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AN APPROXIMATION TO THE ENTROPY FOR QUANTUM DECAYING STATES

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The concept of entropy was initially defined for systems with thermodynamical equilibrium. We try to extend this notion for quantum non-relativistic decaying states. We use a technique based on path integration on coherent states in order to obtain an approximation to the entropy of a decaying state.

Keywords: Quantum unstable states; entropy; path integrals.

1. Introduction

The quantum mechanical treatment of decaying states started with the pioneering work of Gamow [1], which immediately attracted scientists on the various aspects of resonances. Since then, the quantum mechanical principles underlying the physics and mathematics of resonances have been consistently formulated in various ways [2–8]. Considerably less effort was devoted to the understanding of the statistical (or thermodynamical) side of the problem. A decaying system should also obey thermodynamical laws, in a broad sense not limited by the notion of probabilities, exactly as it happens in the just referred quantum mechanical frame for resonances [6, 7]. From the physical point of view the problem has strong links with the measurement of decay properties of resonances and with the role of interactions between resonances and the environment.

The purpose of this communication is to give an approximate value of the entropy for quantum decaying states.

In this context, two approaches are possible. One is the introduction of the entropy operator, as proposed by Misra, Prigogine and Courbage [9]. This approach is time-dependent. The second approach begins with the assumption that if the mean life of a resonance is large (or equivalently if the width is small), this resonance could be considered, in a first approximation, as a system in thermodynamical equilibrium. This approach has been proposed by Kobayashi and Shimbori [10, 11]. This is the point of view that we follow in this discussion.

2. The Friedrichs Model

We shall make use of a theoretical laboratory valid to study qualitative properties of resonances: the Friedrichs model [12]. The basic Friedrichs model is an exactly solvable model for resonances which contains all features of resonant scattering. In particular, the existence of a Hamiltonian pair ($\{H_0, H\}$ where H_0 is a free Hamiltonian and $H = H_0 + V$, where the potential V is the interaction responsible for the existence of resonances), the existence of a scattering matrix, the presence of resonances as poles of an analytic continuation of a reduced resolvent or, equivalently, of the scattering matrix or S-matrix [13].

In the Friedrichs model, the free Hamiltonian H_0 has a stationary state plus an external field without interaction with the stationary state:

$$H_0 = \omega_0 |1\rangle\langle 1| + \int_0^\infty \omega |\omega\rangle\langle\omega| d\omega, \tag{1}$$

where $H_0|1\rangle = \omega_0|1\rangle$ and $H_0|\omega\rangle = \omega|\omega\rangle$. Note that $\omega_0 > 0$, so that the bound state of H_0 is immersed in its continuous spectrum. The total Hamiltonian H is

$$H = H_0 + \lambda V = H_0 + \lambda \int_0^\infty d\omega f(\omega)[|\omega\rangle\langle 1| + |1\rangle\langle\omega|]. \tag{2}$$

Here λ is a real coupling constant. The function $f(\omega)$ that appears under the integral sign in the expression which defines the potential V in (2) is a square integrable function that can be taken as real. We should assume that its square $f^2(\omega)$ admits analytic continuation in an open set including the positive semi-axis $\mathbb{R}^+ \equiv [0, \infty)$. The potential V produces an interaction between the stationary state of H_0 and the external field, so that the bound state $|1\rangle$ is transformed into a resonance. In order to calculate the resonance, let us consider the reduced resolvent:

$$\frac{1}{\eta(z)} := \langle 1|\frac{1}{z-H}|1\rangle. \tag{3}$$

Under the above conditions, the function $\eta(z)$ is analytic on the complex plane, except for a branch cut on the positive semi-axis. Furthermore, it admits analytic continuations from above to below, with a zero at $z_R = E_R - i\Gamma/2$, and from below to above, with a zero at $z_R^* = E_R + i\Gamma/2$. These are the resonance poles of the Hamiltonian pair $\{H_0, H\}$.

The Gamow vectors are the eigenvectors of H with eigenvalues z_R and z_R^*. The eigenvector for z_R, $|\psi^D\rangle (H|\psi^D\rangle = z_R|\psi^D\rangle)$ is called the decaying Gamow vector as it decays exponentially as $t \mapsto \infty$ [6, 7]. The eigenvector of H for z_R^*, $|\psi^G\rangle$, is called the growing Gamow vector and it decays exponentially to the past, i.e. $t \mapsto -\infty$.

We know that a decaying state, i.e. the quantum state corresponding to a quantum resonance, decays exponentially (with good accuracy) for a wide range of times, which do not include very short times or very long times [14]. As the decaying Gamow vector, $|\psi^D\rangle$, decays exponentially for $t > 0$, it is a good approximation for the quantum state within the range of exponential decay. Then, it is somehow reasonable to adopt $|\psi^D\rangle$ as the vector state for a quantum resonance. This idea was first proposed by Nakanishi [2].

The Friedrichs model can also be formulated in terms of second quantization language and this formulation is the appropriate for our discussion. In these terms the total Hamiltonian can be written as [17]:

$$H = \omega_0 a^\dagger a + \int_0^\infty d\omega \omega b_\omega^\dagger b_\omega + \lambda \int_0^\infty d\omega f(\omega)(a^\dagger b_\omega + a b_\omega^\dagger), \tag{4}$$

where a and $a^\dagger$ are the annihilation and creation operators for the stationary state and b_ω and $b_\omega^\dagger$ the annihilation and creation operators for $|\omega\rangle$, from a vacuum state $|0\rangle$. Note that the potential V is given by the last integral in (4).

Let us define:

$$A_{\mathrm{IN}}^\dagger := \int_\gamma d\omega \frac{\lambda f(\omega)}{\omega - z_R} b_\omega^\dagger - a^\dagger, \tag{5}$$

$$A_{\mathrm{OUT}} := \int_\gamma d\omega \frac{\lambda f(\omega)}{\omega - z_R} b_\omega - a, \tag{6}$$

$$B_{\omega,\mathrm{IN}}^\dagger := b_\omega^\dagger + \frac{\lambda f(\omega)}{\tilde{\eta}^+(\omega)} \left\{ \int_0^\infty d\omega' \frac{\lambda f(\omega')}{\omega' - \omega - i0} b_{\omega'}^\dagger - a^\dagger \right\}, \tag{7}$$

$$B_{\omega,\mathrm{OUT}} := b_\omega + \frac{\lambda f(\omega)}{\tilde{\eta}^+(\omega)} \left\{ \int_0^\infty d\omega' \frac{\lambda f(\omega')}{\omega' - \omega - i0} b_{\omega'} - a \right\}. \tag{8}$$

These operators satisfy the following commutation relations:

$$[A_{\mathrm{OUT}}, A_{\mathrm{IN}}^\dagger] = 1; \quad \frac{\eta^+(\omega)}{\eta^-(\omega)} [B_{\omega,\mathrm{OUT}}, B_{\omega',\mathrm{IN}}^\dagger] = \delta(\omega - \omega'). \tag{9}$$

All other commutators vanish. The total Hamiltonian can be diagonalized as

$$H = z_R A_{\mathrm{IN}}^\dagger A_{\mathrm{OUT}} + \int_0^\infty d\omega \omega \frac{\eta^+(\omega)}{\eta^-(\omega)} B_{\omega,\mathrm{IN}}^\dagger B_{\omega,\mathrm{OUT}} \tag{10}$$

and

$$|\psi^D\rangle = A_{\mathrm{IN}}^\dagger |0\rangle, \quad A_{\mathrm{OUT}} |\psi^D\rangle = |0\rangle. \tag{11}$$

Our objective is to give a reasonable expression for the entropy of decaying states using the Friedrichs model.

3. An Approximation to the Canonical Entropy for the Harmonic Oscillator with Coherent States

At this point, the following comment is in order: In the formalism proposed by Prigogine and his team, once we have determined the entropy operator M [9], the entropy of a quantum state ρ is given by $S = \operatorname{tr} \rho M \rho$. For decaying states, they propose the following entropy operator [15]:

$$M := |\psi^G\rangle\langle\psi^G|. \tag{12}$$

One may show that if $\rho(0) = |\psi^D\rangle\langle\psi^D|$ represents the density operator for the Gamow state $|\psi^D\rangle$, its entropy is given by

$$S(t) = e^{-2\Gamma t} \operatorname{tr} \rho(0), \tag{13}$$

for a certain definition of the trace [16]. This result is also given in [15].

Let us consider the canonical entropy for the harmonic oscillator. In terms of the canonical partition function, it can be calculated by means of the following formula:

$$S = k\left(1 - \beta\frac{\partial}{\partial\beta}\right)\log Z, \tag{14}$$

where

$$Z = \operatorname{tr}\{e^{-\beta H}\} = \sum_{n=0}^{\infty}\langle n|e^{-\beta H}|n\rangle, \tag{15}$$

where $|n\rangle$ represent the bound states of the oscillator. The final expression is

$$S = -k\log[2\sinh(\beta\hbar\omega/2)] + k\frac{\beta\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right). \tag{16}$$

The objective is to compute an approximation to this formula using path integration [18] over the coherent states of the oscillator [19]. As is well known, coherent states are defined from a vacuum state $|0\rangle$ as

$$|\alpha\rangle := e^{\alpha a^\dagger - \alpha^* a}|0\rangle, \tag{17}$$

where $a^\dagger$ and a are the creation and annihilation operators for the harmonic oscillator respectively. The vacuum state $|0\rangle$ is the ground state of the harmonic oscillator in the present case.

Take now the canonical state $\rho = e^{-\beta H}$ 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:

$$\langle\alpha_i|\rho|\alpha_f\rangle = \lim_{N\mapsto\infty}\rho_N(\alpha_i,\alpha_f), \tag{18}$$

where,

$$\rho_N(\alpha_i,\alpha_f) = \int \prod_{k=1}^{N} \left(\frac{d^2\alpha_k}{\pi}\right) \exp\left\{-\tau\left[\sum_{n=1}^{N} H_+(\alpha_{n-1},\alpha_n)\right.\right.$$
$$\left.\left. + \sum_{n=1}^{N+1}\left\{\left(\frac{\alpha_n^* - \alpha_{n-1}^*}{2\tau}\right)\alpha_n - \alpha_{n-1}^*\left(\frac{\alpha_n - \alpha_{n-1}}{2\tau}\right)\right\}\right]\right\}, \qquad (19)$$

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

$$H_+(\alpha,\alpha') = \frac{\langle\alpha|H|\alpha'\rangle}{\langle\alpha|\alpha'\rangle}, \quad \langle\alpha|\alpha'\rangle = \exp\left\{-\frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2} + \alpha^*\alpha'\right\} \qquad (20)$$

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

$$\rho(\alpha_i,\alpha_f) := \frac{1}{\langle\alpha_i\,|\,\alpha_f\rangle}\rho_N(\alpha_i,\alpha_f) = \exp\left\{-\frac{1}{2}\beta\hbar\omega\right\} \times \exp\{-\beta\hbar\omega\alpha_i^*\alpha_f\}, \qquad (21)$$

which does not depend on N.

In the way to obtain (21), we have arrived to integrals of the form [20],

$$\frac{1}{\pi}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dy_1 \exp\{-x_1^2 - y_1^2 + \sigma(\alpha_i^*(x_1+iy_1) + \sigma(x_1 - iy_1)\alpha_2\}$$
$$= \frac{1}{\pi}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dy_1 \exp\left\{-\left[x_1 - \frac{\sigma}{2}(\alpha_i + \alpha_2)\right]^2 + \frac{\sigma^2}{4}(\alpha_i^* + \alpha_2)^2\right.$$
$$\left. - \left[y_1 - i\frac{\sigma}{2}(\alpha_i^* - \alpha_2)\right]^2 - \frac{\sigma^2}{4}(\alpha_i^* - \alpha_2)^2\right\}. \qquad (22)$$

These integrals give rise to undesirable infinities which should be removed in order to obtain a reasonable value for the entropy. To this end, we discard the terms $\frac{\sigma}{2}(\alpha_i + \alpha_2)$ and $i\frac{\sigma}{2}(\alpha_i^* - \alpha_2)$ in the above exponents. This approximation is standard in path integrations and it amounts to neglecting infinite vacuum contributions [18].

Once we have followed this procedure, the partition function gives Z in (14) gives:

$$Z = e^{-(\beta\hbar\omega)/2}\frac{1}{\beta\hbar\omega}, \qquad (23)$$

which finally with (14) gives:

$$S \approx k[1 - \log(\beta\hbar\omega)]. \qquad (24)$$

This is an approximation to (16) taken into account that $\coth x = 1/x + \cdots$ and $\sinh x = x + \cdots$.

The moral of this section was that the use of coherent states to approximate the entropy of a system is a technique amenable for future extensions to systems in which the method of calculation of the entropy is not clear. This is the case of the entropy of decaying states, which will be discussed in Sec. 4.

4. An Approximation for the Value of the Entropy for Decaying States

In the sequel, we shall assume that the mean life of a decaying state is sufficiently large so as to consider the state in thermodynamical equilibrium with temperature T. In this case, we shall use the technique employed for the determination of an approximation of the entropy in the harmonic oscillator in order to obtain an approximate entropy for a decaying state.

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:

$$\begin{aligned} |\alpha\rangle &:= \exp\{\alpha A_{\mathrm{IN}}^\dagger - \alpha^* A_{\mathrm{OUT}}\}|0\rangle, \\ \langle\alpha| &:= \langle 0|\exp\{\alpha^* A_{\mathrm{OUT}} - \alpha A_{\mathrm{IN}}^\dagger\}, \end{aligned} \tag{25}$$

where $|0\rangle$ is the vacuum state. Making use of the commutation relations (9), we realize that these coherent states satisfy the same properties than the coherent states for the harmonic oscillator. In particular,

$$\begin{aligned} A_{\mathrm{OUT}}|\alpha\rangle = \alpha|\alpha\rangle; &\quad \langle\alpha|A_{\mathrm{IN}}^\dagger = \alpha^*\langle\alpha|; \\ \int_{\mathbb{C}} \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = 1; &\qquad d^2\alpha = (d\ \mathrm{Real}\,\alpha)(d\ \mathrm{Im}\,\alpha), \end{aligned} \tag{26}$$

where $\mathbb{C}$ denotes the field of complex numbers. The normal expansion (20) is now

$$H_+(\alpha, \alpha') = z_R \alpha^* \alpha'. \tag{27}$$

Then, one reproduces the calculation performed for the case of the harmonic oscillator. As a result, instead of (21), we have the following equation

$$\rho(\alpha_i, \alpha_f) = \exp\{-\beta z_R \alpha_i^* \alpha_f\}, \tag{28}$$

which gives

$$Z = \frac{1}{\beta z_R}. \tag{29}$$

Finally, using (14), we arrive to the desired result:

$$S = k(1 - \log(\beta z_R)) = k\left[1 - \ln\left(\beta\sqrt{E_R^2 + \frac{\Gamma^2}{4}}\right) - i\arctan\left(\frac{\Gamma}{2E_R}\right)\right], \tag{30}$$

where $z_R = E_R + i\Gamma/2$ and ln means natural logarithm. We take the principal branch of $\log z$.

Now, take the limit as $\Gamma \mapsto 0$ and compare with the formula obtained for the harmonic oscillator. Note that the result is the same provided that we replace E_R by $\hbar\omega$. This shows that the result that we have obtained by this means for the unstable state is reliable.

5. Concluding Remarks

After the result obtained for the harmonic oscillator, we admit that (30) is an approximation to the value of the entropy for decaying states. We see that this result gives a complex entropy. This requires of some interpretation on the meaning of the imaginary part. The situation is quite similar to the existence of complex energy for decaying states, where the imaginary part is interpreted as the half-width.

Note that the resonance in the Friedrichs model is caused by the interaction of the system with the background, which plays the role of a thermal bath. Then, we suggest that the real part of the entropy is the entropy of the system and the imaginary part the entropy transferred from the system to the background. Should the total entropy be identified with the modulus of (30), one concludes that the total entropy is bigger than the entropy of the system itself. Thus, a decaying system has bigger entropy than a stable one.

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References

[1] G. Gamow, On the quantum theory of atomic nucleus, *Z. Phys.* **51** (1928) 204–212.
[2] N. Nakanishi, A note on the physical state of unstable particles, *Progr. Theor. Phys.* **21** (1959) 762–763.
[3] A. Bohm, Resonance poles and Gamow vectors in the rigged Hilbert space formulation of quantum mechanics, *J. Math. Phys.* **22** (1981) 2813–2823.
[4] H. M. Nussenzveig, *Causality and Dispersions Relations* (Academic Press, New York, 1972).
[5] V. I. Kukulin, V. M. Krasnopolski and J. Horacek, *Theory of Resonances. Principles and Applications* (Academia, Praha, 1989).
[6] A. Bohm and M. Gadella, *Dirac Kets*, *Gamow Vectors and Gelfand Triplets*, Lecture Notes in Physics, Vol. 340 (Springer, Berlin, 1989).
[7] O. Civitarese and M. Gadella, Physical and mathematical aspects of Gamow vectors, *Phys. Rep.* **396** (2004) 41–113.
[8] R. de la Madrid, A. Bohm and M. Gadella, Rigged Hilbert space treatment of continuous spectrum, *Fortschr. Phys.* **50** (2002) 185–216.
[9] B. Misra, I. Prigogine and M. Courbage, Liapunov Variable-entropy and measurement in quantum mechanics, *Proc. Natl. Acad. Sci. USA* **76** (1979) 4768–4772.
[10] T. Kobayashi and T. Shimbori, Statistical mechanics for unstable states in Gelfand triplets and investigations of parabolic potential barriers, *Phys. Rev. E* **63** (2001) 056101.
[11] T. Kobayashi, New aspects in physics on Gelfand triplets, *Int. J. Theor. Phys.* **42** (2003) 2265–2283.
[12] K. O. Friedrichs, On the perturbation of continuous spectra, *Commun. Appl. Math.* **1** (1948) 361–406.
[13] P. Exner, *Open Quantum Systems and Feynmann Integrals* (Reidel, Dordrecht, 1985).

[14] L. Fonda, G. C. Ghirardi and A. Rimini, Decay theory of unstable quantum systems, *Rep. Progr. Phys.* **41** (1978) 587–631.
[15] E. Karpov, G. Ordóñez, T. Petrosky and I. Prigogine, Microscopic entropy, *Int. J. Quantum Chem.* **98** (2004) 69–77.
[16] O. Civitarese and M. Gadella, On the concept of entropy for quantum decaying systems, to be submitted.
[17] I. E. Antoniou, M. Gadella, E. Karpov, I. Prigogine and G. Pronko, Gamov algebras, *Chaos, Solitons Fractals* **12** (2001) 2757–2775.
[18] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[19] D. ter Haar, *Lectures on Selected Topics in Statistical Mechanics* (Pergamon Press, Oxford, 1977).
[20] O. Civitarese and M. Gadella, On the entropy for quantum unstable states, submitted.