KMS Condition

George V. Bassis

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1 Description of thermal states

1.1 Thermal states in classical statistical mechanics

In classical statistical mechanics, the description of systems which are in thermal equilibrium with respect to each other (thermal states) is achieved with the use of Gibbs' canonical ensemble (Gibbs measure). The canonical ensemble represents the probability distribution of microscopic states of a system which can share its energy with a large heat reservoir. The heat capacity of the reservoir is assumed tobe large enough for the temperature of the coupled system to remain fixed. Given the fact that the exchange of energy is possible, the energy of each of the component systems is not a priori known. What is known is that the total system is also in an equilibrium state. Hence, denoting by $\rho_i = f_i(H_i)$ the probability density functions on phase space for each of the component systems, the following relation must hold

$$f_1(E_1)f_2(E_2) = f(E_1 + E_2) \tag{1}$$

Differentiating (1) with respect to E_1 and E_2 respectively yields the equation

$$f_1'f_2 = f_1f_2' \Rightarrow \frac{f_1'}{f_1} = \frac{f_2'}{f_2}$$
 (2)

Given the fact that each hand-side of (2) depends upon different independent variables, the two hand sides must be constant. So, in thermal equilibrium we will have for the probability density function

$$\rho = Z^{-1} e^{-\beta H} \tag{3}$$

where $\beta \in \mathbb{R}$ is an arbitrary constant which is identified with the inverse of the temperature ($\beta = 1/kT$). Z is called the partition function and is calculated using the normalization condition for the probability density function ρ :

$$Z = \int d^{3N} \vec{q} d^{3N} \vec{p} e^{-\beta H(\vec{q},\vec{p})} = \int d\Omega_H(E) e^{-\beta E}$$

$$\tag{4}$$

where $\Omega_H(E)$ is the phase space volume enclosed by the hypersurface $\{(\vec{q}, \vec{p}), H(\vec{q}, \vec{p})\}$. If in addition to the exchange of energy, the exchange of particles between the coupled systems is also allowed, the probability density function of the equilibrium states will depend on both the energy and the number of particles, i.e. we will have

$$\rho = f(H, N) \tag{5}$$

The equilibrium condition in this case will be given by

$$f_1(E_1, N_1)f_2(E_2, N_2) = f(E_1 + E_2, N_1 + N_2)$$
(6)

which has the general solution

$$f(E,N) = Z_G^{-1} e^{-\beta(E-\mu N)}$$
(7)

where μ is the chemical potential. The states described by the distribution (7) are called the "grand-canonical ensemble".

1.2 Thermal states in quantum statistical mechanics

In order to arrive at a description of equilibrium states in the quantum mechanical case, we can base the theory on the algebra \mathfrak{U} of observables. We start with a 1-component system (a system containing only one type of particles) confined to a box of volume \mathcal{V} . If the total number of particles is known we consider the Hilbert space $\mathcal{H}_{\mathcal{N}}$ of totally antisymmetric (respectively totally symmetric) N-particle wavefunctions. Imposing boundary conditions on the walls of the box gives us the Hamilton operator H. In this context, a general state is described by a positive operator ρ with $tr\rho = 1$ called the density matrix. The expectation value of an observable $A \in \mathcal{B}(\mathcal{H})$ is then given by

$$\omega(A) = tr\rho A \tag{8}$$

The density matrix corresponding to an equilibrium state at inverse temperature $\beta = (kT)^{-1}$ is then

$$\rho_{\beta} = Z^{-1} e^{-\beta H}; Z = tr e^{-\beta H} \tag{9}$$

(generalization of Gibbs' canonical ensemble to quantum mechanics). The internal energy of the system, in the sense of thermodynamics, is then given by

$$E = tr\rho_{\beta}H\tag{10}$$

If in addition to the exchange of energy, we also allow for the exchange of particles, i.e. if we do not fix the number of particles \mathcal{N} , we get the quantum mechanical adaptation of the grand canonical ensemble. In this case, we consider the Fock space $\mathcal{H}_{\mathcal{F}} = \bigoplus_{N=0}^{\infty} \mathcal{H}_{\mathcal{N}}$. The number of particles \mathcal{N} is then an operator in $\mathcal{H}_{\mathcal{F}}$. We then consider the algebra generated by the bosonic and fermionic creation and annihilation operators, which we denote by \mathcal{U} . Denoting by H the Hamiltonian in the Fock space we get the following density matrix in this case

$$\rho_{\beta,\mu} = G^{-1} e^{-\beta(H-\mu N)}; G = tr e^{-\beta(H-\mu N)}$$
(11)

with β being again the inverse temperature and μ the "chemical potential".

2 Description of thermal states with the use of the KMS condition.

2.1 Motivation for the introduction of the KMS condition for thermal state and extraction of the KMS condition.

Before proceeding to the extraction of the KMS condition, we should mention the reasons which led to the pursue of such a condition. The description of thermal states with the use of Gibbs' distribution ($\hat{\rho} = e^{-\beta H}$ works for systems of finite volume. But at the thermodynamic limit ($\mathcal{V} \to \infty, E \to \infty$ with N/\mathcal{V} and E/\mathcal{V} finite) this description breaks down. At the thermodynamic limit the system has an infinite number of degrees of freedom and the usual formulation of classical mechanics and quantum mechanics is not sufficient for the description of such a system. The only way to make predictions about the behaviour of such a system using the usual formulation would be to consider large, but finite systems and take the thermodynamic limit at the end. This leads us to look for an alternative way of describing thermal states. One which would allow us to treat systems with infinitely many degrees of freedom without having to resort to the "solution" of seeing them as limiting cases of systems with finitely many degrees of freedom.

Let A be an observable. Then, the time evolution of A is given by

$$\alpha_t(A) = e^{iHt} A e^{-iHt} \tag{12}$$

Let A,B $\in \mathcal{B}(\mathcal{H})$ and ω_{β} be defined as in equations (7), (8), (9). We have, due to the invariance of the trace under cyclic permutations

$$\omega_{\beta}(\alpha_t(A)B) = Z^{-1}tre^{-\beta(H)}e^{iHt}Ae^{iHt}B =$$
$$Z^{-1}trBe^{iH(t+i\beta)}Ae^{-iHt} = \omega_{\beta}(Be^{iH(t+i\beta)}Ae^{-iH(t+i\beta)})$$

Thus

$$\omega_{\beta}(\alpha_t(A)B) = \omega_{\beta}(B\alpha_{t+i\beta}A) \tag{13}$$

where, replacing t by a complex variable z, we have written

$$\alpha_z A = e^{iHz} A e^{-iHz} \tag{14}$$

We note that α_z is not, in general, a bounded operator. We now introduce for each pair A,B $\in \mathcal{B}(\mathcal{H})$ of observables the following two functions of z

$$F_{A,B}^{\beta}(z) = \omega_{\beta}(B(\alpha_{z}(A)))$$

$$G_{A,B}^{\beta}(z) = \omega_{\beta}((\alpha_{z}A)B)$$
(15)

We see that, with $z = t + i\gamma$

$$F_{A,B}^{\beta}(z) = Z^{-1} tr B e^{iHt} e^{-\gamma H} A e^{-iHt} e^{-(\beta - \gamma)H}$$

is an analytic¹ function of z in the strip

$$0 < \gamma < \beta, \gamma = Im(z) \tag{16}$$

Indeed,

$$e^{iHz}Ae^{-iHz}e^{-\beta H} \stackrel{z=t+i\gamma}{=} e^{iH(t+i\gamma)}Ae^{-iH(t+i\gamma)}e^{-\beta H} = e^{iHt}e^{-H\gamma}Ae^{-iHt}e^{H\gamma}e^{-\beta H} = e^{iHt}e^{-H\gamma}Ae^{-iHt}e^{-(\beta-\gamma)H}$$

will be bounded and of trace class² for $0 \leq \gamma \leq \beta$ because, with these restrictions on γ , all the factors in the above product are bounded and either the second factor or the last (or both) are of trace class. Similarly, $e^{-\beta H}\alpha_z A$ will be of trace class for $-\beta \leq \gamma \leq 0$. Therefore, for $F_{A,B}^{\beta}(z)$ is well defined in the strip $0 \leq \gamma \leq \beta$. In fact it is differentiable, hence analytic in the open strip $0 < \gamma < \beta$ and continuous at the boundaries (follows from the fact that $He^{-\alpha H}$ is a bounded operator for any $\alpha > 0$). Similarly, the function $G_{A,B}^{\beta}(z)$ is analytic in the strip $-\beta < \gamma < 0$ and continuous at the boundaries. For real values of z, F and G are bounded, continuous functions of t and we obtain G(t) as the boundary value of F(z) for $z \to t + i\beta$

$$G^{\beta}_{A,B}(t) = F^{\beta}_{A,B}(t+i\beta) \tag{17}$$

If instead of the canonical ensemble we use the grand canonical one, we arrive at the same relation with μ and H replaced by $H(\mu)$, α_t in (12) replaced by α_t^{μ} , \mathfrak{U} by \mathcal{A} where

$$H(\mu) = H - \mu N, \alpha_t^{\mu} A = e^{iH(\mu)t} A e^{-iH(\mu)t}$$
(18)

Relation (17) survives the thermodynamic limit $(\mathcal{V} \to \infty, E \to \infty \text{ with } N/\mathcal{V})$ and E/\mathcal{V} finite). Specifically we may regard A and B as local quantities, $\omega_{\beta,\mu}$ as the state (normalized, positive, linear form over \mathcal{A}) corresponding to equilibrium with inverse temperature β , chemical potential μ in unlimited space. We can now consider H and N in (11) as generators of symmetries which are realized by automorphism groups on \mathcal{A} , namely the time translations α_t and the U(1) gauge transformations

$$\gamma_{\phi}A = e^{iN\phi}Ae^{-iN\phi} \tag{19}$$

 $H(\mu)$ is an element in the Lie algebra of the symmetry group and

$$\alpha_t^{\mu} = \alpha_t \gamma_{-\mu t} \tag{20}$$

¹We remind that a function is called analytic if it is locally given by a convergent power series. That is, a function f is called analytic if it is equal to its Taylor series in some neighborhood of every point where it is defined.

²Let \mathcal{H} be a separable Hilbert space. An endomorphism of \mathcal{H} is a compact operator for which a trace may be defined, so as to be finite and independent of the choice of basis.

From the previous analysis (for the case of the canonical ensemble) it is suggested that F(t) is the boundary value on the real axis of a function F(z), analytic in the strip given by (16) and that G(t) is obtained as the boundary value for $Im(z) = \beta$ as in (17). We thus reach the relation

$$G_{A,B}^{\beta,\mu}(t) = F_{A,B}^{\beta,\mu}(t+i\beta)$$
(21)

which is analogous to (17) for the grand canonical ensemble. This relation represents the adaptation of the condition satisfied by the Kubo-Martin-Schwinger (KMS) states by Haag, Hugenholtz and Winnink and is called the KMS condition. The KMS condition implies that $\omega_{\beta,\mu}$ is an invariant state with respect to α_t^{μ}

$$\omega_{\beta,\mu}(\alpha_t^{\mu}(A)) = \omega_{\beta,\mu}(A) \tag{22}$$

<u>Remark:</u> The KMS condition (23) is equivalent to requiring that the Fourier transforms of F and G are related by a Boltzmann factor, i.e.

$$\tilde{G}(\epsilon) = e^{-\beta\epsilon} \tilde{F}(\epsilon) \tag{23}$$

where $\tilde{F}(\epsilon) = \int dt F(t) e^{-i\epsilon t}$.

2.2 Equivalence of KMS states and canonical ensemble for finite systems

The question which is raised now is whether the KMS condition suffices to characterize an equilibrium state. We will start by looking at the case of a system enclosed in a box of volume \mathcal{V} . The standard way to describe such a system with an arbitrary number of (internal) particles in non-relativistic quantum theory is by introducing creation and annihilation operators (which act in a Fock space $\mathcal{H}_{\mathcal{F}}$.

The question of the equivalence between the KMS condition and description of the thermal states with the use of Gibbs' canonical ensemble can be stated as follows: Does the requirement that ω is a normal³ state on $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ satisfying the KMS condition imply that ω is given by the density matrix of (8), (9) or (11)? First we note that a normal state on $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ is described by a density matrix ρ such that $\omega(A) = tr\rho A$. Also, all automorphisms of $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ as given by (20) are inner, i.e. are maps of the form $\alpha_t^{\mu} : \mathcal{B}(\mathcal{H}_{\mathcal{F}}) \to \mathcal{B}(\mathcal{H}_{\mathcal{F}}); A \mapsto e^{-i(H-\mu N)t}Ae^{i(H-\mu N)t}$, for every $A \in \mathcal{B}(\mathcal{H}_{\mathcal{F}})$ and so defines a unitary $U^{\mu}(t) \in \mathcal{B}(\mathcal{H}_{\mathcal{F}})$ up to a phase factor and, considering time as a continuous variable defines a generator $H(\mu)$ up to an additive

³A state is called normal if it can be described by a density matrix ρ , i.e. by a positive endomoprhism on $\mathcal{H}_{\mathcal{F}}$ ($\rho \in \mathcal{B}(\mathcal{H}_{\mathcal{F}})$).

constant that plays no role in (11). The expectation values of energy and particle number for a state described by (11) are given by

$$E = tr\rho_{\beta,\mu}H; < N > = tr\rho_{\beta,\mu}N \tag{24}$$

as functions of β , μ and \mathcal{V} . Inserting in (21), (22) for A an invariant element, i.e. one which commutes with all $U^{\mu}(t)$ (that is with all operators of the form $e^{-iH(\mu)t}$ (see equation (18))). In this case, $\alpha_t^{\mu}(A) = A$ and so $F_{A,B}(z)$, $G_{A,B}(z)$ are independent of z and equal to one another, which implies for the density matrix $tr[\rho, A]B = 0$ for all $B \in \mathcal{B}(\mathcal{H}_{\mathcal{F}})$, i.e. $[\rho, A] = 0$ if A commutes with $H(\mu)$. Thus $\rho \in \{\bigcup_t U^{\mu}(t)\}^{\prime\prime}$ (the double prime denotes the commutant of the commutant. We remind here the definition of the commutant: the commutant of a subset S of a semigroup (such as an algebra or a group) A is the subset S' of elements of A commuting with every element of S. i.e. $S' = \{x \in A : sx = xs, \forall s \in S\}$ and ρ must be a bounded function of $H(\mu)$. The fact that this function is of the form $ce^{-\beta H(\mu)}$ follows then by choosing for A and B operators which have non-vanishing matrix elements only between two vectors Ψ_1 and Ψ_2 which are simultaneous eigenvectors of $H(\mu)$ and ρ . Thus $H(\mu)$ and ρ can be simultaneously diagonalized in the basis of Ψ_1, Ψ_2 . And for ρ to be a diagonal finite operator it has to be of the form $ce^{-\beta H(\mu)}$.

The equivalence of the description of thermal states using the KMS condition to the one provided by the canonical ensemble, can be elucidated in the special case where we consider the algebra \mathcal{A} of observables to be the algebra of $n \times n$ matrices with complex entries, which will be denoted by $M_n(\mathbb{C})$. The states on \mathcal{A} are of the form $\omega(A) = tr\rho A$, with $\rho \in M_n(\mathbb{C})$, $\rho = \rho^*, tr\rho = 1, \rho \geq 0$. Using the KMS condition (13) for t = 0 we get

$$tr\rho AB = tr\rho Be^{-\beta H}Ae^{\beta H} = trBe^{-\beta H}Ae^{\beta H}\rho = trB\rho A$$

from which we have

$$\rho A = e^{-\beta H} A e^{\beta H} \rho \Rightarrow [e^{\beta H} \rho, A] = 0, \forall A \in \mathcal{U}$$

Since the algebra is simple, only multiples of the identity commute with all of its elements, hence

$$e^{\beta H}\rho = \lambda \mathbb{1} \Rightarrow \rho = \lambda e^{-\beta H}$$

3 KMS state for a free field and its GNS representation

Let ω be a KMS-state over a C^* -algebra \mathcal{A} . We will now look at the representations π of \mathcal{A} resulting from ω by the GNS-construction. The

representation π has some remarkable properties. We will start by exhibiting these properties for the case of the system in a box where $\mathcal{A} = \mathcal{B}(\mathcal{H}_F)$ and ω is given by (7), (11). The density operator, ρ , is a positive operator with finite trace. Therefore, dropping the indices β and μ , the operator:

ŀ

$$\kappa_0 = \rho^{1/2}$$
 (25)

is well defined and of Hilbert-Schmidt class, that is $\kappa_0 \in \{\kappa : tr\kappa^*\kappa < \infty, \kappa \in \mathcal{B}(\mathcal{H}_F)\}$. We denote this set here by \mathcal{H} because it is a Hilbert space with respect to the scalar product

$$<\kappa|\kappa'>=tr\kappa^*\kappa'$$
 (26)

complete with respect to the norm $||\kappa||_H = (tr\kappa^*\kappa)^{1/2}$. It is also a *-algebra and it is a 2-sided ideal in $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$, i.e.

$$\kappa \in \mathcal{H}\&A \in \mathcal{B}(\mathcal{H}_{\mathcal{F}}) \Rightarrow A\kappa \in \mathcal{H}\&\kappa A \in \mathcal{H}$$
(27)

Since ρ has finite trace, $\kappa_0 \in \mathcal{H}$ and since all spectral values of ρ and hence of κ_0 are non-vanishing, we have:

$$A\kappa_0 \neq 0, \kappa_0 A \neq 0, \omega(A^*A) \equiv trA^*A \neq 0 forA \in \mathcal{B}(\mathcal{H}_{\mathcal{F}})$$
(28)

Thus ω is a faithful state. Hence in the implementation of the GNS construction, $\mathcal{H}_{\omega} = \mathcal{B}(\mathcal{H}_{\mathcal{F}})$. We now consider the following representation of $\mathcal{A} = \mathcal{B}(\mathcal{H}_{\mathcal{F}})$ by operators acting on \mathcal{H} :

$$\pi(A)|\kappa\rangle = |A\kappa\rangle; \kappa \in \mathcal{H}, A \in \mathcal{B}(\mathcal{H}_{\mathcal{F}})$$
⁽²⁹⁾

where by $|\kappa\rangle$ we denote the Hilbert-Schmidt operator κ seen as a vector of the Hilbert space \mathcal{H} . The state $\omega(A)$ can then be written as:

$$\omega(A) = <\kappa_0 |\pi_l(A)| \kappa_0 > \tag{30}$$

From (28) we see that $|\kappa_0\rangle$ is a cyclic vector for the representation π_l . From (29) and (30) it is obvious that the representation π_l is isomorphic to the GNS representation induced by ω and that $|\kappa_0\rangle$ is the state vector corresponding to ω . We thus drop the index "l" and will henceforth write π instead of π_l .

There is obviously another mapping of the form $A \in \mathcal{B}(\mathcal{H}_{\mathcal{F}}) \to \pi_r(A) \in \mathcal{B}(\mathcal{H})$ (the index "r" here stands for "right") defined by:

$$\pi_r(A)|\kappa\rangle = |\kappa A^*\rangle \tag{31}$$

It gives a conjugate linear representation of \mathcal{A} namely:

$$\pi_r(AB) = \pi_r(A)\pi_r(B); \pi_r(A^*) = (\pi_r(A))^*; \pi_r(cA) = \bar{c}\pi_r(A)$$
(32)

It can be shown that the operator norms of $\pi(A)$ and $\pi_r(A)$ are equal, i.e. that $\| \pi(A) \| = \| \pi_r(A) \|$, as well that the commutant of $\pi(A)$ (that is the subset of elements of $\mathcal{B}(\mathcal{H})$ commuting with every element of $\pi(A)$) is equal to the commutant of the commutant of $\pi_r(A)$, or symbolically: $(\pi(A))' = (\pi_r(A))''$. For the relation between the two representations we also have the following theorem:

Theorem 3.1. (i) κ_0 is a cyclic vector for both $\pi(A)$ and $\pi_r(A)$ and

$$\omega(A) = <\kappa_0 |\pi(A)| \kappa_0 > = \overline{<\kappa_0 |\pi_r(A)| \kappa_0 >}$$
(33)

(ii) π and π_r are transformed into each other by an antiunitary conjugation operator J defined by:

$$J|\kappa \rangle = |\kappa^*\rangle \tag{34}$$

with

$$J\pi(A)J = \pi_r(A), J^2 = 1, J|\kappa_0 > = |\kappa_0 >$$
(35)

Proof. The cyclicity of κ_0 for the representation π is related to the faithfulness of ω in the following way: Suppose there is $\kappa \in \mathcal{H}$ such that $\langle \kappa | \pi(A) | \kappa_0 \rangle = 0$ for all $A \in \mathcal{B}(\mathcal{H}_F)$. Since κ can also be ragarded as an element of $\mathcal{B}(\mathcal{H}_F)$ we can choose $A = \kappa \kappa_0$. Then we could get $tr \kappa^* \kappa_0^2 = \omega(\kappa \kappa^*)$ and hence, by faithfulness of ω we have $\kappa = 0$. The first part of (34) results directly from the defining equations. This means that the representation π is the one resulting from the GNS theorem with the state ω . The operator J is defined by

$$J\kappa = \kappa^* \tag{36}$$

J is anti-unitary since:

$$\langle J\kappa_1|J\kappa_2\rangle = \langle \kappa_1^*|J\kappa_2^*\rangle = tr\kappa_1\kappa_2^* = \langle \kappa_2|\kappa_1\rangle$$

Because $J^2 = 1$, the operator J is a conjugation. The remaining statements of the theorem result from the previous.

Given that ω is invariant under the group of automorphisms α_t^{μ} , we can implement this automorphism in the GNS representation by unitary operators $U^{\mu}(t)$ with defining relation:

$$U^{\mu}(t)\pi(A)|\kappa_0\rangle = \pi(\alpha_t^{\mu}A)|\kappa_0\rangle \tag{37}$$

If ω is also invariant under time translations and the gauge symmetry we mentioned earlier, i.e. if ω is invariant under α_t and γ_{ϕ} there will also exist unitary operators U(t), $V(\phi)$ in the GNS representation which will imposing these transformations. The particle number operator N and the operator $H(\mu) = H - \mu N$ can then be regarded as the generators for the symmetries realised by the operators U, V and $U^{\mu}(t)$ respectively. H, N and $H(\mu)$ are operators acting on \mathcal{H} , satisfying:

$$H|\kappa_0\rangle = 0, N|\kappa_0\rangle = 0 \tag{38}$$

(This equation results from the invariance of the expectation functional under the afforementioned groups of automorphisms.) It is obvious though that the operators mentioned in (43) are not the ones defined in (24), (25). The Hamiltonian and particle number of our system cannot be equal to zero. Denoting by $\mathcal{H}_{\mathcal{F}}$, $\mathcal{N}_{\mathcal{F}}$ the Hamiltonian and particle number operators in Fock space and $U_{\mathcal{F}}(t) = expi\mathcal{H}_{\mathcal{F}}t$ as elements of the algebra \mathcal{A} of bounded operators in Fock space, we have:

$$U(t) = \pi(U_{\mathcal{F}}(t))\pi_r(U_{\mathcal{F}}(t))$$
(39)

U(t) is the unitary operator implementing the time translation automorphism in the representation $\pi(A)$. Symbolically we can thus write

$$H = \pi(H_{\mathcal{F}}) - \pi_r(H_{\mathcal{F}}) \tag{40}$$

(Of course there exist analogous expressions for the operators U^{μ} and $V(\phi)$ which implement the other symmetries in the representation π) $\pi_r(\mathcal{A})$ commutes with $\pi(\mathcal{A})$ since

$$\begin{aligned} [\pi(A), \pi_r(A)] |\kappa\rangle &= (\pi(A)\pi_r(A) - \pi_r(A)\pi(A)) |\kappa\rangle \\ &= |A\kappa A^* > -|A\kappa A^* > = 0 \end{aligned}$$

Thus, the factor $\pi_r(H_F)$ in (41) has no impact on the action of the automorphism of time translations. This can be seen with the following quick calculation:

$$<\kappa_{0}|\pi(U_{t})A\pi(U_{-t})|\kappa_{0}> = <\kappa_{0}|e^{iH_{\mathcal{F}}t}Ae^{-iH_{\mathcal{F}}t}\kappa_{0}> =$$
$$= tr\kappa_{0}^{*}e^{iH_{\mathcal{F}}t}Ae^{-iH_{\mathcal{F}}t}\kappa_{0} = tr\rho e^{iH_{\mathcal{F}}t}Ae^{-iH_{\mathcal{F}}t} = tr\rho A = \omega(A)$$

where the relations $\kappa = \rho^{1/2}$ and $\rho = e^{-\beta H_F}$ have been used and similarly:

$$<\kappa_0|\pi(U_t)\pi_r(U_t)A\pi_r(U_{-t})\pi(U_{-t})|\kappa_0> = <\kappa_0|e^{iH_{\mathcal{F}}t}Ae^{-iH_{\mathcal{F}}t}\kappa_0e^{-iH_{\mathcal{F}}t}e^{iH_{\mathcal{F}}t}> = tr\rho A = \omega(A)$$

Hence:

$$\left. \frac{\partial \pi(\alpha_t A)}{\partial t} \right|_{t=0} = i[H, \pi(A)] = i[\pi(H_{\mathcal{H}}), \pi(A)]$$
(41)

The term $\pi_r(H_{\mathcal{F}})$ plays an important role though when taking the thermodynamic limit. The total energy operator at that limit becomes meaningless given the fact that both its expectation value and its fluctuations tend to infinity as $\mathcal{V} \to \infty$. It is then obvious that at the thermodynamic limit the ability to define a meaningful (i.e. bounded) total energy operator depends on the invariance of the state ω which is determined by the evolution operator U(t). In this case, the second term of (41) cancels the infinities which appear (it provides a rescaling of the spectrum of the total energy operator) so that the equilibrium state vector becomes an eigenvector of H corresponding to the eigenvalue zero as in (43). In order to make this procedure of cancelation of infinities more clear, we start by noting that

$$\kappa_0 = Z^{-1} e^{-\beta H_F/2} \tag{42}$$

We then have, acting on κ_0 with $\pi(H_{\mathcal{F}})$

$$\pi(H_{\mathcal{F}})|\kappa_0\rangle = Z^{-1}|H_{\mathcal{F}}e^{-\beta H_{\mathcal{F}}/2}\rangle \equiv \Psi$$

But according to (41) we have

$$H|\kappa_0 > = Z^{-1/2}|[H_{\mathcal{F}}, e^{-\beta H_{\mathcal{F}}}/2] > = 0$$

The norm of the vector Ψ increases to infinity as $\mathcal{V} \to \infty$ at the thermodynamic limit while the equilibrium state vector $|\kappa_0\rangle$ through the use of the Hamiltonian operator given by (41) becomes an eigenvector of H with eigenvalue equal to zero. As a concluding remark we could say the following: For a system in a box there are two equivalent descriptions of the equilibrium states. The first one is the description with the use of the density matrix $\rho_{\beta,\mu} = G^{-1}e^{-\beta}(H - \mu N)$. In this description an irreducible representation⁴ of the algebra \mathcal{A} is used (actually in this description the algebra \mathcal{A} of observables is taken to be the algebra $\mathcal{B}(\mathcal{H}_{\mathcal{F}})$ of bounded operators acting on the Fock space of the system.) In this representation, the mixed⁵ state $\omega_{\beta,\mu}$ is described by the density matrix $\rho = G^{-1}e^{-\beta(H-\mu N)}$. The second description is achieved with the use of a reducible representation of the algebra of observables on the algebra of Hilbert-Schidt class operators acting on the Fock space of the system. The first description breaks down at the thermodynamic limit whereas the second one remains valid after the implementation of the thermodynamic limit.

⁴A *-representation π on a Hilbert space \mathcal{H} is irreducible if and only if there are no closed subspaces of \mathcal{H} which are invariant under all the operators $\pi(x)$ other that \mathcal{H} itself and the trivial subspace 0. If such invariant subspaces exist, the representation π is called reducible.

⁵We remind that extremal states on a C^* -algebra are called pure states. States which are not pure are called mixed. Pure stated can be described by a state vector $|\psi\rangle$ in a Hilbert space (i.e. this vector completely determines the statistical behaviour of a measurement). On the contrary, mixed states are states prepared by statistically combining two or more pure states with certain probabilities. In this case there is no state vector which determines this statistical behaviour (i.e. a state vector $|\xi\rangle$ such that the expectation value of A will be $\langle \xi | A | \xi \rangle$). The description of mixed states is done with the use of the density operator which, in its most general form reads $\rho = \sum_i p_j |\psi_j\rangle \langle \psi_j|$.

To make the reducibility of the representation of the algebra of observables provided by the GNS construction evident, we return to the known example where we consider the algebra of observables to be $\mathcal{A} = M_n(\mathbb{C})$ with the standard representation of a state being achieved with the use of a density matrix. As described above we have the map $\pi: \mathcal{A} \to \mathcal{B}(\mathcal{H})$ where, in this case $\mathcal{H} = \mathbb{C}^{\mathbb{n}}$. For the states on the algebra \mathcal{A} we have $\omega(A^*A) = tr\rho A^*A$, which is different than zero for $A \neq 0$ (faithful state). Thus, we can define the operator $\kappa_0 = \rho^{1/2}$ which is of Hilbert - Schmidt class. Consider now the representation of \mathcal{A} by Hilbert - Schmidt class operators defined by $\pi(A)|\kappa_0\rangle = |A\kappa_0\rangle, |\kappa_0\rangle$ cyclic for π (see equation ((29)). The GNS Hilbert space is $\mathcal{H} = \kappa : tr\kappa^*\kappa < \infty$. But, as we now there is an isomorphism $M_n(\mathbb{C}) \simeq \mathbb{C}^{\mathbb{D}^2}$ given the fact that their dimension is the same. Taking $\lambda_1 \in \mathcal{H}$ to be the diagonal $n \times n$ matrix $\lambda_1 = diag(1, 0, ..., 0)$, we easily see that it defines an invariant subspace. Considering now the matrices λ_i , i = 2, 3, ..., n(i.e. the $n \times n$ diagonal matrices whose only nonzero element is $\lambda_i i = 1$ we see that they also define invariant subspaces for our representation. The previous argument confirms the fact that the representation π of our algebra of observables is reducible. As a final remark we may also note that in the free field case, for quasi-free fields (that is fields for which all expectation values are determined by 2 - point functions, the KMS condition takes the form:

$$\omega(\phi(x), \alpha_t \phi(y)) = \omega(\alpha_{t+i\beta} \phi(y), \phi(x)) \tag{43}$$

where $\omega(\phi(f), \phi(g))$ is the aforementioned 2 - point function.