RELATION TIME-THERMODYNAMICS. A PATH INTEGRAL APPROACH.

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Abstract

Starting from an algebraic approach of quantum physics it has been shown via the Tomita-Takesaki theorem and the KMS condition that the canonical density matrix contains the dynamics of the system provided we use a rescaling of time. In this paper we show that the path integral form of the partition function reveals a dynamics which is complementary of the one given by the Tomita-Takesaki theorem. To do that we work in the spirit of a Feynman’conjecture. We define the entropy as a measure of the disorder in space time. By using an equilibrium condition we introduce a natural time scale that it is precisely the one appearing in the Tomita-Takesaki theorem. For this time scale depending on the temperature but not on the system properties our definition of entropy is identical to the thermodynamic one. The underlying dynamics associated with the partition function allows us to derive a \textbf{H-theorem}. It is obtained in the thermodynamic limit and provided we are in a regime in which the thermal fluctuations are larger than the quantum ones.

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I. INTRODUCTION

When a new field of investigation is developing we frequently observe that different equivalent approaches are proposed. These approaches focusing on different starting points may reveal different and non expected aspects of the theory. Moreover, after sometimes new extensions or new generalizations of the initial description may be proposed. This was the case for classical mechanics (1) where after the Newton laws the Lagrangian and Hamiltonian formalisms have been introduced while, more recently, a symplectic approach has been developed. The last one offers a scheme in which it is possible to recast the general relativity (2). A similar evolution is true in the case of quantum mechanics. Almost at the same time Heisenberg elaborated his matrix mechanics and Schroedinger proposed his famous equation, while later Feynman introduced the path integral formalism. If all these approaches are equivalent at the level of the Schroedinger equation, the path integral formalism has been extended far beyond in order, for example, to describe the partition function near a black hole (3).

The matrix mechanics has giving rise to the so called algebraic approach of quantum mechanics (4) in which the main point is the existence of a C* algebra of non-commutative operators. Then due to the GNS construction (4) it is possible to give a concrete definition of these operators by a representation in a Hilbert space constructed from a given state that is called cyclic and noted Ω. An important result of this approach is the Tomita-Takesaki theorem (5)(for a recent review on this theorem see (6)) that establishes the existence of a one parameter group of automorphisms of the algebra

\[ \alpha_t A = \Delta^{-it} A \Delta^{it} \]  

that is true for any operator A of the algebra and leaves the algebra globally invariant. In \( \Delta \) is a self adjoint positive operator and \( \alpha_t \) is the so called modular group on the algebra. Another consequence of the Tomita theorem is the existence of a relation

\[ (\Omega, B(\alpha_{t_1+t_2} A) \Omega) = (\Omega, (\alpha_{t_1} A) B \Omega) \]  

in which (,) means the inner product. It has been demonstrated that such relation is independent of the particular state but it is an intrinsic property of the von Neumann algebra (7). At this level it is impossible to claim that the parameter t in (2) is a time.
However we may compare (2) with the KMS condition (3) established by Kubo (4) and Martin and Schwinger (5). Haag and his coworkers (6) postulated that the KMS condition is the correct definition of thermal equilibrium for infinite dimensional quantum systems. The KMS condition shows that the correlation function between two variables A and B noted $< (\gamma_t A) B >$ is analytic in the strip $0 < \text{Im}(t) < \beta \hbar$ where $\beta$ is the usual reverse of temperature ($\beta = \frac{1}{k_B T}$) and we have

$$< (\gamma_t A) B >= < B (\gamma_{t+i\beta \hbar} A) >$$

(3)

where $\gamma_t$ introduces the time translation group defined according to

$$\gamma_t A = \exp \frac{i t H}{\hbar} A \exp - \frac{i t H}{\hbar}$$

(4)

in which $H$ is the hamiltonian operator. Finally we find that the result of the Tomita-Takesaki theorem is equivalent to the time evolution of the bounded operators generated by the Hamilton provided the time is measured in units $\beta \hbar$ as already noted in (3). These works show that the canonical density matrix

$$\rho = exp - \frac{\beta H}{N}$$

(5)

where $N$ is a normalization constant contains the dynamics of the system. Connes and Rovelli (12) suggested an extension of the previous results to general covariant theories via the thermal time hypothesis in which the physical time is given by the modular group (11). Hereafter our main task will be to explain the origin of the rescaling $t \to \frac{t}{\beta \hbar}$.

This paper is organized as follows. In section 2 we develop a path integral approach in the spirit of a Feynman’conjecture. We show that the usual partition function involved a given dynamics restricted to time interval $t \leq \beta \hbar$. Then, from simple physical arguments, we introduce an entropy characterizing the disorder in space time. In section 3 we show that a thermal equilibrium condition leads to introduce a time interval $\tau = \beta \hbar$ that is independent of the system but determined by the thermodynamic state via the temperature. This time interval appears as a natural time scale in equilibrium thermodynamics, indeed it is precisely the time scale related to the Tomita-Takesaki theorem. Moreover our definition of equilibrium is very similar to the one introduced by Rovelli (2). Traditionally time and thermodynamics are related via the second law of thermodynamics, which asserts the existence of a state function that is a non-decreasing function of time for any closed system.
In statistical mechanics this leads to the problem of the arrow of time and the so-called **H-theorem** (for a review see for instance (14)). In section 4 we show that the dynamics associated with the partition function allows the derivation of a **H-theorem**, in order to do that we define a **H** function showing the interplay between open and close paths. In section 5, we give some conclusions.

II. STATISTICAL MECHANICS AND PATH INTEGRAL FORMALISM

Starting from (5) Feynman (15) derived a path integral formalism for the partition function $Z$. In order to do that it was needed i) to start from the wave function, the existence of stationary states and eigenvalues, ii) to develop some arguments justifying the use of the canonical form of the density matrix and iii) to introduce some mathematical tricks. Then the partition function can be written as

$$Z = \int dx \int Dx(t) \exp \frac{1}{\hbar} A_0[x(t); 0, \tau]$$

in which $Dx(t)$ is the measure for the functional integral and $A_0[x(t); 0, \tau]$ represents the quantity

$$A[x(t); 0, \tau] = \frac{\tau}{2m} \frac{[dx(t)]^2}{dt} + V(x(t))$$

calculated on loops i.e. on trajectories on which we have $x(t = 0) = x(t = \tau) = x$; for each loop the dummy variable, $t$, varies from 0 to $\tau$, $t$ and $\tau$ have the dimension of a time. In (7) it is assumed that the external potential $V(x(t))$ does not depend explicitly on $t$. The integral (6) is calculated on the all values of $x$ taken in the volume of the system under consideration. The expression of $Z$ given in (6) is just a mathematical transformation of the standard expression of $Z = Tr(\exp[-\beta H])$ provided we use $\tau = \beta \hbar$. Of course in such a formal derivation we cannot claim that $t$ is a time having a physical meaning i.e. that $A_0[x(u); 0, \tau]$ is an action associated to loops in ordinary space time.

After deriving (6) Feynman wrote in (15) a paragraph entitled "Remarks on methods of derivation"on which he suggested that it should be possible to derive the expression of $Z$ directly from the path integral description for the time-dependent motion how he did for the quantum mechanical amplitude in quantum mechanics. Why to search such a short cut that should avoid the wave function and the energy levels ? The Feynman’s answer is the following "in doing that a deeper understanding of physical processes might result or
possibly more powerful methods of statistical mechanics might be evolved”. Hereafter, to be short we will mention these comments as the Feynman’s conjecture (FC). From the FC it is suggested that \( Z = Tr(\exp[-\beta H]) \) contains the dynamics of the system provided we use its path integral version. This is very similar to what has been exposed above where it has been shown that \( \exp[-\beta H] \) may reveal the dynamics of the system if we use an algebraic approach of quantum mechanics.

Hereafter, we will try to explicit the dynamics involved in the path integral version of \( Z \) and to show that \( \tau = \beta \hbar \) is the natural unit of time in equilibrium thermodynamics. In order to do that the first step is to check that all the results obtained via the path integral formalism are meaningful if we consider that \( t \) is a physical time in the action \( A[x(t); 0, \tau] \). In \( (16) \) it has been shown that loops are fractal trajectories with the same Hausdorff dimension as the one calculated from Schroedinger equation. We may also shown, for a free particle, that the trajectories are mainly restricted to a sphere for which the radius corresponds to the thermal de Broglie wavelength, an expected result. Moreover, a first meaning of the time \( \tau \) can be given by an analysis in terms of time/energy uncertainty relation, \( \tau \) appears as the time interval we need to wait in order to reach a regime in which the quantum fluctuations become smaller than those of thermal origin \( (16), (17) \). However these results are not sufficient to give a strong basis to the FC. In order to go beyond we must show that i) the dynamics implicitly involved in \( (6) \) is meaningful and ii) the form of the functional integral can be written down immediately from simple physical arguments.

A. Dynamics implicitly involved in \( Z \)

From \( Z \) we may define the quantity

\[
q(t_0, x_0; t, x) = \int D(x(t)) \exp \left\{ -\frac{1}{\hbar} A[x(t); t_0, t] \right\}
\]

(8)

\( q(t_0, x_0; t, x) \) appears as a weighted sum of all the paths \( x(t) \) connecting the points \( x_0 \) to \( x \) during an interval \( (t - t_0) \). From \( q(t_0, x_0; t, x) \) and a function \( \phi_0(x) \) defined for \( (t = t_0) \) we may form a real-valued function \( \phi(t, x) \) according to

\[
\phi(t, x) = \int \phi_0(y)q(t_0, y; t, x)dy
\]

(9)
By using the Feynman-Kac formula, we can see that \( \phi(t, x) \) is the solution of the equation

\[
- \partial \phi(t, x) / \partial t + \frac{\hbar}{2m} \Delta_x \phi(t, x) - \frac{1}{\hbar} u(t, x) \phi(t, x) = 0
\] (10)

that verifies the initial condition \( \phi(0, x) = \phi_0(y) \) i.e. \( q(t_0, x_0; t, x) \) is the fundamental solution of (10) in which \( \Delta_x \) means the laplacian operator taken at the point \( x \). Note that (10) is not a Chapman-Kolmogorov type equation and consequently \( q(t_0, x_0; t, x) \) is not a density of probability, this quantity can not be normalized in general (18). However \( q(t_0, x_0; t, x) \) verifies the law of composition (18)

\[
q(t_1, x_1; t_2, x_2) = \int dx_3 q(t_1, x_1; t_3, x_3) q(t_3, x_3; t_2, x_2)
\] (11)

provided \( t_1 < t_3 < t_2 \) and therefore it can be used to describe the transitions in space-time. The evolution in space-time is then represented by a semi-group, \( \phi(t, x) \) is defined for \( t \geq t_0 \) and the equation (10) is time-irreversible.

The equation (10) has the classical form of a diffusion equation in an external potential, \( \frac{\hbar}{2m} \) plays the role of a diffusion coefficient. To summarize, if we accept that the parameter \( t \) that appears in (6) is a physical time then the underlying dynamics is given by (10). The next question is: can we accept this dynamics as realistic ? In (19) we have shown how to justify (10) starting from a primarily discrete space-time and to recast (10) in general trends in modern physics. The next step is to show that we can write thermodynamic properties directly in terms of path integral.

### B. Path integral expression of the entropy

From standard thermodynamics we know that \( Z \) is related to the free energy \( F \) by \( F = -k_B T \ln Z \); we have also \( F = U - TS \) in which \( S \) is the entropy and \( U \) the internal energy. We may consider that \( U \) is an external parameter fixed by the mode of preparation of the system. From the previous thermodynamic relations and (6) we introduce a path integral expression of the entropy given by

\[
S = k_B \ln \int dx \int Dx(t) \exp \left( -\frac{1}{\hbar}[A_o[x(t); 0, \tau] - \tau U] \right).
\] (12)

in which we consider temporarily \( \tau \) as a free parameter and the quantity \( \tau U \) as the thermal action. We see that \( S \) is determined by the difference \( A_o[x(t); 0, \tau] - \tau U \). If it
should exist only one possible trajectory for which the euclidean action should exactly compensate the thermal one should say that there is no disorder in the system and from (12) we can see that $S = 0$ as expected. For real systems it may exist some fluctuations of $A_o[x(t); 0, \tau]$ and we may have a lot of trajectories for which the order of magnitude of $A_o[x(t); 0, \tau] - \tau U$ is approximately $\hbar$, all these trajectories contribute to $S$. Larger is this number of trajectories smaller is the order in space time and larger is the entropy. From (12) we see that the calculation of $S$ requires to start from a point $x = x(t = 0)$ in space and to explore during a time interval $\tau$ all the loops around this point and, finally, to perform the same procedure for each value of $x$ in the volume of the sample. It is clear that $S$ characterizes the order in space time. Thus from the dynamics it is possible to write immediately $S$ from physical arguments as suggested by the FC. Because there is no explicit Gibbs ensembles in our definition of entropy there is no direct relation between (12) and canonical or micro-canonical representations of statistical mechanics. In fact (12) is an entropy representation of statistical mechanics as defined by Callen (22). The question is now to see if such a definition of $S$ leads to the thermodynamic result. In order to do that we have to find a manner to determine the free parameter $\tau$.

III. THE NATURAL UNIT OF TIME

The entropy defined above depends on two external parameters $\tau$ and $U$ that are not independent. From the definition (12) we may calculate the derivative $\frac{dS}{dU}$ that is the reverse of the temperature $T$ in the usual thermodynamic definition. In (19), (21) it has been shown that we have

$$\frac{1}{T} = \frac{k_B \tau}{\hbar} + \frac{k_B}{\hbar} \left[ U + \hbar \frac{d}{d\tau} \ln Z \right] \frac{d\tau}{dU}$$

(13)

that we can rewrite as

$$\frac{\hbar}{k_B T} = \tau + [U - \int dx < u_K(x) >_{path} + < u_P(x) >_{path}] \frac{d\tau}{dU}$$

(14)

in which $< u_K(x) >_{path}$ is the regular part of the mean value of the kinetic energy calculated over the paths localized around the initial point $x$ and $< u_P(x) >_{path}$ is a similar quantity but associated to the potential energy coming from the external potential. From (14) we
may deduce a natural equilibrium condition

\[ U = \int dx [\langle u_K(x) \rangle_{\text{path}} + \langle u_P(x) \rangle_{\text{path}}] \quad (15) \]

It means that the mean value of the energy calculated on the paths corresponds to the internal energy needed to create the system. This equilibrium condition is very similar to the one used in (12), it does not imply a time but as the consequence it leads to a time scale since from (11) we get \( \tau = \beta \hbar \) that is related to the temperature but not to the particular properties of the system as the mass of the particle or the external potential. When we introduce this value of \( \tau \) into the expression of the path entropy we recover the thermodynamic result. Thus there is two equivalent definitions of the entropy; starting from the usual form of the partition function we recover the Boltzmann definition that we can relate to a number of states but from (12) we may also define the entropy as the disorder in space time. This second definition is closely connected with the Gibbons Hawking (13) approach of the black holes thermodynamics in which the partition function is related to the euclidean action of the gravitational field and this action is associated with a time interval \( \beta \hbar \). From our definition of entropy, it is also possible to establish a relation between action and entropy (21), a relation that is verified in the case of black holes. Thus the definition of entropy as the disorder in space time is equivalent to the Boltzmann one but may have a validity in more extended situations.

Clearly \( \tau \) appears as the unit of time characterizing the thermodynamic equilibrium. From standard textbooks in statistical mechanics (13) it is well known that there is no entropy on a short period of time. Here there is no thermodynamics for time intervals smaller than \( \tau \) since for \( 0 \leq t \leq \tau \) the quantum fluctuations are larger than the thermal ones having \( \frac{1}{\beta} \) as order of magnitude. Thus to describe the thermodynamic evolution any time interval must be considered as a multiple of \( \tau \) that appears as the natural unit of time.

The dynamics associated with the partition function allows us to derive a \textit{H-theorem} as illustrated below.

\section*{IV. DERIVATION OF A H-theorem}

In Section 3 we have seen that the evolution in space time is characterized by the transition function \( \phi(t, x) \) which is the solution of (10) verifying the initial condition \( \phi_0(x) \). We have
shown that the calculation of thermodynamic equilibrium properties requires to explore some loops during a time $\tau$. To this time interval we may associate a length $\Lambda = (D\tau)^{1/2}$ that is the thermal de Broglie wavelength multiplied by a numerical factor; $D = \frac{\hbar}{2m}$. Other lengths in the problem are the range of the external potential and, $L$, the one dimensional extension of the system. However $\phi(t, x)$ allows to investigate physical properties more general than just the equilibrium ones.

Let consider the conditions in which Boltzmann derived the so called $H$-theorem. A system of particles is prepared in a given state by an external constraint. At $t = t_0$ the particles are distributed in space according to a distribution function $\phi_0(x)$ that is positive and normalized. At a given time $t = t_0$ the constraint is removed i.e. the external potential is switched off, the system becomes free and relaxes towards an equilibrium state. The second law of thermodynamics asserts that during the relaxation it exists a given function that increase monotonically with $(t - t_0)$ and tends to the thermal entropy when $(t - t_0) \to \infty$.

Hence for $t \geq t_0$, $\phi(t, x)$ is the solution of

$$- \frac{\partial \phi(t, x)}{\partial t} + \frac{\hbar}{2m} \Delta_x \phi(t, x) = 0 \quad (16)$$

In a one dimensional system of extension, $L$, the solution of (16) is, taking $t_0 = 0$,

$$\phi(t, x) = \frac{1}{L} + \sum A_n \exp \left( -\left( \frac{\pi n \Lambda}{L} \right)^2 \frac{t}{\tau} \right) \cos \left( \frac{\pi n \Lambda}{L} \right) x \quad (17)$$

on which the summation runs from $n = 1$ to $n = \infty$ and the $A_n$ are the Fourier coefficients in the expansion of $\phi_0(x)$. $\phi(t, x)$ is normalized and it reduces to $\frac{1}{L}$ in the limit $t \to \infty$, it gives the probability of being in $x$ at time $t$. Now we may introduce a new definition of the entropy taking into account the evolution of $\phi(t, x)$. The equilibrium entropy defined in (12) can be written as

$$S_{eq} = k_B \ln(L\Gamma(\tau))$$

with

$$\Gamma(\tau) = k_B \int Dx(t) \exp -\frac{1}{\hbar} [A_o [x(t); 0, \tau] - \tau U]. \quad (18)$$

we may rewrite (18) as

$$S_{eq} = k_B \int dx \frac{1}{L} \ln(L\Gamma(\tau)) \quad (19)$$

That we can generalize by replacing $\frac{1}{L}$ by $\phi(t, x)$, we get

$$S(t) = k_B \int dx \phi(t, x) \ln \frac{\Gamma(\tau, t)}{\phi(t, x)} \quad (20)$$
In [20] the entropy $S(t)$ has two origins. One, related to $\phi(t, x)$, is associated with the evolution of the overall system and therefore with open paths. Smaller is $\phi(t, x)$ larger is the matter distribution and larger is $\ln \frac{1}{\phi(t, x)}$ i.e. the contribution to $S(t)$. The second contribution is determined by $\Gamma(\tau, t)$ that is a generalization of $\Gamma(\tau)$ when the probability of space occupation is given by $\phi(t, x)$. This contribution is local and related to close paths. Thus, $S(t)$ defined by [20] contains the interplay between a global and a local relaxation.

Let assume that we are in the thermodynamic limit $\frac{A}{L} \to 0$ and focusing on $t >> \tau$. We may expand $\phi(t + \tau, x)$ according to

$$\phi(t + \tau, x) = \phi(t, x) + \frac{\partial \phi(t, x)}{\partial \tau} + ... = \phi(t, x) - \frac{\partial^2 \phi(t, x)}{\partial x^2} + ... \quad (21)$$

It is easy to calculate the partial derivatives using the explicit expression of $\phi(t, x)$ given in [17]. For $n$ finite $\frac{\partial^2 \phi(t, x)}{\partial x^2}$ goes to zero due to the thermodynamic limit, while if $(\frac{\pi n A}{L})$ becomes very large the partial derivatives are cancelled due to the condition $\frac{t}{\tau} >> 1$. Thus, there are realistic conditions for which the two contributions to $S(t)$ are uncoupled. Let consider now the function $H(t)$ defined by $H(t) = (\frac{1}{k_B})(S(t) - S_{eq})$, it is given by

$$H(t) = -\int dx \phi(t, x) \ln \phi(t, x) - \ln L \quad (22)$$

It is easy to verify (21) that $H(t)$ is a monotonic function of time. Hence, in the thermodynamic limit, $\frac{A}{L} \to 0$, and provided we inspect the system for times much larger than $\tau$ we have been able to define a monotonic increasing function of time $S(t)$ for which the limit $t \to \infty$ corresponds to the equilibrium entropy. The condition $t >> \tau$ leads to analyze the system for time interval $t$ on which the thermal fluctuations are much larger than the quantum ones, it corresponds to thermodynamic regime; at room temperature $\tau$ is approximately 20 femtoseconds.

Starting from the the transition function $\phi(t, x)$ it was easy to derive a $H - theorem$ because $\phi(t, x)$ is the solution of a time irreversible equation [10]. Now to be really convincing we have to show that our approach can be extended in a natural way in order to describe reversible behaviors. This has been done in (21) where it has been shown that we may introduce a second transition function to describe the reverse motion. The two transition functions can be mixed into a complex valued function that verifies a Schroedinger like equation (21), more details will be given in (22).
V. CONCLUSIONS

From the Gibbs expression of the density matrix several approaches have been developed. Starting from an algebraic approach of quantum mechanics the Tomita-Takesaki theorem shows the existence of a one parameter isomorphism group. By comparing this result with the KMS condition it seems natural to identify the parameter to a rescaled time. Then the partition function contains all the dynamics of the system for time larger than $\beta \hbar$. Starting from the path integral version of the partition function we may also discover a motion in space time but this one is restricted to a time interval smaller than $\beta \hbar$. If the dynamics issued of the Tomita-Takesaki theorem is generated by the hamiltonian in the path integral approach the dynamics is associated with a time irreversible equation. We have shown that it exists an equilibrium condition not based on a time condition but leading to introduce a time scale $\beta \hbar$ independent of the system properties like the mass or the external potential. The introduction of the equilibrium condition is similar to what has been done in (2). We have shown that a $H$-theorem can be derived in the thermodynamic limit provided we focus on times larger than $\beta \hbar$. We may conclude that the Feynman’s conjecture leads to new aspects in statistical physics as expected by Feynman.

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