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On K.M.S. evolutions and liouville in quantum statistical mechanics.

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*Document Version*

Publisher's PDF, also known as Version of record

*Publication date:*

1977

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Brinke, G. T. (1977). *On K.M.S. evolutions and liouville in quantum statistical mechanics*. s.n.

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## INTRODUCTION AND SUMMARY

Statistical mechanics is the study of macroscopic properties of large systems starting from the microscopic properties. A system in a box is inadequate as a model for large systems since it presupposes the unphysical fiction of a completely isolated system. For instance a system in a box neither exhibits phase transitions (cf. [1] theory of Yang and Lee) nor approach to equilibrium (cf. [1] Poincaré cycle), both well known phenomena for physical systems. To reproduce the thermodynamic behaviour one performs the so-called thermodynamic limit, i.e. one uses the "Gibbs Ansatz" to calculate the expectation values of observables and takes the limit  $V$  (volume),  $N$  (number of particles)  $\rightarrow \infty$ , keeping  $N/V$  fixed.

For the precise description of the above mentioned phenomena one has to consider as a model a thermodynamic system, i.e. a system consisting of an infinite number of particles in an infinite volume with finite density. Such a description is most adequately given in an algebraic setting, thereby assuming that the observables generate a  $C^*$ -algebra  $\mathcal{U}$  and the dynamics is described by a one-parameter group of  $*$ -automorphisms  $\{\alpha_t\}$  of  $\mathcal{U}$ . The expectation values of the observables, in particular correlation functions, are given by positive linear functionals (i.e. states) on  $\mathcal{U}$ .

We restrict ourselves to equilibrium quantum statistical mechanics. It can be argued that equilibrium states of thermodynamic systems satisfy the so-called K.M.S. condition, which is a direct generalization of the "Gibbs Ansatz" (cf. [2]), with respect to  $\{\alpha_t\}$  at inverse temperature  $\beta > 0$ .

An important problem is to mathematically describe the dynamics that gives rise to a thermodynamical equilibrium state. It is therefore of interest to investigate which automorphism groups are *evolutions*, i.e. admit a K.M.S. state. For this one has, among other things, to consider the properties of the infinitesimal generator of the automorphism group  $\{\alpha_t\}$ . Generally speaking the infinitesimal generator

is an *unbounded* derivation. (In chapter I we present a short introduction to this subject, whereas in chapter III we specialize to separable U.H.F. algebras. A more complete survey can be found in [3].)

For the finite system, where the algebra of observables consists of all the bounded operators on a suitable infinite dimensional separable complex Hilbertspace, one knows which automorphism groups, characterized by a selfadjoint operator  $H$  ("Hamiltonian"), admit of K.M.S. states. In this case the automorphism group admits of a K.M.S. state iff there is a  $\beta > 0$  such that  $e^{-\beta H}$  is a trace class operator. A K.M.S. state admitted by such a dynamics is the well known Gibbs state and this state is, in accordance with the Yang-Lee theory, the only one.

For a thermodynamic system there is no Hamiltonian. We have to look for other means to distinguish automorphism groups that admit of a K.M.S. state from automorphism groups that do not admit of a K.M.S. state. One proves that only strongly continuous automorphism groups are candidates for evolutions in case of a separable algebra of observables.

We will treat this problem for two models, namely quantum lattice systems and Fermi systems. For these models the  $C^*$ -algebra of observables is of a particular, technically simple, nature. It is a so-called separable U.H.F. algebra. It has a local structure built in that permits of a natural discussion of thermodynamic systems starting from finite systems. This local structure gives rise to the so-called approximately inner automorphism groups, i.e. automorphism groups that can be approximated by a sequence of uniformly continuous one-parameter groups of inner  $*$ -automorphisms. In particular the physically important class of dynamics obtained as a limit of finite volume dynamics is approximately inner.

Closely connected with any strongly continuous automorphism group  $\{\alpha_t\}$  of a separable U.H.F. algebra is a set of K.M.S. states (*not with respect to  $\{\alpha_t\}$ !*). This set has a cluster point  $\omega$ . (Its properties are investigated in chapter IV). It is known [4] that, if  $\{\alpha_t\}$  is approximately inner,  $\omega$  satisfies the K.M.S. condition with respect to  $\{\alpha_t\}$ . It has been conjectured [4] that every strongly continuous one-parameter group of  $*$ -automorphisms of a separable U.H.F. algebra is approximately

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inner. Obviously the truth of this conjecture gives a unique characterization of evolutions. An example of an approximately inner group of automorphisms is provided by the usual quantum lattice dynamics (cf. section 3.3).

We will prove (proposition 4.3) that all the quasi-free evolutions of the Clifford algebra (a particular U.H.F. algebra appropriate for the description of Fermion systems) are approximately inner<sup>\*</sup>). Furthermore we extend the above result to a large class of automorphisms, connected in some way with the quasi-free evolution. In particular we show (proposition 4.8) that certain global perturbations of these automorphism groups again give approximately inner automorphism groups.

The approximately inner property of  $\{\alpha_t\}$  is sufficient to ensure that the cluster point  $\omega$  is a suitable K.M.S. state. Whether this property is necessary is not clear. It is quite possible that all strongly continuous automorphism groups of a separable U.H.F. algebra admit a K.M.S. state, without all being approximately inner. To investigate this it is natural to consider in more detail the clusterpoint  $\omega$ , mentioned above. We prove (proposition 4.12) that  $\omega$  satisfies some interesting inequalities, which may be useful in solving this problem. For instance we show (proposition 4.13) that a state on a general C<sup>\*</sup>-algebra which satisfies these inequalities is separating. Hence this state satisfies the K.M.S. condition on the level of the von Neumann algebra.

The observables of continuous quantum systems, as opposed to quantum lattice systems, are described by the so-called quasi-local algebra. The temporal behaviour of correlation functions is determined by the spectral properties of the so-called *Liouville operator*. In the last chapter we will study, also for general continuous quantum systems, the spectral properties of the Liouville operator, which is defined as follows: a state  $\omega$  that satisfies the K.M.S. condition with respect to

<sup>\*</sup>) Professor Sakai brought to our attention that R. McGovern obtained related results [8].

an automorphism group  $\{\alpha_t\}$  is  $\alpha_t$ -invariant and gives rise to a G.N.S. representation in which  $\{\alpha_t\}$  is implemented by a strongly continuous group of unitary operators. The infinitesimal generator  $H_\omega$  of this unitary group is called a Liouville operator. It is the direct generalization of the well known Liouville operator of ordinary classical statistical mechanics.

With the help of the notion of Arveson spectrum (cf. [5]), to be defined in chapter I, we show that the spectrum of a Liouville operator is symmetric around the origin. This is a well known result from the Tomita-Takesaki theory. Our proof, however, shows in a very simple way the role of the separating character of the state.

Let  $\omega_1$  and  $\omega_2$  be K.M.S. states with respect to an evolution  $\{\alpha_t\}$  of a  $C^*$ -algebra  $\mathcal{U}$  at inverse temperatures  $\beta_1$  and  $\beta_2$  (possibly  $\beta_1 = \beta_2$ ). Denote the Liouville operators by  $H_{\omega_1}$  and  $H_{\omega_2}$ . We show that in many cases the spectra of these operators coincide as sets. For the non-separable quasi-local algebra  $\mathcal{U}$  this is true if  $\{\alpha_t\}$  satisfies some *regularity* conditions. For a separable  $C^*$ -algebra, for instance the separable U.H.F. algebra, the spectra of the Liouville operators belonging to the same automorphism group are always the same (cf. [6]). Moreover for the free Bose gas, where the algebra of observables is neither separable nor quasi-local, this is also true, due to the fact that  $\{\alpha_t\}$  acts in an asymptotically abelian way.

Suppose we have a non-primary K.M.S. state  $\omega$  at an inverse temperature  $\beta$  that admits of a decomposition into extremal K.M.S. states  $\omega_\gamma$ , i.e.  $\omega = \int d\mu_\omega(\gamma)\omega_\gamma$ , where  $\omega_\gamma$  represent the pure phases. Without any further assumption one can prove that a discrete point in the spectrum of  $H_\omega$  appears as discrete point ("survives the decomposition") in the spectra of  $H_{\omega_\gamma}$  for  $\gamma$  in some set with non-zero  $\mu$ -measure [7].

For the particular case that all the G.N.S. representation spaces are separable we show that a real number  $\lambda$  is a discrete point of  $\sigma(H_\omega)$  iff it is a discrete point of  $\sigma(H_{\omega_\gamma})$  for  $\gamma$  in some set with non-zero  $\mu$ -measure. ( $\sigma(H_\omega)$  is the spectrum of  $H_\omega$ ).

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Similar statements are made with respect to generators of unitary groups that implement other groups of automorphisms, such as space translations.

In section 5.3 and 5.5 we apply the foregoing to the two-dimensional Ising model and the ideal Bose gas.