On the definition of entropy for quantum unstable states

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Abstract. The concept of entropy is central to the formulation of the quantum statistical mechanics, and it is linked to the definition of the density operator and the associated probabilities of occupation of quantum states. The extension of this scheme to accommodate for quantum decaying states is conceptually difficult, because of the nature of these states. Here we present a way to treat quantum unstable states in the context of statistical mechanics. We focuss on the definition of the entropy and avoid the use of complex temperatures.

1. Introduction

The fact that decaying states can be accommodated in the context of extensions of the framework of ordinary quantum mechanics [1] suggests that, in principle, they can also be accommodated in the framework of quantum statistical mechanics. However, the subject has been rarely treated in the literature, perhaps because of the inherent difficulty of having to deal with complex energy states in a formalism strongly limited by the notion of probabilities. Thus, one encounters here the same conceptual difficulties of the quantum mechanical treatment of complex energy states, which, as said before, can be avoided by adopting the notion of analytic extensions of the representations [1, 2, 3]. Kobayashi and Shimbori [4], and Kobayashi [5]have elaborated on the notion of entropy for complex-energy systems. In these papers the real and imaginary parts of the energy of a resonance are treated independently, and the canonical partition function for the resonance is given as a product of canonical partition functions for the real and imaginary parts of the energy, so that the total entropy is the sum of both contributions. Then, decaying processes transfer entropy from the imaginary part to the real part and the rate of this transference depends on time. Each part has its own temperature, which suggest a notion of a complex temperature. Another approach has been advanced by the Brussels group [6], by the notion of entropy operator for Gamow states, in the spirit of the entropy operator of Misra, Prigogine and Courbage [6]. This operator belongs to a family of operators defined on an extended space. The difficulty associated to this approach consists on the construction of the entropy operator.

In our approach, we give an expression for the entropy, without the introduction of the entropy operator of Misra et al.[6]. We assume thermodynamical equilibrium for decaying systems, which is a valid approximation if the half life of the state is sufficiently large, or equivalently if the width is sufficiently small, and use the Friedrichs model [7] as a laboratory, because it has the advantage of being a solvable model for resonance phenomena. We have formulated the Friedrichs model in second quantization language to construct coherent state and used of path integral method

to obtain the canonical partition function of a system with resonances, which naturally leads to an expression for the canonical entropy of decaying states. The resulting entropy is complex, a fact that requires an interpretation. For the sake of the present work, and in order to introduce this method of calculation of the entropy for decaying systems, we have illustrated it to evaluate the canonical entropy for the harmonic oscillator. Although the path integration over coherent states yields a first approximation to the exact result, it shows its power to handle the problem of dealing with complex energy states. Further details of the formalism are presented in [8, 9]

2. The Friedrichs model in second quantification language.

The Friedrichs model [7], is an exactly solvable model for decaying phenomena in quantum mechanics, which shows all the features of resonant scattering. The point of departure is a unperturbed Hamiltonian H_0 with a simple absolutely continuous spectrum, and a positive eigenvalue, i.e., imbedded in the continuous spectrum. H_0 is written

$$H_0 = \omega_0 \, a^\dagger a + \int_0^\infty d\omega \, \omega \, b_\omega^\dagger b_\omega \,, \tag{1}$$

where $a^\dagger$ (a) is the creation (annihilation) operator of a bound state of energy ω_0, and $b_\omega^\dagger$ (b_ω) is the creation (annihilation) operator for the state of energy ω. The potential V is given by

$$V = \int_0^\infty d\omega \, f(\omega) \, (a^\dagger b_\omega + a b_\omega^\dagger) \,. \tag{2}$$

The function $f(\omega)$ in (2) is the form factor. The total Hamiltonian is $H = H_0 + \lambda V$, where λ is a real coupling constant. Creation and annihilation operators fulfill the following commutation relations:

$$[a, a^\dagger] = 1 \,; \qquad [b_\omega, b_{\omega'}^\dagger] = \delta(\omega - \omega') \tag{3}$$

and all other commutators vanish. For the states we use the notation

$$|1\rangle = a^\dagger |0\rangle \,; \qquad |\omega\rangle = b_\omega^\dagger |0\rangle \,. \tag{4}$$

where $|0\rangle$ is the vacuum. Note that

$$a|0\rangle = b_\omega |0\rangle = 0 \,. \tag{5}$$

As consequence of the interaction, the bound state of H_0 vanishes, and it is replaced by a resonance that, under some conditions on the form factor $f(\omega)$, depends analytically on the coupling constant λ. This resonance is a pole of the analytic continuation through the real axis of the function

$$g(z) = \langle 1| \frac{1}{z - H} |1\rangle \,. \tag{6}$$

The function $g(z)$ is often called the reduced resolvent of H at the complex number z, not in the spectrum of H. This function is analytic with no poles on (an open set of) the complex plane with a branch cut on the positive semi-axis, admitting an analytic continuation through this cut. It is interesting to use the explicit form of its inverse $\eta(z)$ ($g(z) = 1/\eta(z)$) given by [10, 11]

$$\eta(z) = \omega_0 - z - \int_0^\infty d\omega \, \frac{\lambda^2 \, f^2(\omega)}{\omega - z} \,. \tag{7}$$

The function representing the boundary values of $\eta(z)$ on the positive semiaxis from above to below $\eta(\omega + i0)$ and from below to above $\eta(\omega - i0)$ are here denoted as $\eta^+(\omega)$ and $\eta^-(\omega)$

respectively. They are complex conjugate of each other. The analytic continuation of $\eta(\omega + i0)$ has a zero located at $z_R = E_R - i\Gamma/2$, the resonance pole of $g(z)$. The real part E_R of z_R is identified with the resonance energy and the imaginary part $\Gamma/2$ with the half width. Its inverse $\tau = 2/\Gamma$ is the half life. In [10], the following creation and annihilation operators are defined:

$$A^\dagger_{IN} := \int_\gamma d\omega \, \frac{\lambda f(\omega)}{\omega - z_R} \, b^\dagger_\omega - a^\dagger \,, \tag{8}$$

$$A_{OUT} := \int_\gamma d\omega \, \frac{\lambda f(\omega)}{\omega - z_R} \, b_\omega - a \,, \tag{9}$$

$$B^\dagger_{\omega,IN} := b^\dagger_\omega + \frac{\lambda f(\omega)}{\tilde{\eta}^+(\omega)} \left\{ \int_0^\infty d\omega' \, \frac{\lambda f(\omega')}{\omega' - \omega - i0} \, b^\dagger_{\omega'} - a^\dagger \right\} \,, \tag{10}$$

$$B_{\omega,OUT} := b_\omega + \frac{\lambda f(\omega)}{\tilde{\eta}^+(\omega)} \left\{ \int_0^\infty d\omega' \, \frac{\lambda f(\omega')}{\omega' - \omega - i0} \, b_{\omega'} - a \right\} \,, \tag{11}$$

where,

$$\frac{1}{\tilde{\eta}^+(\omega)} := \frac{1}{\eta^+(\omega)} + 2\pi i A \delta(\omega - z_R) \,, \tag{12}$$

In these equations γ is the circular contour around the pole and A is the residue of $1/\eta^+(\omega)$ on the pole at z_R. Operators (8-11) satisfy the following commutation relations:

$$[A_{OUT}, A^\dagger_{IN}] = 1 \,; \qquad \frac{\eta^+(\omega)}{\eta^-(\omega)} \, [B_{\omega,OUT}, B^\dagger_{\omega',IN}] = \delta(\omega - \omega') \,. \tag{13}$$

All other commutators vanish.

The Hamiltonian H can be written in terms of these operators as:

$$H = z_R \, A^\dagger_{IN} \, A_{OUT} + \int_0^\infty d\omega \, \omega \, \frac{\eta^+(\omega)}{\eta^-(\omega)} \, B^\dagger_{\omega,IN} \, B_{\omega,OUT} \,. \tag{14}$$

the operators $A^\dagger_{IN}$ and A_{OUT} are, respectively, the creation and annihilation operators of the decaying) Gamow vector $|\psi^D\rangle$:

$$|\psi^D\rangle = A^\dagger_{IN}|0\rangle \,, \qquad A_{OUT}|\psi^D\rangle = |0\rangle \,. \tag{15}$$

From the point of view of the time asymmetric quantum theory [12, 13], both operators are defined for $t > 0$, that is the "decaying part" of a resonance process. In (15), we have seen that they play the role of creation and annihilation operators of the decaying Gamow vector, which is defined for $t > 0$ only [3].

3. The entropy for the harmonic oscillator from the path integrals approach.
The procedure to obtain the canonical entropy corresponding to a system with Hamiltonian H is well known. Consider the partition function Z for a system with time independent Hamiltonian H and let $\beta := 1/(kT)$, where k is the Boltzmann constant and T is the absolute temperature. Then, the canonical entropy is given by

$$S = k \left(1 - \beta \frac{\partial}{\partial \beta}\right) \log Z \,. \tag{16}$$

Now, let us assume that H represents the Hamiltonian of the harmonic oscillator in one dimension. Let us denote by $|n\rangle$ the eigenvectors of H, thus $H|n\rangle = \hbar\omega(n+1/2)|n\rangle$. As is well known, the partition function is now defined as

$$Z = \mathrm{tr}\{e^{-\beta H}\} = \sum_{n=0}^{\infty} \langle n|e^{-\beta H}|n\rangle. \tag{17}$$

Then, the value of the canonical entropy for the one dimensional harmonic oscillator can be directly obtained from (16). A straightforward calculation gives:

$$S = -k\log[2\sinh(\beta\hbar\omega/2)] + k\frac{\beta\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right). \tag{18}$$

The use of path integrals to give an approximate expression for the entropy was introduced by Feynman and Hibbs [14]. Here, the idea is firstly to express the canonical ensemble in terms of coherent states , and then use the path integrals to compute the density operator. As it is well known, coherent states are defined from a vacuum state $|0\rangle$ as

$$|\alpha\rangle := e^{\alpha a^\dagger - \alpha^* a}|0\rangle, \tag{19}$$

where $a^\dagger$ and a are the creation and annihilation operators for the harmonic oscillator, respectively, acting on the vacuum state $|0\rangle$, which is the ground state of the harmonic oscillator.

Take now the density operator $\rho = e^{-\beta H}$ and use the strategy of path integrals to estimate its matrix elements with respect to the coherent states. This is for any pair of complex numbers α_i and α_f:

$$\langle\alpha_i|\rho|\alpha_f\rangle = \lim_{N\mapsto\infty} \rho_N(\alpha_i, \alpha_f), \tag{20}$$

where

$$\rho_N(\alpha_i, \alpha_f) = \int \prod_{k=1}^{N}\left(\frac{d^2\alpha_k}{\pi}\right) \exp\left\{-\tau\left[\sum_{n=1}^{N} H_+(\alpha_{n-1}, \alpha_n)\right.\right.$$

$$\left.\left. + \sum_{n=1}^{N+1}\left\{\left(\frac{\alpha_n^* - \alpha_{n-1}^*}{2\tau}\right)\alpha_n - \alpha_{n-1}^*\left(\frac{\alpha_n - \alpha_{n-1}}{2\tau}\right)\right\}\right]\right\}, \tag{21}$$

with $\alpha_0 = \alpha_i$, $\alpha_{N+1} = \alpha_f$ and $\tau = \beta/N$. We write $\alpha_i = x_i + iy_i$ and $d\alpha_i = dx_i dy_i$, so that we have $2N$ integrals in the variables $x_1, \ldots, x_N, y_1, \ldots, y_N$. The integration limits are $-\infty$ and ∞ in all cases, since there must be one coherent state for any complex number. The term

$$H_+(\alpha, \alpha') = \frac{\langle\alpha|H|\alpha'\rangle}{\langle\alpha|\alpha'\rangle}, \qquad \langle\alpha|\alpha'\rangle = \exp\left\{-\frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2} + \alpha^*\alpha'\right\} \tag{22}$$

is called the normal expansion of the Hamiltonian H. The final result is

$$\rho(\alpha_i, \alpha_f) := \frac{1}{\langle\alpha_i|\alpha_f\rangle}\rho_N(\alpha_i, \alpha_f) = \exp\left\{-\frac{1}{2}\beta\hbar\omega\right\} \times \exp\{-\beta\hbar\omega\alpha_i^*\alpha_f\}, \tag{23}$$

which does not depend on N. Thus, (23) represents approximate matrix elements, in terms of the coherent states, of the canonical partition function of the harmonic oscillator.

Let us use now (16) in order to obtain an approximate expression for the entropy. First of all, let us calculate an (approximate) partition function by taking the trace of ρ as obtained in (23) with the aid of coherent states. It gives ($\alpha = x + iy$):

$$Z = \int \frac{d^2\alpha}{\pi} \, \rho(\alpha, \alpha) = \frac{1}{\pi} \, e^{-(\beta\hbar\omega)/2} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \, e^{-\beta\hbar\omega(x^2+y^2)} = e^{-(\beta\hbar\omega)/2} \, \frac{1}{\beta\hbar\omega} \, .$$

$$\log Z = -\frac{1}{2} \, \beta\hbar\omega - \log(\beta\hbar\omega) \, , \qquad (24)$$

which leads to

$$S \approx k(1 - \log(\beta\hbar\omega)) \, , \qquad (25)$$

which certainly gives an approximation for (18). To see it, let us note that $\coth x = 1/x + \dots$ and $\sinh x = x + \dots$. Applying these approximations in (18) leads to (25).

The moral of the present Section is that the use of coherent states to calculate the matrix representing the density operator is a technique amenable for extensions to systems where the standard notion of probabilities cannot be applied.

4. A notion of entropy for quantum decaying states

Now we face the problem of giving an approximate expression for the canonical entropy of a quantum system with resonances. This partition function will be find again with the use of the path integral method and coherent states, as we did for the harmonic oscillator in the previous section. The most natural basis to compute the trace is by taking the object $\{|\psi^D\rangle, |\omega^+\rangle\}$, where $|\psi^D\rangle$ is the decaying Gamow vector and $|\omega^+\rangle$ is a complete set of generalized eigenvectors of the total Hamiltonian H. The expression of these vectors in the basis $\{|1\rangle, |\omega\rangle\}$ of eigenvectors of the unperturbed Hamiltonian H_0 ($H_0|1\rangle = \omega_0|1\rangle$, $H_0|\omega\rangle = \omega|\omega\rangle$, $\omega_0 > 0$, $\omega \in [0, \infty)$) is

$$|\psi^D\rangle = |1\rangle + \int_0^\infty \frac{\lambda f(\omega)}{z_R - \omega + i0} \, |\omega\rangle \, d\omega \qquad (26)$$

$$|\omega^+\rangle = |\omega\rangle + \frac{\lambda f(\omega)}{\eta^+(\omega)} \left(|1\rangle + \int_0^\infty d\omega' \frac{\lambda f(\omega')}{\omega - \omega' + i0} \, |\omega'\rangle \right) \, , \qquad (27)$$

where λ and $f(\omega)$ are the coupling constant and the form factor, respectively. From (26) and (27), one sees that expressions like $\langle\psi^D|\psi^D\rangle$ or $\langle\omega^+|\omega^+\rangle$ are ill defined. In fact, since discrete and continuous subspaces of a self adjoint operator are mutually orthogonal, we have that

$$\langle 1|1\rangle = 1 \, ; \quad \langle 1|\omega\rangle = \langle\omega|1\rangle = 0 \, ; \quad \langle\omega|\omega'\rangle = \delta(\omega - \omega') \, . \qquad (28)$$

Take now the expression for $|\psi^D\rangle$ in (26) and use the products in (28) to obtain

$$\langle\psi^D|\psi^D\rangle = 1 + \int_0^\infty d\omega \, \frac{\lambda f(\omega)}{(z_R^* - \omega - i0)(z_R - \omega + i0)} \, . \qquad (29)$$

The integral represents the action of a distribution on the function $f(\omega)$. This distribution is the product of $(z_R^* - \omega - i0)^{-1}$ and $(z_R - \omega + i0)^{-1}$, which is not well defined. A similar problem would arise if we consider $\langle\omega'^+|\omega^+\rangle$.

Since in the Friedrichs model, $H|\psi^D\rangle = z_R|\psi^D\rangle$ and $H|\omega^+\rangle = \omega|\omega^+\rangle$, we conclude that a trace of the form

$$\text{tr} \, e^{-\beta H} = \langle\psi^D|e^{-\beta H}|\psi^D\rangle + \int_0^\infty \langle\omega^+|e^{-\beta H}|\omega^+\rangle \, d\omega \qquad (30)$$

is not well defined. Then, we shall follow a similar approximation that the one discussed in Section III, not only to obtain an approximate value of the entropy for a system with a decaying state, but also to extent on the concept itself. As in the case of the harmonic oscillator, we define the coherent state $|\alpha\rangle$ and its bra $\langle\alpha|$, for all complex number α, as:

$$|\alpha\rangle := \exp\{\alpha\, A_{IN}^\dagger - \alpha^*\, A_{OUT}\}\, |0\rangle\,,$$

$$\langle\alpha| := \langle 0|\exp\{\alpha^*\, A_{OUT} - \alpha\, A_{IN}^\dagger\}\,, \tag{31}$$

where $|0\rangle$ is the vacuum state. Making use of the commutation relations (31) it becomes evident that these coherent states satisfy the same properties than the coherent states (19). In particular,

$$A_{OUT}|\alpha\rangle = \alpha|\alpha\rangle\,;\qquad \langle\alpha|A_{IN}^\dagger = \alpha^*\langle\alpha|\,;$$

$$\int_C \frac{d^2\alpha}{\pi}\, |\alpha\rangle\langle\alpha| = 1\,;\qquad d^2\alpha = (d\,\mathrm{Real}\,\alpha)(d\,\mathrm{Im}\,\alpha)\,, \tag{32}$$

where C denotes the field of complex numbers. The normal expansion (23) is now

$$H_+(\alpha,\alpha') = z_R\,\alpha^*\alpha'\,. \tag{33}$$

Then, instead of (23), we have the following equation

$$\rho(\alpha_i,\alpha_f) = \exp\{-\beta\, z_R\, \alpha_i^*\alpha_f\}\,, \tag{34}$$

which gives

$$Z = \frac{1}{\pi}\int_{-\infty}^{\infty} dx\, e^{-\beta\, z_R\, x^2}\int_{-\infty}^{\infty} dy\, e^{-\beta\, z_R\, y^2} = \frac{1}{\beta\, z_R}\,. \tag{35}$$

where $z_R = E_R - i\frac{\Gamma}{2}$. Finally, using (16), we arrive at the result:

$$S = k(1 - \log(\beta z_R)) = k\left[1 - \ln(\beta\sqrt{E_R^2 + \frac{\Gamma^2}{4}}) - i\arctan\left(\frac{\Gamma}{2E_R}\right)\right]\,, \tag{36}$$

In (36) we have taken the principal branch of $\log z$. The result (36) reminds the case of the harmonic oscillator, (25), except for the presence of an imaginary term. If $\Gamma \to 0$ both results do indeed coincide, after replacing $\hbar\omega$ by E_R. The presence of a complex entropy, for the case of Gamow vectors, requires of some interpretation on the meaning of its imaginary part. The situation is quite similar to the existence of complex energy for decaying states, where the imaginary part is interpreted as the inverse of the half life. Note that the resonance in the Friedrichs model is caused by the interaction of the system with the background, which plays the role of the thermodynamical bath. Then, we suggest that the real part of the entropy (36) is the entropy of the system and that the imaginary part of it is the entropy transferred from the system to the background. Should the thermodynamical entropy be identified with the modulus of (36), one concludes that the total entropy for a decaying state is bigger than the entropy of a stable system.

5. Conclusions.

In this work we have pointed out to some of the difficulties concerning the application of concepts of Statistical Mechanics to complex-energy vectors. We have presented a suitable alternative to the probabilistic description, by implementing a representation of the decaying vectors, obtained in the framework of the Friedrisch model, written them in terms of coherent states and by performing a path integration over these states to get the density matrix operator. The results are quite encouraging, because at the level of approximation used to calculate the density operator, we do not have to introduce some ad-hoc notions like complex temperatures or treat independently real and imaginary entropies. We think that this is a promising first step towards a novel formulation of the statistical mechanics for decaying systems. We hope to be able to complete this program in the near future.

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