Information and thermodynamics properties of a non-Hermitian particle ensemble

Francisco Cleiton Lima[1], Allan Moreira[1], and CARLOS ALBERTO ALMEIDA[2]

[1]Universidade Federal do Cear
[2]Universidade Federal do Ceara

December 2, 2020

Abstract

In the context of non-relativistic quantum mechanics, we use information theory to study Shannon's entropy of a non-Hermitian system and understand how the information is modified with the cyclotron frequency. Subsequently, we turn our attention to the construction of an ensemble of these spinless particles in the presence of a uniform magnetic field. Then, we study the thermodynamic properties of the model. Finally, we show how information and thermodynamic properties are modified with the action of the magnetic field.

Keywords: Non-relativistic Quantum Mechanics; Quantum Information; Shannon Entropy.

Introduction

In the initial course of quantum mechanics, we learned that the Hamiltonian operator must be Hermitian (2005; Sakurai & J. Napolitano, 2014). This premise is extremely important for us to have the guarantee of obtaining an energy spectrum with real eigenvalues (2005). As a consequence of this premise, we have a unitary theory with the probability conserved in time, once the inner product in Hilbert's space will have a definite positive norm.

On the other hand, in recent years, it has been observed that the requirements for real energy eigenvalues and the unitarity of the theory can be obtained in non-Hermitian Hamiltonian operators. Indeed, in 1998, Bender and Boettcher (Bender & S. Boettcher, 1998) demonstrated that the hermiticity condition can be replaced by a condition analogous to the space-time reflection symmetry, i. e., the $\mathcal{PT}$-symmetry (Bender & S. Boettcher, 1998). Therefore, if the Hamiltonian operator is invariant under the $\mathcal{PT}$-symmetry operator it will satisfy all the conditions of quantum mechanics mentioned above (Bender & S. Boettcher, 1998; S. Weigert, 2003; C. M. Bender, 2007). If the $\mathcal{PT}$ symmetry is violated in the model, the energy eigenvalues would not be physically acceptable.

After the publication of the paper of Ref. (Bender & S. Boettcher, 1998), there has been a significant increase in the interest of many researchers and supporters of the concept of non-Hermitian Hamiltonian. As a matter of fact, this paper allowed a new branch for studies involving these systems, for example, studies in quantum optics (C. M. Bender, 2015; S. Longhi, 2010; Razzari & R. Morandotti, 2012), superconductivity (J. Rubinstein & Q. Ma, 2007; N. ChtcheLkatchev & V. Vinokur, 2012), lasers (Y. D. Chong & A. D. Stone, 2011; 2012), microwave cavities (2011; 2012), electronic circuits (2011), graphene (2011), among others. However, after the seminal work of Bender (Bender & S. Boettcher, 1998), interesting developments arise towards the structures of theories with non-Hermitian and non-$\mathcal{PT}$ symmetric Hamiltonians, but with real eigenvalues (M. Swanson, 2004; A. de Souza Dutra & V. G. C. S. dos Santos. Europhys. Lett., 2005; F. B. Ramos & K. Bakke, 2019).

In 1948, Claude E. Shannon constructed the concept that would be known as Shannon's entropy or Shannon's Information (C. E. Shannon, 1948). Initially, this concept was formulated within the framework of the mathematical theory of communication or information theory (C. E. Shannon, 1948; Shihan Dong & J. P. Draayer, 2014; Xu-Dong Song & Shi-Hai Dong, 2015). Information theory has allowed the study of cryptography (Grosshans & N. J. Cerf, 2004), coding (B. Schumacher, 1995), noise theory (Wyner & S. Shamai, 1998), and others. In the context of quantum mechanics the interpretation of Shannon's entropy in the space of positions is related to the uncertainty of the location of the particle in space (M. Born, 1989; Shihan Dong & J. P. Draayer, 2014; Xu-Dong Song & Shi-Hai Dong, 2015). Similarly, entropy in the momentum space is related to the uncertainty of the particle momentum measurements. Thus, Shannon's entropy presents itself in quantum mechanics as a new formalism for the study of uncertainties and information related to quantum systems (C. E. Shannon, 1948; 1997).

Theoretical studies on information measures for different quantum systems have been carried out in several studies. There are many models in which we have the investigation of information theory. For instance, models involving the Schrödinger equation for several potentials, such as Dirac-delta potential (P. A. Bouvrie & J. S. Dehesa, 2011), hyperbolic potential (R. Valencia-Torres & S. H. Dong, 2015), harmonic oscillator in D dimensions and hydrogen atom (R. J. Yanez & J. S. Dehesa, 1994; J. S. Dehesa & A. I. Aptekarev, 2019), Morse and Pöschl-Teller potentials (J. S. Dehesa & V. N. Sorokin, 2006), infinite potential well (V. Majernik & E. Majernikova, 1999), double well (S. T. Tserkis & C. P. Panos, 2014), hydrogen atom confined and free (Mukherjee & A. K. Roy, 2018), Eckart potential (P. R. Kumar & A. Kumar, 2016), among others.

The principal aim of this work is to obtain the thermodynamics properties of a physical system described by a non-Hermitian Hamiltonian. In particular, we investigate Shannon's entropy of the system when submitted to a magnetic field, and we conclude that this entropy is strongly influenced by this magnetic field.

This work is organized as follows. In Section II, we introduce a brief review of the model considered. Then, through the information theory we studied Shannon's entropy of a non-Hermitian spinless particle in Section III. Also we present here the numerical and graphical results related to information density and Shannon's entropy. In Section IV, we build a canonical ensemble of these particles and study the thermodynamic properties of the system. We present our conclusions and discuss perspectives of the work in Section V.

A brief review

In this study, we will use the model recently introduced by Ramos et. al. (F. B. Ramos & K. Bakke, 2019) and in this section we follow closely that work. We consider a spinless charged particle interacting with the magnetic field. The respective Schrödinger equation is written as

$$i\hbar\partial_t\Phi(\vec{r},t) = \frac{1}{2m}[\hat{p} - e\vec{A}(\vec{r})]^2\Phi(\vec{r},t) + V(\vec{r})\Phi(\vec{r},t), \tag{1}$$

where e is the electric charge, m is the mass of the particle, $\vec{A}(\vec{r})$ is the electromagnetic vector potential and $V(\vec{r})$ is the scalar potential of the system.

For convenience, we assume that

$$\vec{A}(\vec{r}) = Bx\hat{y},$$

(2)

where B is a constant that represent the magnitude of the magnetic field. With the expression (2), we observe that

$$\vec{B}(\vec{r}) = \vec{\nabla} \times \vec{A}(\vec{r}) \rightarrow \vec{B}(\vec{r}) = B\hat{z}.$$

(3)

Therefore, the electron moves in a plane perpendicular to the magnetic field, which gives rise to a spectrum of energy well known in the specialized literature as the levels of Landau (2005; F. B. Ramos & K. Bakke, 2019).

We know that when we work with non-relativistic quantum systems, it is necessary to formulate a Hermitian Hamiltonian operator. However, as discussed by Ramos *et. al* (F. B. Ramos & K. Bakke, 2019), it is possible to describe some systems with non-Hermitian operators that have real eigenvalues. In other words, although the operator is non-Hermitian, these operators can describe physical aspects of the systems.

As our start point, we will assume a non-Hermitian operator of the form (F. B. Ramos & K. Bakke, 2019)

$$V(\vec{r}) = i\sqrt{2}\alpha\hat{r} \cdot [\hat{p} - e\vec{A}],$$

(4)

with $\hat{r} = \frac{1}{\sqrt{2}}(\hat{x}, \hat{y}, 0)$ and α a real parameter.

Observing Eq. (4), we notice that the potential is not invariant under $\mathcal{PT}$ transformations. Thus, we note that the Hamiltonian operator that describes the Landau system is non-Hermitian and is not symmetric by $\mathcal{PT}$.

Assuming variable separation $\Phi(\vec{r}, t) = \mathrm{e}^{-i\mathcal{E}t/\hbar}\psi(x, y)$ in the model, we observe that

The equation above is independent of the y variable. From the fundamental of quantum mechanics, this implies that the momentum operator component $\hat{p}_y$ commutes with the Hamiltonian. In other words, this physical quantity is a conserved one. Indeed, it worth to comment here that the system is effectively bidimensional. Then, the solution of the system can be written as $\psi = \mathrm{e}^{i\frac{p_y}{\hbar}y}f(x)$ with $-\infty < p_y < \infty$ corresponding to the eigenvalue associated with the momentum operator in the y-component.

Rewriting the previous equation, now we have for the function $f(x)$, where $\omega = eB/m$ is the frequency of the cyclotron. We assume the parameters

$$\beta = \frac{2m\mathcal{E}}{\hbar^2} \qquad \text{and} \qquad \theta = \frac{2m\alpha}{\hbar}.$$

(5)

In addition, we consider the respective changes in the independent and dependent variables as

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\left(x - \frac{p_y}{m\omega} - i\frac{\theta\hbar}{2m\omega}\right),$$

(6)

and

$$f(\xi) = \xi \mathrm{e}^{-\frac{\xi^2}{2}} \mathrm{e}^{\frac{\theta}{2}\sqrt{\frac{\hbar}{m\omega}}} F(\xi).$$

(7)

Replacing the equations (6) and (7), we reduced the expression (**??**) to

$$F''(\xi) + \left(\frac{2}{\xi} - 2\xi\right)F'(\xi) + \left[\frac{\beta\hbar}{4m\omega} - \frac{\theta^2\hbar}{8m\omega} - \frac{3}{4}\right]F(\xi) = 0.$$

(8)

Now after we make $\zeta = \xi^2$, we obtain the equation known as confluent hypergeometric equation, namely,

$$\zeta F''(\zeta)\left(\frac{3}{2} - \zeta\right)F'(\zeta) + \left[\frac{\beta\hbar}{4m\omega} - \frac{\theta^2\hbar}{8m\omega} - \frac{3}{4}\right]F(\zeta) = 0.$$

(9)

Remembering that $\Psi(\vec{r} \to 0, t) \to 0$, we finally obtain that the wave function is described by with $n = 0, 1, 2, ...$

Corresponding eigenvalues of energy are given by

$$\mathcal{E}_n = \left(2n + \frac{3}{2}\right)\hbar\omega + m\alpha^2.$$

(10)

Information theory: Shannon's entropy

Based on thermodynamics, the Shannon entropy concept provides the irreversibility of the physical system. According to statistical physics, the measure of entropy appears as a measure associated with the degree of disorder of the system.

Shannon's concept of entropy was first proposed in 1948 by Claude E. Shannon in the paper entitled *A mathematical theory of communication* (C. E. Shannon, 1948). In this work, Shannon describes entropy as an element of information theory. In this context, entropy is a measure of uncertainty in a given probability distribution, so it is called Shannon's entropy or information entropy.

The entropy can be interpreted as a starting point for measuring the uncertainty of a probability distribution associated with an information source. According to Born (M. Born, 1989), the statistical interpretation of a quantum system is described by the probability density that is defined by

$$\rho(x) \equiv |\Psi(\vec{r}, t)|^2.$$

(11)

Thus, for a probability density of a continuous system in one-dimensional space, Shannon's entropy for the n-th state is described by

$$S_x^n = -\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \mathrm{Ln}(|\Psi(x,t)|^2)\, dx,$$

(12)

while in the momentum-k space it is

$$S_k^n = -\int_{-\infty}^{\infty} |\Psi(k,t)|^2 \mathrm{Ln}(|\Psi(k,t)|^2)\, dk,$$

(13)

where $\Psi(k,t)$ is the wave function in the reciprocal space or in the momentum space (2005; C. E. Shannon, 1948).

Numerical result of the information

From now on, we analyzed Shannon's information of a charged non-Hermitian spinless particle interacting with the magnetic field. In this context, we investigate how information is modified due to the influence of the magnetic field on the model. For this, we analyzed the wave functions for the first energy levels of the model, that is, $n = 0, 1, 2, 3$. With the wave function described for the first energy levels of the model, we can observe the influence of the magnetic field on the uncertainties related to the solutions of the model, through information theory. With this in mind, we replace the normalized wave eigenfunctions described by the expression (**??**) of the first energy levels in the expression (12), and later through the Fourier transform

$$\Psi(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k,t)\, \mathrm{e}^{ikx}\, dx,$$

(14)

we will investigate the information in the reciprocal space.

Let us now to recall the work of Bialynicki-Birula and Mycielski (BBM) (Bialynicki-Birula & J. Mycielski, 1975). In that work they derive a new uncertainty relation in quantum mechanics. As a matter of fact, this new relation has an interpretation in terms of information theory. Thus, the entropic uncertainty relationship that relates the position and momentum uncertainties must respect the relation

$$S_x^n + S_k^n \geq d[1 + \mathrm{Ln}(\pi)],$$

(15)

where d denotes the dimension of the position and momentum space (Bialynicki-Birula & J. Mycielski, 1975).

Although the system is bidimensional, since the variable y is cyclic, the solution in this coordinate will not contribute to the measurement of information or uncertainties of the physical system. Therefore the equation above turns to

$$S_x^n + S_k^n \geq [1 + \mathrm{Ln}(\pi)] \cong 2,14473.$$

(16)

Numerically calculating the quantities S_x^n and S_k^n, we obtain the results as the cyclotron frequency increases (Table I). In other words, we obtain the information when magnetic field becomes stronger.

The Shannon's information can be well illustrated through the graphics of the entropic density in the position space and in the momentum space for several values of the magnetic field (cyclotron frequency). The results are shown in Figs. (1), (2), (3) and (4).

n	ω	S_x	S_k	$S_x + S_k$
	10	0,07511	2,58794	2,66305
0	100	-1,24617	3,93031	2,68415
	1000	-2,44074	5,12615	2,68541
	10	0,29949	2,51618	2,81568
1	100	-1,33164	3,91697	2,58533
	1000	-2,59974	5,15778	2,55804
	10	0,34254	2,33426	2,67681
2	100	-1,35202	3,89831	2,5463
	1000	-2,62173	5,16562	2,54389
	10	0,35207	2,19412	2,54619
3	100	-1,35095	3,88301	2,53205
	1000	-2,62896	5,16816	2,53919

Table 1: Numerical result of the Shannon's entropy in the system for several values of the cyclotron frequency.

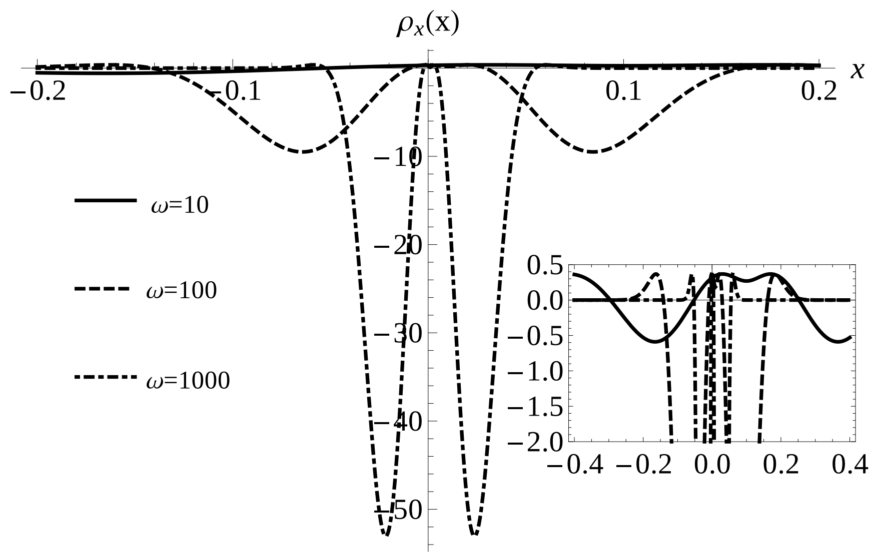

Figure 1: Entropic density in the position space when $n = 0$ for several values of the cyclotron frequency.

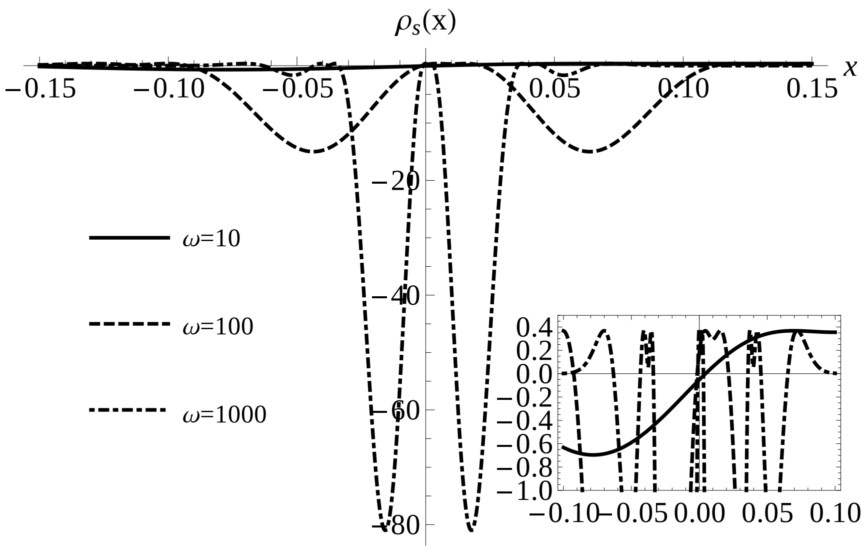

Figure 2: Entropic density in the position space when $n = 1$ for several values of the cyclotron frequency.

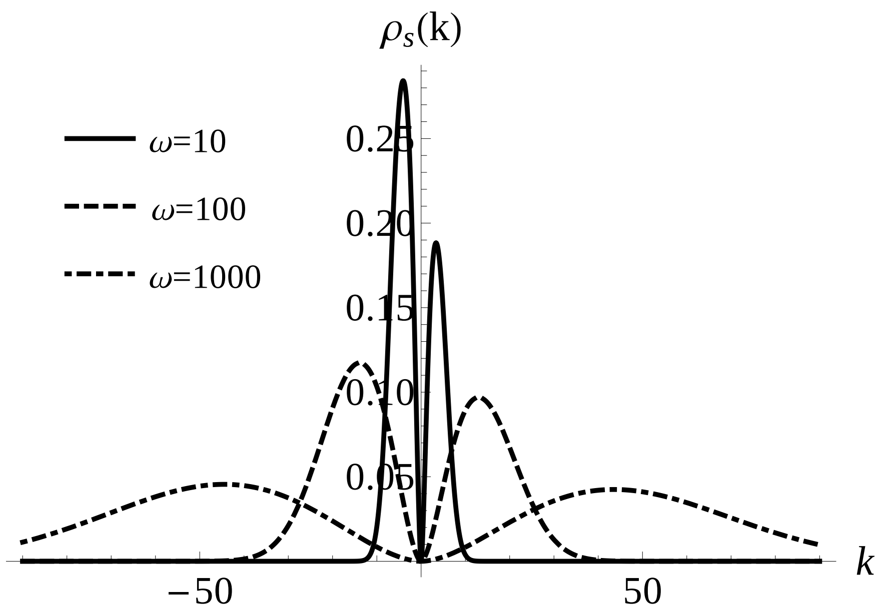

Figure 3: Entropic density in the momentum space when $n = 0$ for several values of the cyclotron frequency.

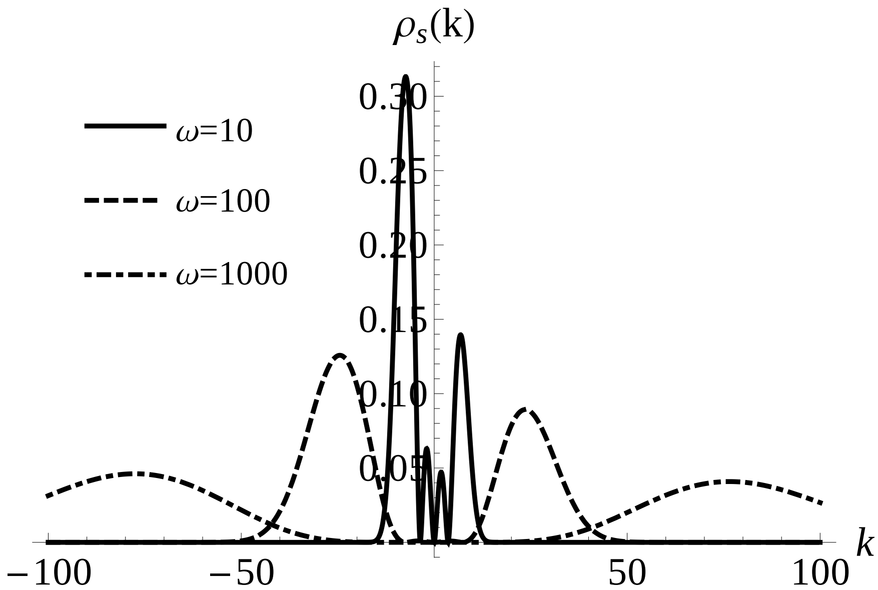

Figure 4: Entropic density in the momentum space when $n = 1$ for several values of the cyclotron frequency.

We can make an analysis of the numerical results for Shannon's entropy in the table (I). We interpolate the functions that represent Shannon's information and present the graphical results as a function of the cyclotron frequency. The results are shown in Figs. (5) and (6).

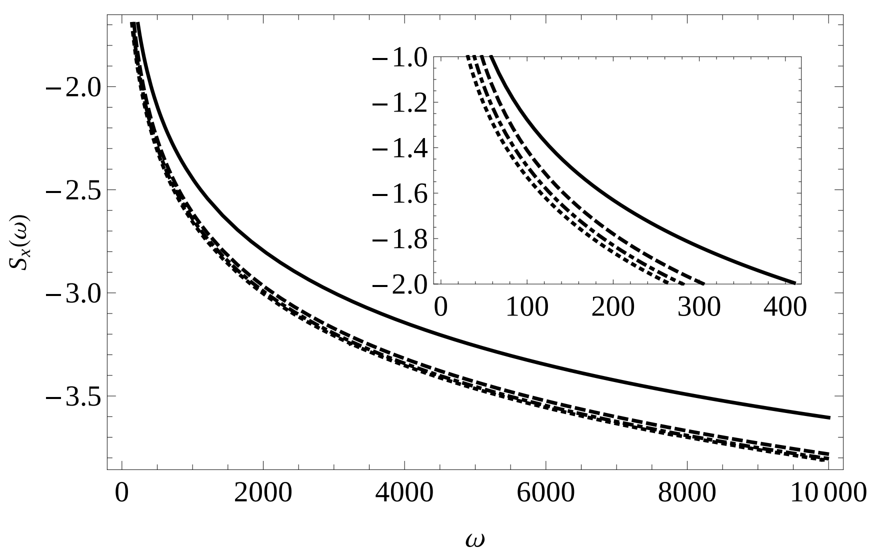

Figure 5: Shannon's entropy in the position space in function of the cyclotron frequency. The energy states are described for $n = 0$ (continuous line), $n = 1$ (dashed line), $n = 2$ (dotted-dashed) and $n = 3$ (dotted line).

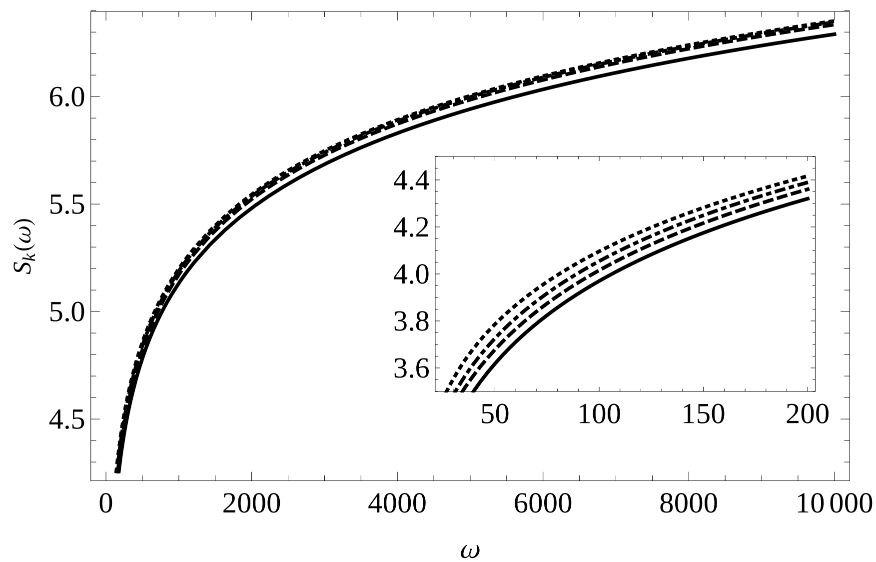

Figure 6: Shannon's entropy in the momentum space in function of the cyclotron frequency. The energy states are described for $n = 0$ (continuous line), $n = 1$ (dashed line), $n = 2$ (dotted-dashed) and $n = 3$ (dotted line).

Thermodynamic properties

Motivated to carry out the study of the thermodynamic properties of the system, we built a canonical ensemble consisting of spinless particles and under the influence of the magnetic field. Initially, for the calculation of the properties we start by defining the well known partition function. We recall that the partition function plays a fundamental role in statistical mechanics, where all thermodynamic quantities are constructed from it. Since the model is not degenerate, the partition function that describes the accessible states of the particles in a thermal bath is described by

$$Z_1 = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta \mathcal{E}_n}, \tag{17}$$

where $\beta = 1/k_B T$; k_B is the Boltzmann constant and T is the temperature of the ensemble in thermodynamic equilibrium. For later convenience in the analysis of the graphical results, we will assume the variable $\tau = k_B T$.

After obtaining the partition function, it is possible to study all the Boltzmann thermodynamic properties of the model. In this work, we will turn our attention to the study of the main thermodynamic functions and the influence of the magnetic field on their properties. Namely, the main properties are the Helmholtz free energy $\mathcal{F}(\tau)$, the mean energy $\mathcal{U}(\tau)$, the entropy $\mathcal{S}(\tau)$ and the heat capacity $\mathcal{C}_v(\tau)$. Mathematically, these quantities for a canonical ensemble are given by where Z_N is the total partition function and N is the amount of particles that make up the ensemble.

The results

Now, we consider Eq. (10) to build the partition function of the model. Then, we obtain that

$$Z_1 = \mathrm{e}^{-m\alpha^2\beta}\sum_{n=0}^{\infty}\mathrm{e}^{-(2n+\frac{3}{2})\hbar\omega\beta} = \frac{\mathrm{e}^{-(m\alpha^2+\frac{3}{2}\hbar\omega)\beta}}{1-\mathrm{e}^{-2\hbar\omega\beta}}.$$

(18)

From the partition function, we obtain the main thermodynamic functions. Namely,

and

$$\mathcal{C}_v = \frac{4\mathrm{e}^{-2\hbar\omega\beta}N\hbar^2\omega^2\beta^2k_B}{(\mathrm{e}^{-2\hbar\omega\beta}-1)^2}.$$

(19)

Analyzing the behavior of properties when the frequency $\omega \to 0$. We note that, $\mathcal{F}(\omega \to 0) \to -\infty$, $\mathcal{U}(\omega \to 0) \to 0$, $\mathcal{S}(\omega \to 0) \to \infty$ and $\mathcal{C}_v(\omega \to 0) \to 0$.

The thermodynamic functions are displayed together in Fig. (7). Subsequently, in the concluding remarks, we present a detailed analysis of these graphs. Also, we discuss the results of the information theory obtained for the system.

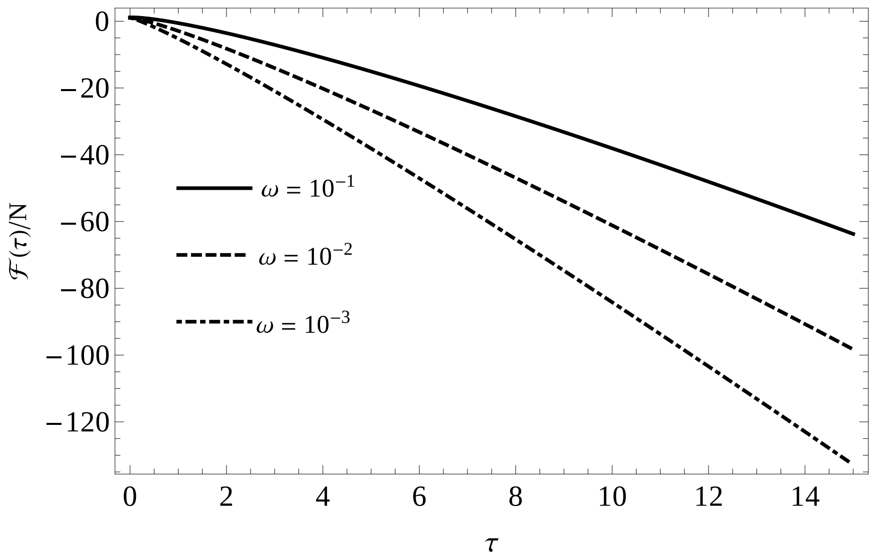

Figure 7: Helmholtz free energy $\mathcal{F}(\tau)$, the mean energy $\mathcal{U}(\tau)$, the entropy $\mathcal{S}(\tau)$ and the heat capacity $\mathcal{C}_v(\tau)$, for several value of the cyclotron frequency.

Concluding remarks

In this work, we study Shannon's information theory of a spinless particle subject to a potential that generates a non-Hermitian Hamiltonian. The system is submitted to a magnetic field. We observe how the information changes with the cyclotron frequency. We realized that depending on the intensity of the magnetic field the probability densities can be more or less located in both spaces.

Through the numerical and graphical results, we noticed that the information tends to decrease in the space of the positions with increasing field. In contrast, it increases in the space of momentum, respecting the entropic uncertainty relationship. We also concluded that the cyclotron frequency, that is, the magnetic field of the system, plays an essential role in Shannon's entropy. We observe that the more intense the magnetic field, the more localized is the Shannon probability density in the position space. Thus, we can conclude that the uncertainties in the particle localization measure will be less.

In contrast, in the momentum space, we have less localized probability densities when the field is intense. This fact leads us to conclude that the uncertainties in the measures related to the particle's momentum are more significant. Therefore, we conclude that with the results obtained from Shannon's entropy, we directly observe the validity of the Heisenberg uncertainty principle for the system studied.

Motivated by the study carried out on Shannon's entropy, we built a canonical ensemble through static arguments and analyzed the thermodynamic properties of the model. Initially, with the Landau spectrum of the system described by Eq. (10), we calculate the partition function of the system. Then, we investigate all the main thermodynamic quantities that could be derived, namely, the Helmholtz free energy $\mathcal{F}$, the mean energy $\mathcal{U}$, the entropy $\mathcal{S}$ and the heat capacity $\mathcal{C}_v$. All these functions are displayed for several values of the cyclotron frequency. As a result, we note that the well-known Dulong-Petit law is satisfied independently of the value of the magnetic field, that is, $\mathcal{C}_v(T \to \infty) \to k_B$. Concluding, it is important to remark the role of the magnetic field in this context. Indeed, when $\omega \to 0$, all the thermodynamic functions turn more relevant, as we can see from Fig. (7).

Acknowledgments

The authors thank the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), grant nº 308638/2015-8 (CASA), and Coordenaçao de Aperfeiçoamento do Pessoal de Nível Superior (CAPES), for financial support.

References

(2005).

(2014).

(1998).

(2003).

(2007).

(2015).

(2010).

(2012).

(2007).

(2012).

(2011).

(2012).

(2011).

(2012).

(2011).

(2011).

(2004).

(2005).

(2019).

(1948).

(2014).

(2015).

(2004).

(1995).

(1998).

New York. (1989).

(1997).

(2011).

(2015).

(1994).

(2019).

(2006).

(1999).

(2014).

(2018).

(2016).

(1975).