})}}\right)^2 + V\,(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}), \tag{2.21}$$

where, $V(\vec{r})$ is the interaction potential energy. Furthermore, we follow the PDM-momentum operator, defined by Mustafa and Algadhi [15], for the PDM Schrödinger equation,

$$\widehat{\boldsymbol{P}}\,(\vec{\boldsymbol{r}}) = -i\left[\vec{\nabla} - \frac{1}{4}\left(\frac{\vec{\nabla}\,m(\vec{r})}{m\,(\vec{r})}\right)\right]. \tag{2.22}$$

This PDM-operator is shown to satisfy the PDM kinetic energy operator of equation (2.19). At this point, equation (2.22) can be used to rewrite equation (2.21) as

$$\left[-\frac{1}{m\,(\vec{r})}\nabla^2+\left(\frac{\vec{\nabla}\,m\,(\vec{r})}{m\,(\vec{r})^2}\right).\vec{\nabla}+\frac{1}{4}\left(\frac{\vec{\nabla}^2 m\,(\vec{r})}{m\,(\vec{r})^2}\right)-\frac{7}{16}\left(\frac{\left(\vec{\nabla}\,m\,(\vec{r})\right)^2}{m\,(\vec{r})^3}\right)+V\,(\vec{r})\right]\psi\,(\vec{r})\;=$$

$$E\psi\,(\vec{r}). \tag{2.23}$$

Let us assume that $m\,(\vec{r})$ is just radially-dependent, so that

$$m\,(\vec{r})=m(r,\varphi,z)=\mathrm{g}\,(r)\,f(\varphi)\,k(z)=\mathrm{g}\,(r);\;f(\varphi)=k(z)=1\,, \tag{2.24}$$

and

$$\mathrm{g}\,(r)\,V(r,\varphi,z)=V(r)+V(\varphi)+V(z)=V(r)+V(z);V(\varphi)=0. \tag{2.25}$$

It should be noted that $V(\varphi)=0$ implies azimuthal symmetry, while the scalar multiplier $m\,(\vec{r})=\mathrm{g}\,(\mathrm{r})$ has only radially-dependent part. This would, secure the separation of the PDM-Schrödinger equation (2.23). We now use the substitution

$$\psi\,(\vec{r})=\psi\,(r,\varphi,z)=R\,(r)\,Z\,(z)\,e^{im\varphi}, \tag{2.26}$$

(with, $m=0,\pm1,\pm2,\ldots.,\pm\ell$ the magnetic quantum number, and ℓ the angular momentum quantum number) and obtain

$$\left[\frac{R''(r)}{R\,(r)}-\left(\frac{\mathrm{g}'(r)}{\mathrm{g}\,(\mathrm{r})}-\frac{1}{r}\right)\frac{R'\,(r)}{R\,(r)}-\frac{1}{4}\left(\frac{\mathrm{g}''(r)}{\mathrm{g}\,(\mathrm{r})}+\frac{\mathrm{g}'(r)}{\mathrm{rg}\,(\mathrm{r})}\right)+\frac{7}{16}\left(\frac{\mathrm{g}'(r)}{\mathrm{g}\,(\mathrm{r})}\right)^2-\frac{m^2}{r^2}+\mathrm{g}\,(\mathrm{r})\,E-\right.$$

$$\left.V\,(r)\right]+\left[\frac{Z''(z)}{Z\,(z)}-V\,(z)\right]=0, \tag{2.27}$$

where, the z-dependent part of the eigenvalues is presented by k_z^2, i.e.,

$$[-\partial_z^2+V\,(z)]Z\,(z)=k_z^2\,Z\,(z), \tag{2.28}$$

and, the corresponding radially-dependent part is

$$\left[\frac{R''(r)}{R\,(r)}-\left(\frac{\mathrm{g}'(r)}{\mathrm{g}\,(\mathrm{r})}-\frac{1}{r}\right)\frac{R'\,(r)}{R\,(r)}-\frac{1}{4}\left(\frac{\mathrm{g}''(r)}{\mathrm{g}\,(\mathrm{r})}+\frac{\mathrm{g}'(r)}{\mathrm{rg}\,(\mathrm{r})}\right)+\frac{7}{16}\left(\frac{\mathrm{g}'(r)}{\mathrm{g}\,(\mathrm{r})}\right)^2-\frac{m^2}{r^2}-k_z^2+\mathrm{g}\,(\mathrm{r})\,E-\right.$$

$$\left.V\,(r)\right]=0. \tag{2.29}$$

Additionally, the radial equation can be further simplified through the use of

$$R\,(r)=\sqrt{\frac{\mathrm{g}\,(\mathrm{r})}{r}}\,U\,(r), \tag{2.30}$$

to obtain the one-dimensional formulation of equation (2.29) as

$$\left[-\frac{d^2}{dr^2}+\frac{m^2-1/4}{r^2}+V_{eff}(r)\right]U(r)=\tilde{\mathrm{E}}\,U(r), \tag{2.31}$$

where,

$$V_{eff}(r)=V(r)-\mathrm{g(r)}\,E+\left[\frac{5}{16}\left(\frac{\mathrm{g'}(r)}{\mathrm{g(r)}}\right)^2-\frac{1}{4}\left(\frac{\mathrm{g''}(r)}{\mathrm{g(r)}}\right)-\frac{1}{4}\left(\frac{\mathrm{g'}(r)}{\mathrm{r\,g(r)}}\right)\right], \tag{2.32}$$

and,

$$\tilde{\mathrm{E}}=-k_z^2 \tag{2.33}$$

At this point of the current study, two types of Schrödinger equations have been constructed and developed. Namely, the z-dependent part (2.28) and the radial-dependent part (2.31). These differential equations will be vital in finding an exact solution to the problem in terms of eigenvalues and eigenfunctions for a power-low type position-dependent mass in a pseudoharmonic potential.

Chapter 3

A PDM IN A PSEUDOHARMONIC POTENTIAL

This chapter is intended to discuss the PDM-Schrödinger equation (2.31), in its one-dimensional radial form, with a pseudoharmonic potential given by [30]

$$V(r) = v_1 r^2 + \frac{v_2}{r^2} - 2v_0; v_1 = \frac{v_0}{r_0^2} \ , v_2 = v_0 r_0^2, v_0 > 0. \tag{3.1}$$

Where, r_0 is the point of zero pseudoharmonic potential, and v_0 is the chemical potential. However, this potential comprises a harmonic quantum dot potential $(v_1 r^2)$ as well as an antidote potential (v_2 / r^2) [29, 30]. For a sample of PDM settings, it has been reported that a pseudoharmonic potential, is befitted to achieve an exact solution for one-dimensional radial PDM-Schrödinger equation. Therefore, the corresponding models to reach the desired solutions are presented in the followings.

3.1 A radially-dependent PDM with $m(\vec{r}) = g(r) = -\xi/r^2$

Having the radial PDM with $m(\vec{r}) = g(r) = -\xi/r^2$ allows for equation (2.31) to be rewritten as

$$\left[-\frac{d^2}{dr^2} + \frac{\tilde{\ell}^2 - 1/4}{r^2} + v_1 r^2\right] U(r) = E_{eff}\, U(r), \tag{3.2}$$

where,

$$\tilde{\ell}^2 - 1/4 = m^2 + v_2 + \xi E \Leftrightarrow |\tilde{\ell}| = \sqrt{m^2 + v_2 + \xi E + 1/4} \tag{3.3 a}$$

$$E_{eff} = 2v_0 - k_z^2 \tag{3.3 b}$$

Equation (3.2) is, in fact, the one-dimensional form of the two-dimensional radial harmonic oscillator [46] which has the exact eigenvalues

$$E_{eff} = 2\sqrt{v_1}\ \left(2n_r + \left|\tilde{\ell}\right| + 1\right) = 2v_0 - k_z^2, \tag{3.4}$$

where n_r is described the radial quantum number. Upon substituting the magnetic quantum number ℓ from (3.3 a) the following can be obtained

$$E_{eff} = 2\sqrt{v_1}\ \left(2n_r + \sqrt{m^2 + v_2 + \xi E + 1/4} + 1\right) = 2v_0 - k_z^2, \tag{3.5}$$

with the corresponding eigenenergies

$$E_{n_r,m} = -\frac{1}{\xi}\left(m^2 + v_2 + 1/4\ - \left(\frac{2v_0 - k_z^2}{2\sqrt{v_1}} - (2n_r + 1)\right)^2\right). \tag{3.6}$$

Furthermore, the radial eigenfunctions can be then determined as

$$R_{n_r,m}(r) \sim r^{-1+|\tilde{\ell}|} exp\left(-\frac{\sqrt{v_1}}{2} r^2\right)\ {}_1F_1\left(-n_r\ ;\ \left|\tilde{\ell}\right| + 1;\ \frac{\sqrt{v_1}}{2}\ r^2\right). \tag{3.7}$$

At the instant, eigenenergies equation (3.6) and eigenfucntions equation (3.7) are obtained by using the radial-dependent of the PDM in a pseudoharmonic potential. In the next section, the partition function will be determined by using eigenenergies equation (3.6).

3.2 Thermal properties for the position-dependent mass in pseudoharmonic potential

In this context, the partition function of our PDM system at a specified temperature T is given by [47, 48]

$$Z(\beta) = \sum_{n=0}^{n_{max}} e^{-\beta\, E_{n_r,m}}\ ,\ \beta = \frac{1}{k_\beta T}, \tag{3.7}$$

where $E_{n_r,m}$ are the energies in equation (3.6) , and k_β is the Boltzmann constant. The thermodynamic properties of our PDM in the pseudoharmonic potential, associated with the energies in (3.6), are obtained by rewriting (3.6) as

$$E_{n_r,m} = \frac{1}{\xi}\ ((\sigma_2 - 2n_r)^2 - \sigma_1), \tag{3.8}$$

where,

$$\sigma_1 = m^2 + v_2 + \frac{1}{4}\ , \tag{3.9}$$

$$\sigma_2 = \frac{2\,v_0 - k_z^2}{2\sqrt{v_1}} - 1. \tag{3.10}$$

Then, equation (3.8) is substituted in (3.7) to obtain

$$Z(\beta) = \sum_{n=0}^{n_{max}} e^{-\frac{\beta}{\xi}\left((\sigma_2 - 2n)^2 - \sigma_1\right)}, \tag{3.11}$$

where we take $n = n_r$ for simplicity of notation and n_{max} is obtained by requiring

$$\frac{dE_{n,m}}{dn} = \frac{1}{\xi}\,[2(\sigma_2 - 2n_{max})(-2)] = 0,$$

$$\Rightarrow \sigma_2 - 2n_{max} = 0,$$

$$n_{max} = \left|\frac{\sigma_2}{2}\right|. \tag{3.12}$$

At this point, an integral in the classical limit is used to replace the summation term in equation (3.11), hence

$$Z(\beta) = \int_0^{n_{max}} e^{-\frac{\beta}{\xi}\left((\sigma_2 - 2n)^2 - \sigma_1\right)}\, dn, \tag{3.13}$$

to yield.

$$Z(\beta) = \frac{1}{4}\,\frac{\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)\,\sqrt{\pi}\,e^{\frac{\beta\,\sigma_1}{\xi}}}{\sqrt{\frac{\beta}{\xi}}}. \tag{3.14}$$

Using the partition function (3.14), the mean energy U, mean free energy F, entropy S and specific heat capacity C can be easily derived following [47, 48]:

(i) mean energy, U

$$U(\beta) = -\frac{\partial\,\ln Z(\beta)}{\partial\beta}, \tag{3.15}$$

$$U(\beta) = \frac{1}{2}\,\frac{\left((-2\beta\sigma_1 + \xi)\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)\sqrt{\frac{\beta}{\xi}}\sqrt{\pi} - 2\beta e^{-\frac{\beta\sigma_2^2}{\xi}}\sigma_2\right)\sqrt{\frac{\beta}{\xi}}}{\sqrt{\pi}\,\beta^2\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)}. \tag{3.16}$$

(ii) mean free energy, F

$$F(\beta) = -\frac{1}{\beta}\ln Z(\beta), \tag{3.17}$$

$$F(\beta) = -\frac{\ln\left(\frac{1}{4}\frac{\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)\sqrt{\pi}\, e^{\frac{\beta\sigma_1}{\xi}}}{\sqrt{\frac{\beta}{\xi}}}\right)}{\beta}. \tag{3.18}$$

(iii) Entropy, S

$$S(\beta) = k\ln Z(\beta) - k\beta\,\frac{\partial \ln Z(\beta)}{\partial\beta}, \tag{3.19}$$

$$S(\beta) = \frac{\sqrt{\frac{\beta}{\xi}}k\left(\frac{1}{2}\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)\sqrt{\frac{\beta}{\xi}}\left(-2\beta\sigma_1+\left(2\ln\left(\frac{1}{4}\frac{\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)\sqrt{\pi}\, e^{\frac{\beta\sigma_1}{\xi}}}{\sqrt{\frac{\beta}{\xi}}}\right)+1\right)\xi\right)\sqrt{\pi}-\beta e^{-\frac{\beta\sigma_2^2}{\xi}}\sigma_2\right)}{\beta\sqrt{\pi}\operatorname{erf}\left(\frac{1}{4}\frac{\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)\sqrt{\pi}\, e^{\frac{\beta\sigma_1}{\xi}}}{\sqrt{\frac{\beta}{\xi}}}\right)}. \tag{3.20}$$

(iv) Specific heat capacity, C

$$C(\beta) = k\beta^2\frac{\partial^2 \ln Z(\beta)}{\partial\beta^2}, \tag{3.21}$$

$$C(\beta) = \frac{1}{2}\frac{\left(\beta\xi\pi^{3/2}\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)^2-4\sigma_2\pi\left(-\frac{3}{4}\sqrt{\frac{\beta}{\xi}}\beta+\left(\frac{1}{2}\beta\sigma_2^2+\xi\right)\left(\frac{\beta}{\xi}\right)^{3/2}\right)e^{-\frac{\beta\sigma_2^2}{\xi}}\xi\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)-2\beta^2\sqrt{\pi}\left(e^{-\frac{\beta\sigma_2^2}{\xi}}\right)^2\sigma_2^2\right)k}{\beta\xi\pi^{3/2}\operatorname{erf}\left(\frac{\beta\sigma_2}{\sqrt{\xi\beta}}\right)^2}. \tag{3.22}$$

In figure 1, the pseudoharmonic potential (3.1) is plotted for different values of the harmonic quantum dote potential parameter v_1. it could be seen from the figure that potential energy rapidly converges to infinity as the related potential parameters

increase. The harmonic quantum dote potential parameter v_1 appears to rapidly influence V(r) as it greatly increases with higher parameter v_1 values.

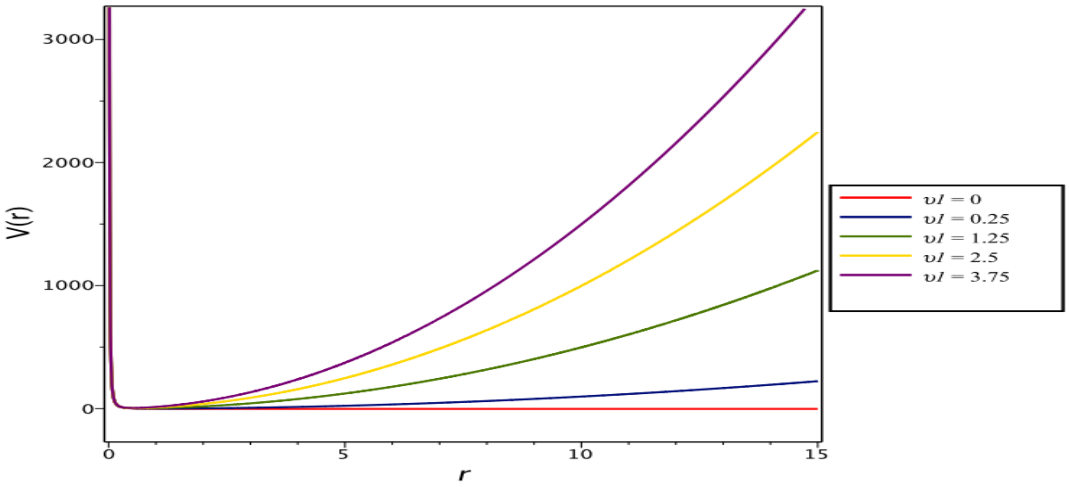

Figure 1. The pseudoharmonic potential (3.1) for different values of the harmonic quantum dote potential parameter v_1 and fixed values for $v_0 = 1$ and $v_2 = 1$.

In the Figure 2, the shape of the pseudoharmonic potential with the change in the antidote potential parameter v_2. It could be seen that figure of the potential energy increases directly in one line as the potential parameters ξ increase.

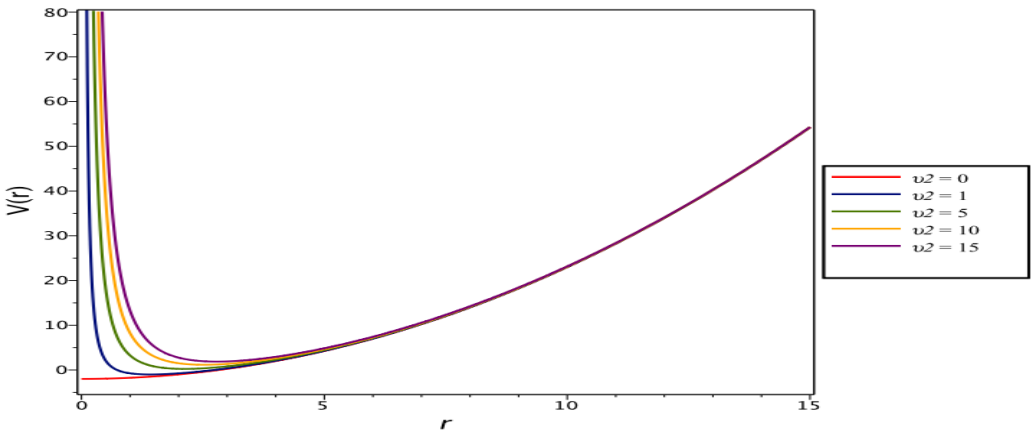

Figure 2. The pseudoharmonic potential (3.1) for different values of the harmonic quantum antidote potential parameter v_2 and fixed values for $v_0 = 1$ and $v_1 = 0.25$.

Whereas, figure 3 shows the effect of chemical potential parameter v_0 on the shape of the pseudoharmonic potential. Generally, it could be seen that the potential energy spreads to infinity as the related potential parameters ξ increases.

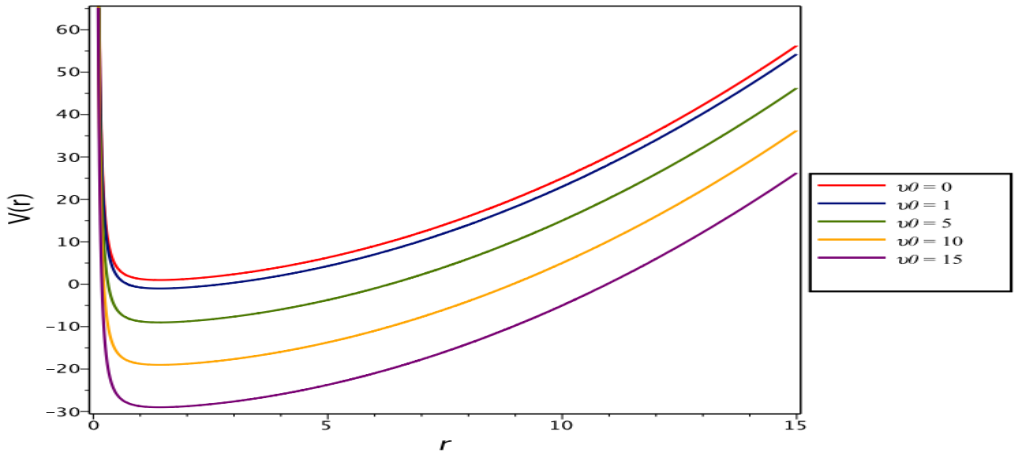

Figure 3. The pseudoharmonic potential (3.1) for different values of the chemical potential parameter v_0 and fixed values for $v_1 = 0.25$ and $v_2 = 1$.

Figures 4-8, we show a graphical representation of the thermal properties obtained via the standard Boltzmann approach. The aim is to analyze and present the interrelationship of the thermodynamical properties with β at different form factors (ξ = 0.1, 0.2, 0.5, 0.6, 0.9). Figure 4 shows the partition function variation with β. It can be seen that the function increases as the temperature decreases for small ξ. However, the line is almost constant with higher ξ values.

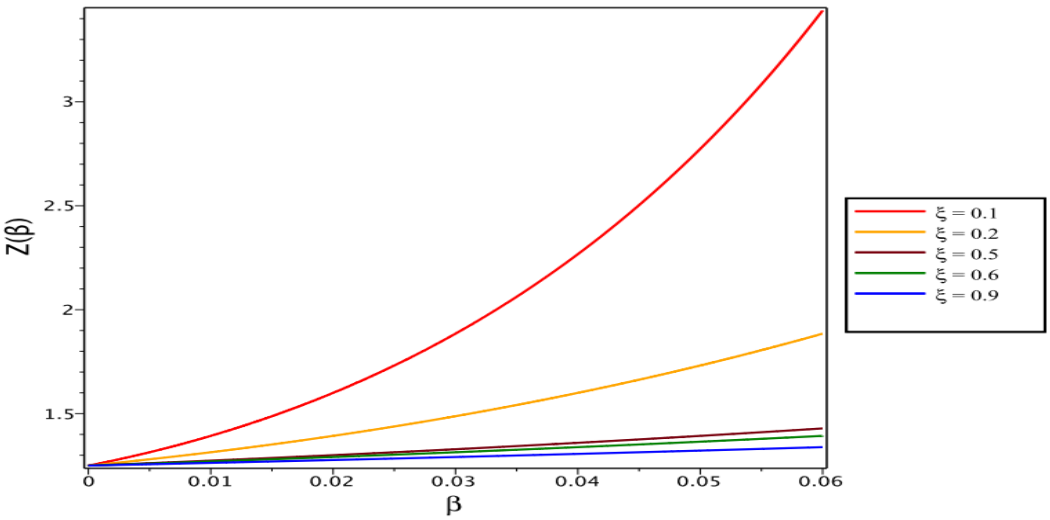

Figure (4). The partition function $Z(\beta)$ (3.14) as a function of β for different values of ξ, when m=1, $v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 1$.

On the other hand, is depicted in figure 5, the mean energy $U(\beta)$ decreases with decreasing temperature T.

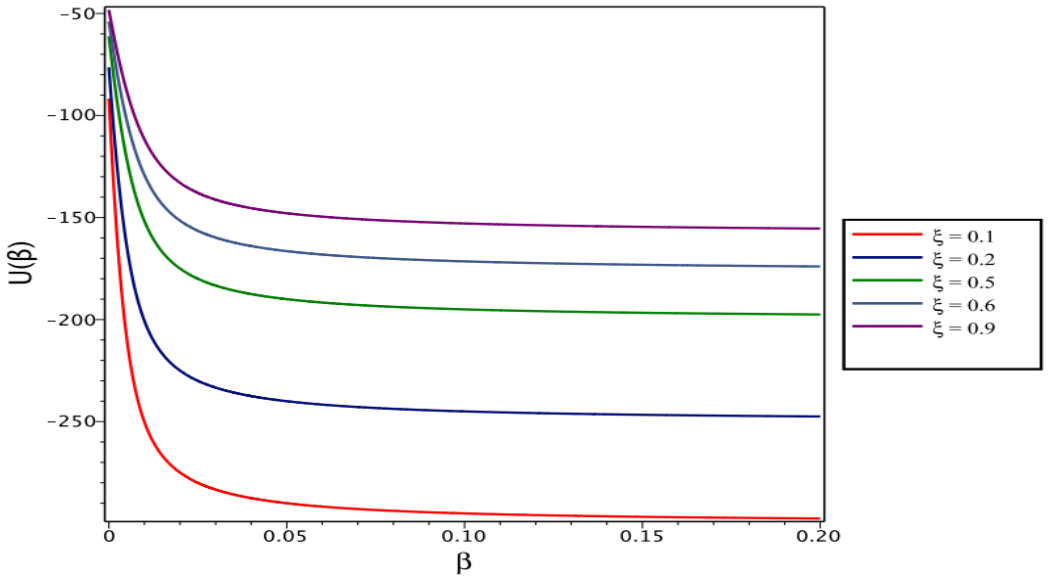

Figure (5). The mean energy $U(\beta)$ (3.16) as a function of β for different values of ξ, when m=1, $v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 1$.

The mean free energy $F(\beta)$ increases monotonically as the temperature T decreases as shown in figure 6.

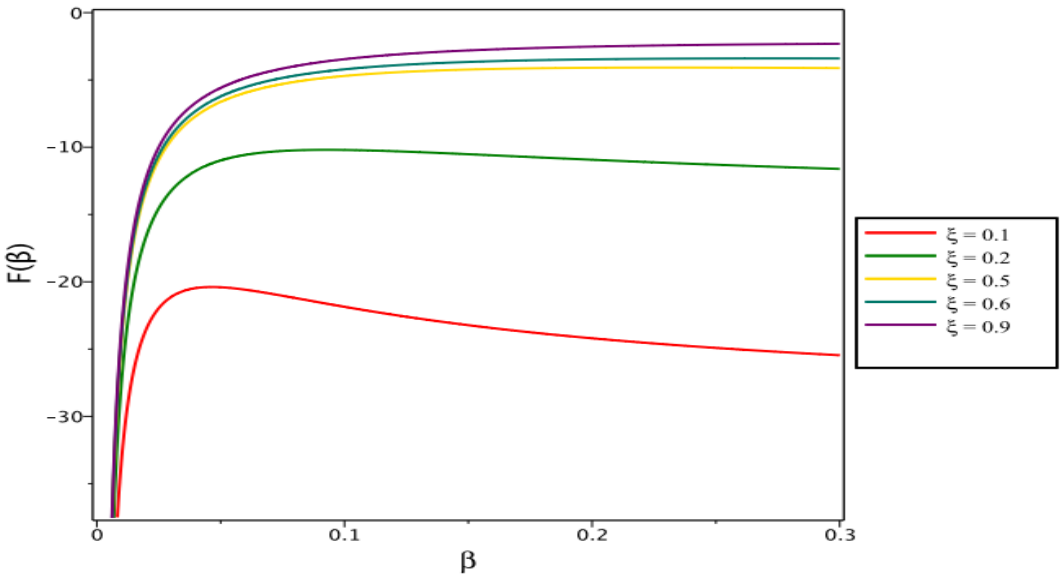

Figure (6). The mean free energy $F(\beta)$ (3.18) as a function of β for different values of ξ, when m=1, $v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 1$.

Figure 7, illustrates the Entropy $S(\beta)$ exponential decrease with decreasing T values and, similar to the case of mean energy $U(\beta)$, the increase in ξ yields higher entropy.

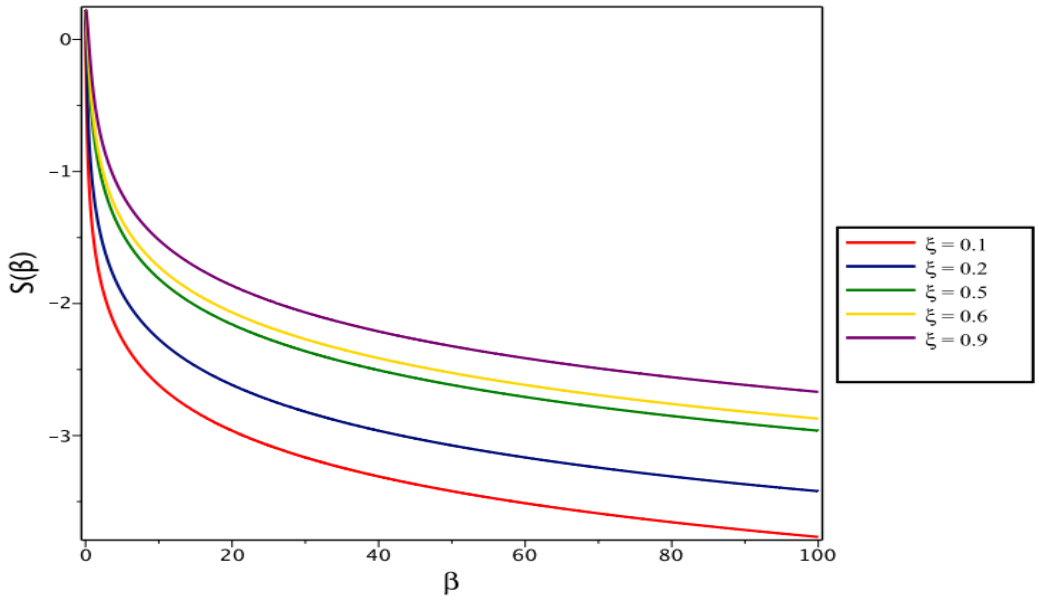

Figure (7). Entropy $S(\beta)$ (3.20) as a function of β for different values of ξ, when m=1, $v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 1$.

Figure 8, shows a decrease in specific heat from the value of $C(\beta) = 1$ as the temperature T decreases. Here, it is observed that the curve for the form factor ξ = 0.1 distinguishes itself from other curves, as it shows a rapid exponential decrease.

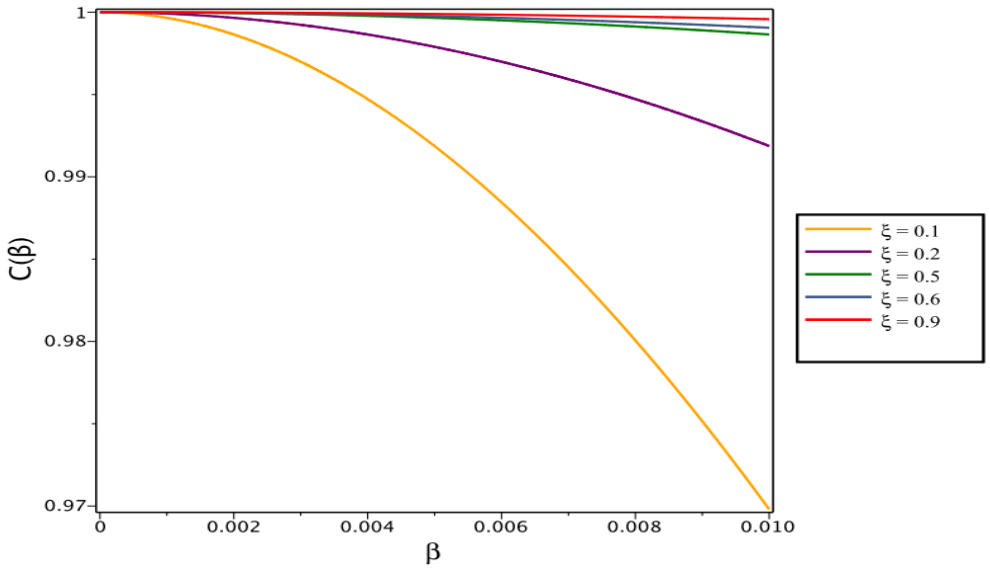

Figure (8). Specific heat capacity $C(\beta)$ (3.22) as a function of β for different values of ξ, when m=1, $v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 1$.

Finally, figures 9-11 show a graphical representation of the energy eigenvalues variation against the parameter ξ for various magnetic quantum number denoted by m m = 0,1,2,3,4. Figure 9 illustrates the energy eigenvalue for n_r=0. As shown, the eigenvalue increases rapidly as the parameter ξ increases, the function however approaches zero with higher ξ values.

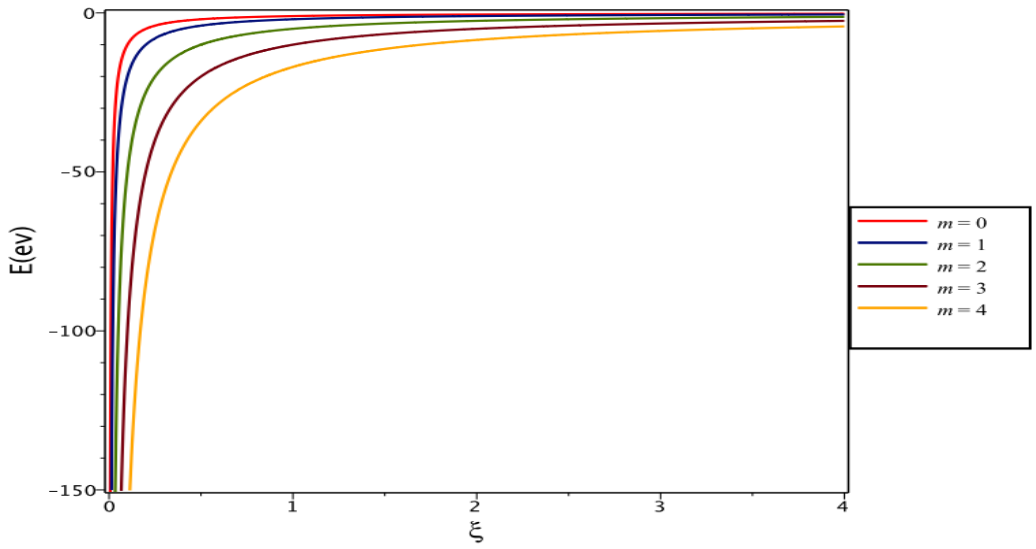

Figure (9). Plot of energy eigenvalue (3.8) as a function of ξ for various magnetic quantum number m, for n_r=0, $v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 2$.

In figure 10, the energy eigenvalue for n_r=1 appears to take a shape having the zero-x-axis as a horizontal asymptote with the eigenvalues being positive when m<2 and negative when m>2.

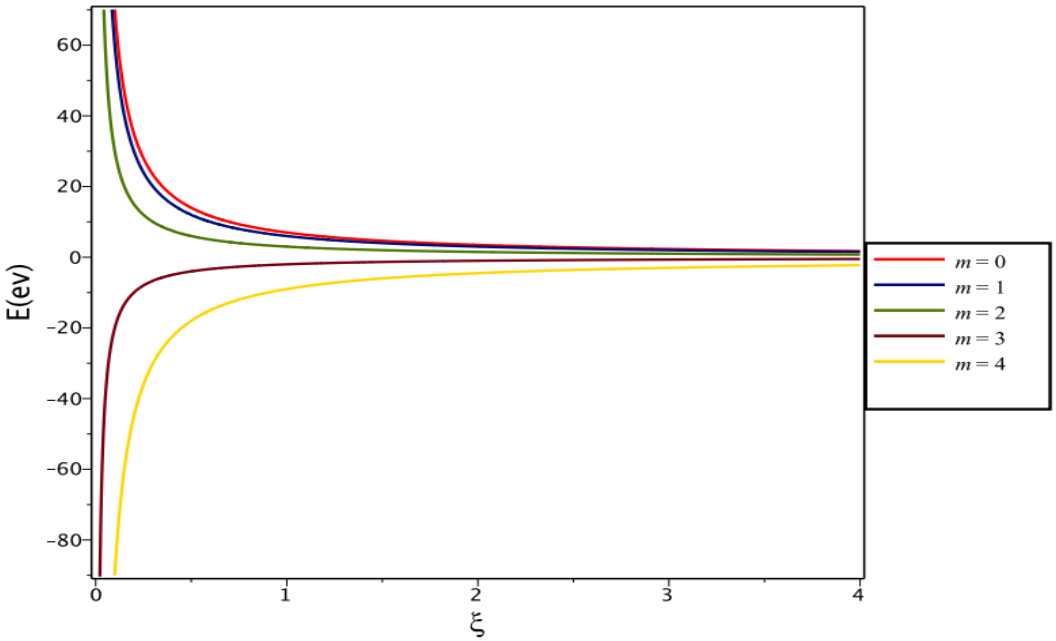

Figure (10). Plot of energy eigenvalue (3.8) as a function of ξ for various magnetic quantum number m, for n_r=1,$v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 2$.

Moreover, for n_r=2 the energy eigenvalue for the various magnetic quantum numbers is almost the mirror version of data observed for n_r=0 (figure 9) about the x-axis, and illustrates the energy eigenvalue decreases rapidly as the parameter ξ increases, which can be seen in figure 11.

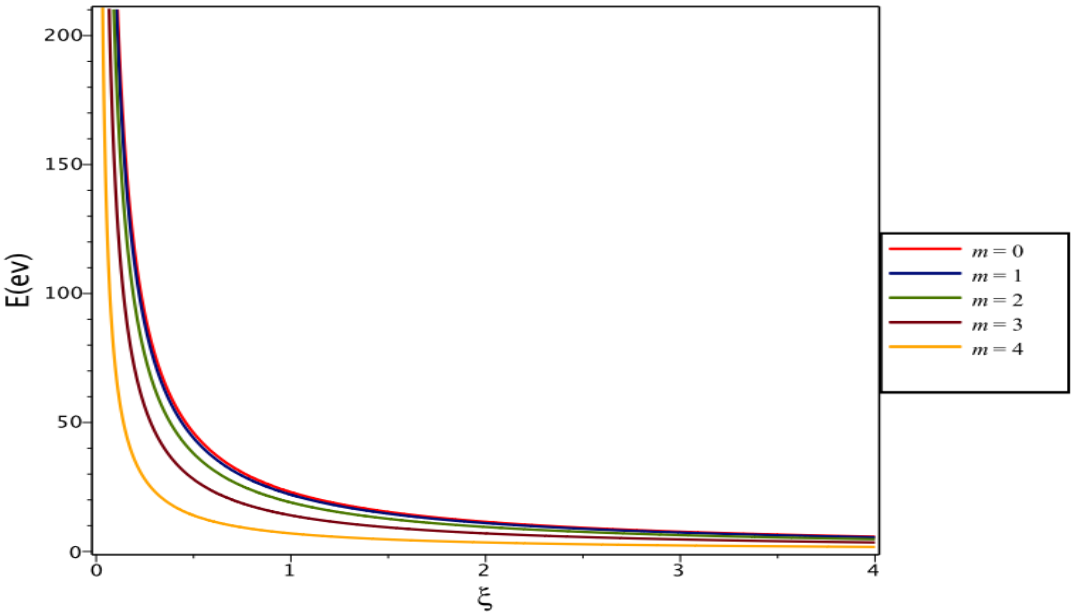

Figure (11). Plot of energy eigenvalue (3.8) as a function of ξ for various magnetic quantum number m, for n_r=2, $v_0 = 2$, $v_1 = 1$, $v_2 = 1.75$, $k_z = 2$.

Chapter 4

CONCLUSION

The thermodynamic properties for a PDM in the pseudoharmonic potential is discussed in this thesis extensively. We have started with the PDM creation and annihilation operators for the PDM harmonic oscillators through the von Roos PDM- Hamiltonian (2.1). The PDM of Schrödinger equation is implemented (2.21), and the formulation of the one-dimensional radial Schrödinger equation (2.31) is obtained. The partition function and thermodynamical properties for PDM-particles in the pseudoharmonic potential have been studied. Their variations with temperature are also presented carefully. Thermodynamical properties like mean energy $U(\beta)$, mean free energy $F(\beta)$, entropy $S(\beta)$ and specific heat capacity $C(\beta)$ are determined in equation (3.16, 3.18, 3.20, 3.22). Results have been discussed extensively using plots. We noted that, mean energy $U(\beta)$ and entropy $S(\beta)$ are reduced as temperature T is decreased, see figure (7,9). We illustrated mean free energy $F(\beta)$ is raised with temperature T decreased monotonically. In contrast to specific heat capacity $C(\beta)$, it has shown the exponentially decreased specific heat capacity $C(\beta)$ for value ($C(\beta)$= 1) with reducing temperature T in figure (6,8). It was found that our results agree with the existing literature. Also the partition function $Z(\beta)$ is growth up as temperature T decreased in figure (4). As we expected, the pseudoharmonic potential is increased with change of the values of the harmonic quantum dote parameter v_1, the harmonic quantum antidote parameter v_2 and the chemical potential parameter v_0, we have shown in figure (1-3). Moreover, effective of the pseudoharmonic potential to our

eigenenergies is illustrated the graphical context. It is noted that in the results, our eigenenergies for the radial quantum number n_r=0 are increased swiftly as the parameter ξ is increased. In contrast to our eigenenergies for n_r=2 is almost mirror version of data about x-axis to observed for n_r=0. Which could be seen in figure (9,11). And our eigenenergies for n_r=1 are positive when m<2 and negative when m>2 as shown in Figure (10).

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