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THERMODYNAMIC PROPERTIES OF INVERTED ISOTROPIC OSCILLATOR WITH DELTA FUNCTION POTENTIAL IN A MAGNETIC FIELD

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Abstract

The thermal properties of inverted isotropic harmonic oscillator with delta function potential in a magnetic field was examined theoretically. The radial form of the Schrodinger equation with a formulated generalized potential was solved using the Frobenius series solution method and the energy eigenvalues was obtained to describe the thermal properties. Analysis of the results showed that, an increase in the strength of the delta function potential leads to a corresponding increase in the even parity energy eigenvalues of the generalized potential and degeneracy removed. An increase in the magnetic field, enhances the generalized potential about a mean point as well as the energy eigenvalues. As the magnetic field and the strength of the delta function potential increases, the thermodynamic functions are enhanced, especially, the additive property of entropy was established.

Keywords**:** Inverted isotropic oscillator, Frobenius method, Thermodynamic functions, Magnetic field, Radial Schrodinger equation, Delta function potential.

Introduction

The linear harmonic oscillator problem is one of the most interesting problems in quantum mechanics owing to the presentation of its closed form solution and its transition to classical domain. It has applications in diverse areas and problems in physics; for example, in studying the vibrational spectra of molecules, in quantum theory of radiation and many more. An expression of the linear isotropic harmonic oscillator is given as

$$V(r) = \frac{1}{2}\mu\omega^2 r^2 \tag{1}$$

where μ is the mass of the oscillator, ω is the frequency and r is the symmetric radius of the oscillator.

If the frequency ω in equation (1) is replaced by $i\omega$, the resulting expression is termed inverted oscillator [1] and is given as

$$V(r) = -\frac{1}{2}\mu\omega^2 r^2 \tag{2}$$

Tackling equation (2) as a problem has attracted attention in many applications and branches of physics varying from high energy physics to solid state theory [2-7]. Several studies that involve inverted harmonic oscillator problem are abounded. Guth and Pi [8], examined the inverted harmonic oscillator as a toy model to describe the early time evolution of inflation from a Gaussian quantum state centred on the peak of the potential. In another study, Boyanovsky et al [9], advocated that the decay of a metastable state is turned into a quantum mechanical inverted oscillator. In the study of chaotic systems, Miller and Sarkar [10] and Gaioli et al [11], used the square of the frequency ω^2 as an instability parameter to determine the expansion and contraction of phase space distributions. The inverted harmonic oscillator Hamiltonian is also used to study statistical fluctuation of fission dynamics [12]. The study of delta (δ) function potential was vigorously pursued by scholars. Prominent among them, are the works of [13 - 14], where it was reported that degeneracy was observed when the strength of the δ -function term tends to unity. According to Patil [15], the harmonic oscillator with a δ -function potential is given as

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$$V(r)=\frac{1}{2}\mu\omega^2 r^2+Z\delta(r) \qquad (3)$$

where Z is the strength of the potential. The author used negative and positive values of Z to obtain some even parity eigenstates of the harmonic oscillator.

Ngiangia and Harry [16], examined the inverted harmonic oscillator with delta (δ) function potential of the form

$$V(r)=-\frac{1}{2}\mu\omega^2 r^2+Z\delta(r) \qquad (4)$$

They reported that an increase in the delta (δ) function potential corresponds to a decrease in the wave function, which is the general characteristics for the inverted excited states. It was suggested that the study can be used to map dimensional string theory on the problem of non-interacting fermions.

Magnetic field is said to deflect alpha decay particles and also in the equidistant splitting of the energy levels generally referred to as the Zeeman effect [17]. Ni and Chen [18] reported that external magnetic field destroyed the superconductivity state of a given element or compound by turning it into normal state. Ikhdair et al [19] examined the effect of magnetic field in non-relativistic molecular models and supporting literatures, showed that the model fit some experimental data. Hayashi [20], opined that magnetic field, alter the rate and yield of chemical reactions. Ngiangia et al [21], reported that in the absence of the centrifugal term in the radial form of the Schrodinger equation, the effect of magnetic field hastened the alpha decay process. Others [22 - 24] also discussed the effect of magnetic field potential in their studies. The thermodynamic properties on classical and quantum systems cannot be underestimated. The heat generated or absorbed and the disorderliness of a system are some of the descriptions of thermodynamic functions. Some studies [25 - 30], highlighted some select thermodynamic functions to describe the energy fluctuations, degeneracy and stability of the systems from the grand partition function. Having examined the works of [1], [15] and [16], the aim is to discuss this work with a potential of the form

$$V(r)=-\frac{qBm\hbar}{2\mu}-\frac{1}{2}\mu\omega^2 r^2+Z\delta(r) \qquad (5)$$

In addition, another new entrance is made, where $\delta(r)$ takes a polynomial of the form

$$\delta(r)=ar^2+br-\frac{c}{r}+\frac{d}{r^2} \qquad (6)$$

where q is the charge, B is the magnetic induction, m is the magnetic quantum number, $\hbar$ is the Planck's constant divided by 2π , a, b, c, and d are potential parameters. The presentation of this work is as follows; in section 2, we analysed the radial Schrödinger equation and presents the bound state energy eigenvalue, section 3, some special cases presented, section 4, the partition function is defined and from it the thermodynamic functions of Hemholtz free energy, internal energy, entropy and specific heat at constant volume were examined, section 5, results and discussion presented, section 6, conclusion, section 7, references.

Radial Schrodinger equation with the effective potential

The study examined the symmetric radial Schrodinger equation of the form

$$\frac{d^2R(r)}{dr^2}+\frac{2}{r}\frac{dR(r)}{dr}+\frac{2\mu}{\hbar^2}\left(E-V(r)-\frac{l(l+1)\hbar^2}{2\mu r^2}\right)R(r)=0 \qquad (7)$$

where l is the orbital quantum number and E is the energy eigenvalues of the system.

Equations (5) and (6) is put into equation (7) and slight repositioning made, the result is given as

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}\right]R(r)+\left[\frac{2\mu}{\hbar^2}\left(E+\frac{qBm\hbar}{2\mu}+\left(\frac{1}{2}\mu\omega^2r^2-Z\left(ar^2+br-\frac{c}{r}+\frac{d}{r^2}\right)\right)\right)\right]R(r)=0 \qquad (8)$$

Simplifying equation (8), results into the form

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{L(L+1)}{r^2}+\left(\varepsilon+Ar^2+B_0r+\frac{C}{r}\right)\right]R(r)=0 \qquad (9)$$

where

$$\varepsilon=\frac{2\mu}{\hbar^2}\left(E+\frac{qBm\hbar}{2\mu}\right) \qquad (9a)$$

$$A=\frac{2\mu}{\hbar^2}\left(\frac{\mu\omega^2}{2}-Za\right) \tag{9b}$$

$$B_0=-\frac{2\mu}{\hbar^2}Zb \tag{9c}$$

$$C=\frac{2\mu}{\hbar^2}Zc \tag{9d}$$

$$L(L+1)=l(l+1)-\frac{2\mu}{\hbar^2}Zd \tag{9e}$$

$$L=\frac{-1\pm\sqrt{(2l+1)^2-\frac{8\mu Zd}{\hbar^2}}}{2} \tag{9f}$$

In order to transform equation (9) into a suitable expression, the symmetric radial wave function is proposed of the form

$$R(r)=Exp\left(-\alpha r^2-\beta r\right)F(r) \tag{10}$$

Equation (10) is put into equation (9) and the resulting expression takes the form

$$F''(r)+\left[\left(-4\alpha r-2\beta+\frac{2}{r}\right)\right]F'(r)+ \\ \left[\left(4\alpha^2-A\right)r^2+\left(4\alpha\beta-2\alpha+B_0\right)r-\frac{L(L+1)}{r^2}+\frac{C}{r}+\left(\beta^2-2\alpha\beta+e\right)\right]F(r)=0 \tag{11}$$

A series solution of the Frobenius type of the form [31] is stated as

$$F(r)=\sum_{n=0}^{\infty}a_n r^{2n+L} \tag{12}$$

Equation (12) is substituted into equation (11) and expand, results into

$$\sum_{n=0}^{\infty}a_n\left\{\left[(2n+L)(2n+L-1)+2-L(L+1)\right]r^{2n+L-2}+\left[-2\beta+C\right]r^{2n+L-1}\right. \\ +\left[-4\alpha(2n+L)+\left(\beta^2-2\alpha\beta+\varepsilon\right)\right]r^{2n+L}+\left[4\alpha\beta-2\alpha\beta+B_0\right]r^{2n+L+1} \\ \left.\left[4\alpha^2-A\right]r^{2n+L+2}\right\}=0 \tag{13}$$

Equation (13) is a linearly independent function, since $a_n\neq 0$ and r is a non – zero function, each of the expressions or terms equal zero and the following relations exist;

$$(2n+L)(2n+L-1)+2-L(L+1)=0 \tag{14}$$

$$\beta=\frac{C}{2} \tag{15}$$

$$-4\alpha(2n+L)+\left(\beta^2-2\alpha\beta+\varepsilon\right)=0 \tag{16}$$

$$B_0+2\alpha\beta=0 \tag{17}$$

$$\alpha=\frac{\sqrt{A}}{2} \tag{18}$$

The values of α , β and L from equations (18), (15) and (9f) respectively and the values of A and C from equations (9b) and (9d) are put into equation (16) and the resulting expression with equation (9a), the energy eigenvalues of the problem under consideration is

$$E_{n,l}=\frac{qBm\hbar}{2\mu}-\frac{\mu}{\hbar^2}\sqrt{\mu\omega^2-2Za}\left(4n-1+\sqrt{(2l+1)^2-\frac{8\mu Zd}{\hbar^2}}-\frac{\mu Zc}{\hbar^2}\right)+\frac{\mu Z^2c^2}{2\hbar^2} \tag{19}$$

The authors observed that this eigenvalue expression is new in view of available literatures.

Some special cases considered

The pseudoharmonic potential

The pseudoharmonic potential is reported to study the anharmonicity of diatomic molecules [32], the interaction of some diatomic molecules [33] and the expression for the mass spectra of heavy quarkonium systems [33]. By adjusting our proposed generalized model using

$\frac{qBm\hbar}{2\mu} = -2D_e, \quad a = \frac{D_e}{r_e^2}$, Z = 1, $d = D_e r_e^2$, $\omega^2 = 0$, b = 0, c = 0, it is reduced to

$$V(r) = -2D_e + \frac{D_e r^2}{r_e^2} + \frac{D_e r_e^2}{r^2} \tag{20}$$

Also, equation (19) reduced to

$$E_{n,l} = 2D_e - \frac{\mu}{\hbar^2}\sqrt{\frac{-2D_e}{r_e^2}}\left(4n - 1 + \sqrt{(2l+1)^2 - \frac{8\mu D_e r_e^2}{\hbar^2}}\right) \tag{21}$$

Comparison of equation (21) with the works of [31], [32] and [33], show acceptable agreement.

The Inverted isotropic harmonic oscillator

From equations (5) and (6), if B = 0, Z = 0, then the resulting expression takes the form of equation (2) and which in turn reduced equation (19) to

$$E_{n,l} = -\left(\sqrt{\mu}\right)^3 (4n + 2l)\frac{\omega}{\hbar^2} \tag{22}$$

Equation (22) is in substantial agreement with [1] and confirmed that the energy eigenvalues decreases and admit discrete energy levels. It also shows that there exist no zero energy associated with the inverted isotropic harmonic oscillator, which was earlier reported by [1]. However, the presence of no zero energy associated with isotropic oscillator is in contrast to the standard harmonic oscillator. This explains that the isotropic harmonic oscillator has some distinguishing characteristics from the inverted counterpart.

Radial wave function

To obtain the radial wave function $R_{n,l}(r)$, equation (12) is put into equation (10) and results in

$$R_{n,l}(r) = Exp\left(-\alpha r^2 - \beta r\right)\sum_{n=0}^{\infty} a_n r^{2n+L}$$

$$= \Pr^L Exp\left(-\alpha r^2 - \beta r\right)\sum_{n=0}^{\infty} a_n r^{2n} \tag{23}$$

where P is a normalization constant.

The associate Laguerre polynomial is defined [17] by

$$L_k^N(r) = \frac{d^N L_k(r)}{dr^N} \tag{24}$$

where $L_k(r) = e^r \frac{d^k}{dr^k}\left(r^k e^{-r}\right)$

The wave function is given as

$$R_{n,l}(r) = \Pr^L Exp\left(-\alpha r^2 - \beta r\right)L_k^N(r) \tag{25}$$

where P can be obtained by normalizing the radial function

$$\int_0^{\infty} r^2 R_{n,l}^2(r)dr = 1 \tag{26}$$

α, β already obtained in equations (18) and (19) and A , C in equations (9b) and (9d) respectively.

If the natural unit $\mu = \hbar = 1, \omega = 2\pi$ [15] is chosen and assume a = c = d = 1, equation (19) reduced to

$$E_{n,l} = -\frac{qBm}{2} - \sqrt{4\pi^2 - 2Z}\left(4n - 1 + \sqrt{(2l+1)^2 - 8Z} - Z\right) + \frac{Z^2}{2} \tag{27}$$

Table 1: Values of energies (J) obtained from equation (27) for the first four even parity for some values of the strength Z of the delta function (imaginary part of Z = 1, 5, 10 is discarded), B = 0.25T, $q = 1.602x10^{-19}C$, m = 1

Z	E_{00}	E_{22}	E_{44}	E_{66}
-10	-88.39026609	-160.1346204	-199.5507694	-326.2002928
-5	-60.12384801	-128.6197201	-166.4049042	-286.1451658
-1	-17.71612859	-88.02012428	-123.3248098	-231.6008063
0	6.283185307	-75.39822368	-113.0973355	-226.1946711
1	-11.74392382	-61.47326703	-99.91930175	-211.8621503
5	-20.07641837	1.641193877	-36.36462756	-146.8954198
10	-1.452203653	63.24030809	-45.58656397	-49.01094067

Table 2: Energy (J) values obtained from equation (2) (for l = 0, the imaginary part is discarded)), B = 0.25T, $q = 1.602x10^{-19}C$, m = 1

Z	N	l	$E_{n,l}$
1	1	0	-11.74392382
	2	0	-36.23177145
		1	-42.35373336
	3	0	-60.71961908
		1	-66.84158099
		2	-85.96111466
	4	0	-85.20746671
		1	-91.32942862
		2	-110.4489623
		3	-124.9071494
	5	0	-109.6953143
		1	-115.8172763
		2	-134.9368099
		3	-148.8949970
		4	-162.0013798

Thermodynamic functions

To study or describe the thermodynamic properties of the system, the grand partition function of ensemble of particles determination is of necessity. The partition function is a statistical measure of the extent to which energy is distributed among the different states of a system or molecules and a function of the degeneracy of the system [35]. The partition function of a quantum mechanical system is given as

$$Z_{n,l}(T) = \sum_{n,l=0}^{\infty} Exp\left(-\frac{E_{n.l}}{k_B T}\right) \tag{28}$$

where k_B is the Boltzmann constant and T is the temperature of the system.

The thermodynamic functions whose properties to be considered for the description of the inverted oscillator are; Helmholtz free energy F(T), internal energy U(T), entropy S(T) and the specific heat at constant volume $C_V(T)$

The Helmholtz free energy is determined by the relation

$$F(T) = -\frac{1}{T}\ln Z_{n,l}(T) = \frac{E_{n,l}}{k_B T^2} \tag{29}$$

The internal energy is stated as

$$U(T) = -\frac{\partial}{\partial T}\ln Z_{n,l}(T) = -\frac{E_{n,l}}{k_B T^2} \tag{30}$$

The entropy is of the form

$$S(T) = -k_B \frac{\partial F(T)}{\partial T} = \frac{2E_{n,l}}{T^3} \tag{31}$$

The specific heat at constant volume results in

$$C_V(T) = k_B \frac{\partial U(T)}{\partial T} = -\frac{2E_{n,l}}{T^3} \tag{32}$$

Results and Discussion

Results

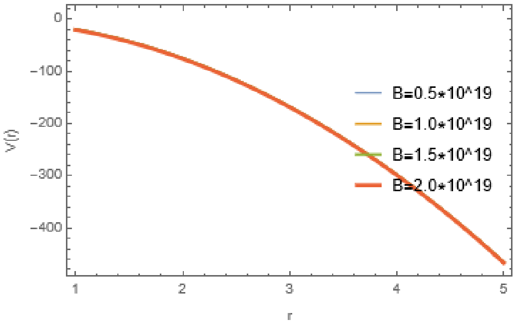

Figure 1: Plot of generalized potential as a function of the radius with magnetic field potential varying

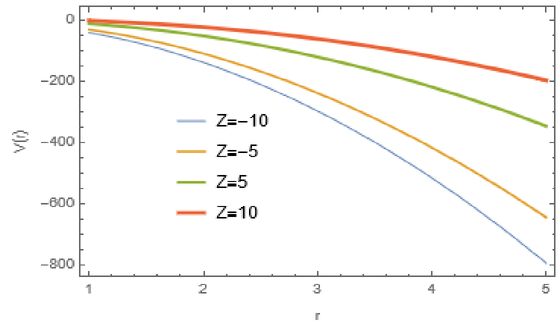

Figure 2: Plot of generalized potential as a function of the radius with strength of delta potential varying

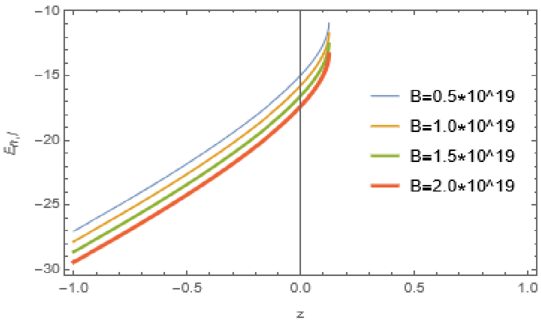

Figure 3: Plot of energy eigenvalues in Joules as a function of the strength of the delta function potential with magnetic field potential varying

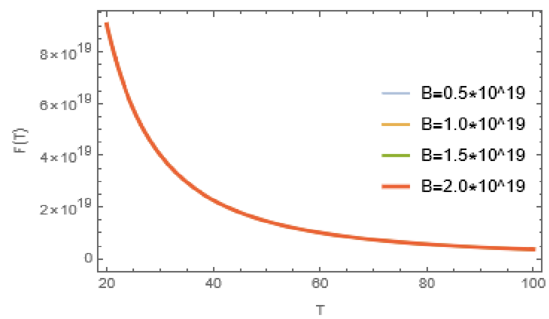

Figure 4: Plot of Helmholtz free energy in joules as a function of temperature with magnetic field potential varying

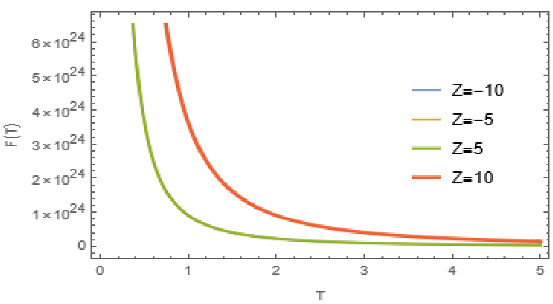

Figure 5: Plot of Helmholtz free energy in joules as a function of temperature with strength of delta function potential varying

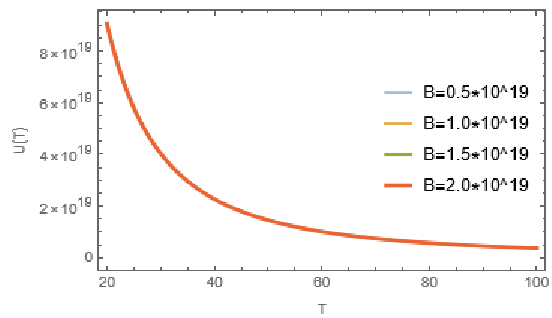

Figure 6: Plot of internal energy in joules as a function of temperature with magnetic field potential varying

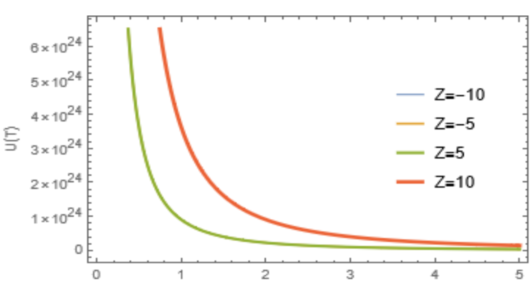

Figure 7: Plot of internal energy in joules as a function of temperature with strength of delta function potential varying

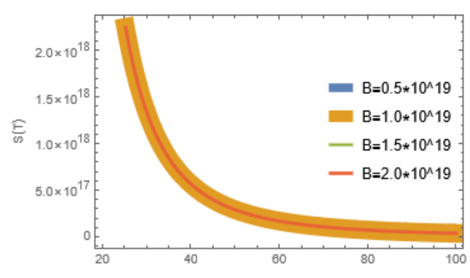

Figure 8: Plot of entropy as a function of temperature with magnetic field potential varying

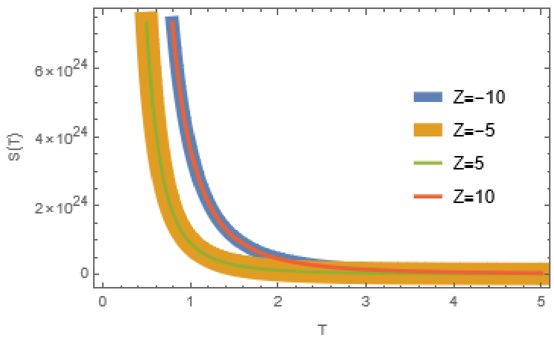

Figure 9: Plot of entropy as a function of temperature with strength of delta function potential varying

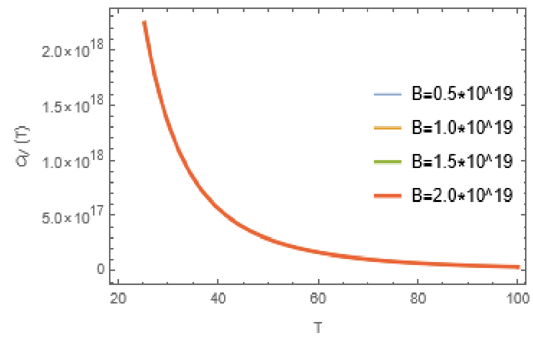

Figure 10: Plot of specific heat at constant volume as a function of temperature with magnetic field potential varying

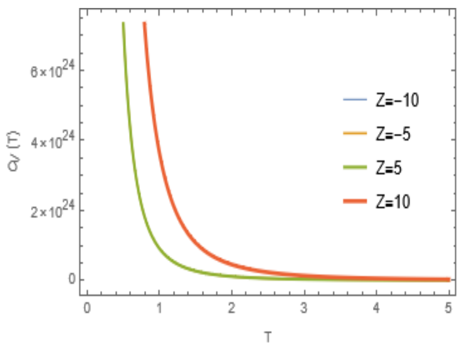

Figure 11: Plot of specific heat at constant volume as a function of temperature with strength of delta function potential varying

Discussion

This work introduced magnetic field and polynomial expression into an isotropic harmonic oscillator with delta function potential and solution to the governing radial form of the Schrodinger equation was obtained using the Frobenius series solution method. The energy eigenvalues has discrete energy spectrum and zero-point energy associated with the generalized potential is present. This results is different from the work of [1] because only inverted harmonic oscillator was considered in their study. The allowed energy eigenvalues of the pseudoharmonic potential and inverted harmonic oscillator potential were deduced as special cases after adjustment of some parameters. The radial eigenfunction of the wave equation was determined though not explicitly. **Table 1**, shows the values of the energies obtained for the first four even parity as the strength Z of the delta function potential increases. As Z increases, degeneracy is removed and the energies increases. It also reveals that the energy tends to the energy of the delta function potential as $Z \rightarrow -\infty$. This findings is in accord with the work of [1]. Although, the presence of the magnetic field increases the energies of the even parity, its effect is proportional to its strength, implying that, it can only be observed if the magnetic field strength is enhanced significantly. **Table 2**, reveals that the energy eigenvalues decreases as the quantum numbers varies and degeneracy is completely removed. However, the effect of the magnetic field is prevalent but not felt owing to the value of the electron charge. **Figure 1**, shows that, as the magnetic field intensity is increased, the generalized potential assumed an increase about a mean position while in **Figure 2**, an increase in the strength of the delta function potential results in an increase in the generalized potential. **Figure 3** depicts that, an increase in the magnetic field, increases the energy eigenvalues and tends to converge at a point. **Figure 4** reveals that, as the magnetic field intensity increases, the Helmholtz free energy increases while an increase in the strength of the delta function potential corresponds to a marginal enhancement of the Helmholtz free energy as shown in **Figure 5**. **Figure 6** displayed graphically, that a marginal increase is observed in the internal energy as the magnetic field increases. However, an increase in the strength of the delta function potential, brought about an increase in the internal energy with a superposition between Z = -5 and 5 and Z = -10 and 10 as shown in **Figure 7**. **Figure 8**, shows an increase in the entropy as the magnetic field intensity increase and as the strength of the delta function potential increases, there exist an overlap on the entropy between the negative value and positive value (- 5 and 5, -10 and 10) . This suggest a fluctuation between the odd parity and even parity and the additive property of entropy [36] as displayed in **Figure 9**. An increase in the magnetic field potential and the strength of the delta function potential enhanced the specific heat at constant volume as shown in **Figures 10 and 11**.

Conclusion

The study shows that an imposed magnetic field of about $10^{19}T$ is required to alter the behaviour of the generalized potential considered. The key results is that, the distinguishing characteristics of inverted isotropic oscillator from harmonic oscillator of other works was also confirmed. Since the allowed energy eigenvalues obtained is new, available literatures to compare the effectiveness of the generalized potential was a challenge. However, the trend with available literatures showed significant agreement. The special cases also laid credence to the agreement with the works of [1], [31], [32] and [33].

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