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On the classical KMS boundary condition

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Summary. — We discuss some properties of the classical KMS boundary condition and find some sufficient conditions for its equivalence to the Kirkwood-Salsburg equations.

1. – Introduction

The KMS boundary condition is an abstract equilibrium condition for quantum statistical mechanics. If ρ is a state and A, B are two observables and $\alpha_t(A)$ is the observable into which A evolves in time t, the condition

$$\rho(AB) = \rho(B\,\alpha_{i\hbar\beta}(A)) \tag{1.1}$$

is supposed to characterize the equilibrium states at temperature $T = \beta^{-1}$. The observables $\alpha_{i\hbar\beta}(A)$ are a kind of "analytical continuation" of the observables $\alpha_t(A)$.

We refrain here from explaining the exact meaning of the above formulae.[1] We rather try to take the formal limit as $\hbar \to 0$. To do this let us write (1.1) as

$$\rho(\frac{AB - BA}{i\hbar}) = \rho(B\,\frac{A_{i\hbar\beta} - A}{i\hbar\beta}) \tag{1.2}$$

and then use the well known classical limit prescription

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[1] R. Haag, N. Hugenholtz and M. Winnink: Comm. Math. Phys., **5**,215 (1967); D. Robinson: Comm. Math. Phys., **7**,337 (1969).

(1.3) $$\frac{AB - BA}{i\hbar} \;\to\; \{A, B\}$$

where in the r.h.s. of (1.3) A and B represent classical observables and $\{\cdot,\cdot\}$ denotes the Poisson bracket.

Then (1.2) becomes

(1.4) $$\rho(\{A, B\}) = \rho\big(B\,\frac{d\alpha_t(A)}{dt}\big|_{t=0}\big)\,\beta,$$

or, also,

(1.5) $$\rho(\{A, B\}) = \beta\,\rho(B\,\{A, H\}),$$

where H is the Hamiltonian of the classical system.

In this paper we shall not consider the ≪dynamical KMS condition≫ (1.4) but only the ≪static KMS condition≫ (1.5) and we shall examine its properties.

Of course our first task will be to give a rigorous meaning to (1.5): roughly ρ is a probability measure on the phase space, A, B, H are functions on it and $\{\cdot,\cdot\}$ is the Poisson bracket.

Equation (1.5) has been known for a long time for some finite systems and its nicest application can be found in ref.([2]) where it is used to show the nonexistence of two dimensional crystals.

2. – The classical observables

The configuration space consists in the sequences $(p_i, q_i)_0^\infty$ where $(p_i, q_i) \in \mathbb{R}^d \times \mathbb{R}^d$, enjoying the ≪local finiteness≫ property: number of points in $(\Lambda \cap \cup_{i=0}^\infty q_i) < +\infty$ for all finite cubes $\Lambda \subset \mathcal{R}^d$.

The above configuration space will be denoted $\mathcal{H}$.

The elements of $\mathcal{H}$ will be denoted by X or (P, Q) or $(p_i, q_i)_0^\infty$ or $(x_i)_0^\infty$.

Let $\mathcal{U}^{(h)}$ denote the set of the real functions $f : \mathcal{H} \to \mathbb{R}$ which can be described in terms of a sequence $\{f^{(m)}\}_0^\infty$ of k-times continuously differentiable ≪potentials≫ $f^{(m)}$: $(\mathbb{R}^d \times \mathbb{R}^d)^m \to \mathbb{R}$ which are bounded, symmetric, have compact support in the second variable and vanish for all but finitely many m's. The form of f is

$$f(X) = f((p_i, q_i)_0^\infty) = f(x_i)_0^\infty = \sum_{m\geq 0}^{\infty} \sum_{i_1<\ldots<i_m} f^{(m)}(x_{i_1}, x_{i_2}, \ldots, x_{i_m}).$$

The set $\mathcal{U}^{(k)}$ is the set of k–times differentiable observables([3]). If $f, g \in \mathcal{U}^{(1)}$ we define $\{f, g\} \in \mathcal{U}^{(0)}$ as

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([2]) R. Kubo,: Journ. Phys. Soc. Japan, **12**, 570 (1957); N.D. Mermin: Journ. Math. Phys., **8**, 1061 (1967).

([3]) D. Ruelle, *Statistical Mechanics* (New York, N.Y., 1969), p. 171.

$$\{f,g\}(X)=\sum_{i=0}^{\infty}\Big(\frac{\partial f(X)}{\partial q_i}\frac{\partial g(X)}{\partial p_i}-\frac{\partial f(X)}{\partial p_i}\frac{\partial g(X)}{\partial q_i}\Big),$$

where $\partial/\partial q_i\,\partial/\partial p_i$ means scalar product of the gradients.

3. – Smooth states

A state ρ ([4]) is a sequence $\{\rho_\Lambda\}$ of probability measures indexed by the open cubes Λ of $\mathbb{R}^d$ and defined on $\mathcal{H}_\Lambda=\oplus_{i=0}^{\infty}(\mathbb{R}^d\times\Lambda)$ which have the following properties:

(a) on $(\mathbb{R}^d\times\Lambda)^i$ the measure ρ_Λ has the form

$$\rho_\Lambda(dx_1\dots dx_i)=\rho_\Lambda^{(i)}(x_1,\dots,x_i)\frac{dx_1\dots dx_i}{i!}, \tag{3.1}$$

where $\rho_\Lambda^{(i)}(x_1,\dots,x_i)$ is a symmetric measurable function.

(b) If $\Lambda'\supset\Lambda$

$$\rho_\Lambda^{(m)}(x_1,\dots,x_m)=\sum_{i=0}^{\infty}\int_{y_i\in\mathbb{R}^d\times(\Lambda'/\Lambda)}\rho_\Lambda^{(m+i)}(x_1,\dots,x_m,y_1,\dots,y_i)\frac{dy_1\dots dy_i}{i!} \tag{3.2}$$

$$(c)\qquad \rho_\Lambda^{(i)}(x_1,\dots,x_i)\le C_\Lambda^i\prod_{i=1}^{i}\eta_\Lambda(|p_i|)\qquad \text{if}\quad x_i=(p_i,q_i) \tag{3.3}$$

where C_Λ is a suitable constant and $\eta_\Lambda(|p|)\in L_1(\mathbb{R}^d)$.

(d) The bound (c) allows one to define

$$\rho_n(x_1,\dots,x_n)=\sum_{i=0}^{\infty}\int_{y_i\in\mathbb{R}^d\times\Lambda}\rho_\Lambda^{(m+i)}(x_1,\dots,x_m,y_1,\dots,y_i)\frac{dy_1\dots dy_i}{i!} \tag{3.4}$$

where Λ is an arbitrary region such that $x_i\in\mathbb{R}^d\times\Lambda,\ \forall\ i=1,2,\dots,n$.

The above functions are called the correlation functions of the state $\{\rho_\Lambda\}$.

(e) There are $\xi>0$, $\eta(|p|)\in L_1(\mathbb{R}^d)$ such that

$$\rho_n(x_1,\dots,x_n)\le\xi^n\prod_{i=1}^{n}\eta(|p_i|), \tag{3.5}$$

and $|p|\eta(|p|)\in L_1(\mathbb{R}^d)$.

A state ρ is smooth if

([4]) D. Ruelle, *Statistical Mechanics* (New York, N.Y., 1969), p. 170.

(f) The correlation functions are once continuously differentiable and

$$|\frac{\partial \rho_n}{\partial p_i}| \le C_n \, \xi^n \prod_{i=1}^{n} \eta(|p_i|), \tag{3.6}$$

$$|\frac{\partial \rho_n}{\partial q_i}| \le C_n \, \xi^n \prod_{i=1}^{n} \eta(|p_i|), \tag{3.7}$$

It can be shown that properties (a)-(e) allow one to define a probability measure ρ on the Borel sets of $\mathcal{H}$ thought of as a topological space with the topology that confuses configurations which differ only by the labeling and that makes all functions $f \in \mathcal{U}^0$ continuous ([5]).

Furthermore ([5]), $\mathcal{U} \subset L_1(\rho)$ and if $f(X) = \sum_{m=0}^{\infty} \sum_{i_1 < \ldots < i_m} f^{(m)}(x_{i_1}, \ldots, x_{i_m})$, then

$$\int_{\mathcal{H}} f d\rho = \sum_{m=0}^{\infty} \int_{\mathbb{R}^g \times \mathbb{R}^d} f^{(m)}(x_1, \ldots, x_m) \rho_m(x_1, \ldots, x_m) \frac{dx_1, \ldots, dx_m}{m!}$$

If a smooth state ρ is such that

$$\int p_1 \, \rho_n(p_1, q_1, \ldots p_n, q_n) \, dp_1 = 0, \qquad \forall n, \forall q_1, p_2, q_3, \ldots, p_n, q_n,$$

we say that ρ is "flowless".

4. – Formal Hamiltonians and Poisson brackets

If $\varphi \in C^{(2)}(\mathbb{R}^d)$ is an even rotation-invariant function on $\mathbb{R}^d$ with compact support, we define the following formal function on $\mathcal{H}$:

$$H(X) = \sum_{i=0}^{\infty} \frac{p_i^2}{2} + \sum_{i<j}^{0,\infty} \varphi(q_i - q_j). \tag{4.1}$$

If $A \in \mathcal{U}^{(1)}$ is an observable we can define

$$\{A, H\}(X) = \sum_{i=0}^{\infty} \Big(\frac{\partial A(X)}{\partial q_i} p_i - \frac{\partial A(X)}{\partial p_i} \big(\sum_{j \neq i} \frac{\partial \varphi(q_i - q_j)}{\partial q_i} \big) \Big).$$

It is easy to check that if $A \in \mathcal{U}^{(1)}$, $B \in \mathcal{U}^{(0)}$ then

$$\{A, H\} \in L_1(\rho) \quad \text{and} \quad B\{A, H\} \in L_1(\rho)$$

([5]) D. Ruelle, *Statistical Mechanics* (New York, N.Y. 1969); p. 171.

if ρ is a smooth state.

5. – The static KMS condition

Definition. Let ρ be a smooth state. We say that ρ is a static KMS *state with respect to the formal Hamiltonian (4.1), with parameter β if*

$$\rho(\{A,B\}) = \beta\,\rho(B\{A,H\}), \qquad \forall A,B\in\mathcal{U}^{(1)}. \tag{5.1}$$

The hope is that the above KMS condition is equivalent to the condition that the state ρ is a thermodynamic limit of a sequence of finite volume Gibbs stats with a suitable sequence of boundary conditions ([6])

Notice that for finite systems the KMS condition can be true for a Gibbs state only for special boundary conditions or, alternatively, the H appearing in (5.1) should be adapted to the particular boundary condition by addition of suitable "boundary terms" ([2]). If the system is infinite we can hope that (5.1) describes all Gibbs states without specification of the boundary conditions: the price that is paid for this nicer formulation is that, in general, (5.1) will have more than one solution (in correspondence with the different possible phases).

6. – KMS smooth states

Let ρ be a KMS smooth flowless state associated to the formal Hamiltonian (5.1). The following theorem holds:

Theorem 1. The correlation functions $\rho_n(p_1,q_1,\ldots,p_n,q_n)$ are of the form

$$\rho(x_1,\ldots,x_n) = \Big(\prod_{i=1}^n \frac{e^{-\beta p_i^2/2}}{\sqrt{2\pi\beta}^d}\Big)\,\widetilde\rho_n(q_1,\ldots,q_n) \tag{6.1}$$

where $x_i=(p_i,q_i)$; and, if $W_{q_1}(q_2,\ldots,q_n)=\sum_{i=2}^n\varphi(q_1-q_i)$,

$$\begin{aligned}\frac{\partial\widetilde\rho(q_1,\ldots,q_n)}{\partial q_1} &= -\beta\frac{\partial W_{q_1}(q_2,\ldots,q_n)}{\partial q_1}\widetilde\rho(q_1,\ldots,q_n)\\ &\quad-\beta\int_{\mathbb{R}^d}\frac{\partial\varphi(q_1-q')}{\partial q_1}\widetilde\rho(q_1,\ldots,q_n,q')\,dq'\end{aligned} \tag{6.2}$$

i.e. if ρ is a smooth KMS *state, it has a Maxwellian velocity and the position space distributions obey the stationary* BBGKY *hierarchy.*

The reader will have no trouble recognizing in (6.2) the stationary BBGKY hierarchy for a "Maxwellian" family of correlation functions ([7]).

([6]) O. Lanford and D. Ruelle: Comm. Math. Phys. **13**, 1921 (1969); R. L. Dobrushin: Funct. Anal. Appl. **2**, 302 (1968).

([7]) G. Gallavotti: *Nuovo Cimento*, **57** B, 208 (1968).

7. – KMS states and Gibbs states

The first to notice the equivalence of (6.2) with the Kirkwood-Salzburg (KS) equation was Morrey in his remarkable (and almost unknown) paper ([8]) under assumptions (say) of Euclidean invariance, low density and "strong" cluster properties.

We say that the smooth Maxwellian state ρ has strong cluster properties ([9]) if $\exists\, C > 0$, $\kappa > 0$ such that the functions

$$\begin{aligned} \widetilde{\rho}^T(q_1,q_2) =& \widetilde{\rho}(q_1,q_2) - \widetilde{\rho}(q_1)\widetilde{\rho}(q_2) \\ \widetilde{\rho}^T(q_1,q_2,q_3) =& \widetilde{\rho}(q_1,q_2,q_3) - \widetilde{\rho}(q_1,q_3)\widetilde{\rho}(q_2) - \widetilde{\rho}(q_1,q_2)\widetilde{\rho}(q_3) \\ & - \widetilde{\rho}(q_2,q_3)\widetilde{\rho}(q_1) + 2\widetilde{\rho}(q_1)\widetilde{\rho}(q_2)\widetilde{\rho}(q_3), \end{aligned} \tag{7.1}$$

etc., are such that

$$\widetilde{\rho}^T(q_1,q_2) \le C^n e^{-\kappa|q_1-q_n|} \tag{7.2}$$

A Maxwellian state is said to have a ξ–low density if it has the strong cluster property (7.2) with parameters C, κ and

$$\widetilde{\rho}(q_1,\ldots,q_n) < \xi^n, \qquad C, e^{-\kappa} \le \xi. \tag{7.3}$$

The meaning of "Euclidean invariant Maxwellian state" is self-explanatory. The following theorem holds:

Theorem 2. If an Euclidean invariant Maxwellian smooth state satisfies the stationary BBGKY *hierarchy (6.2) and if its density is ξ–low with ξ small enough then $\exists\, z = z(\rho) \le 2\xi$ such that*

$$\begin{aligned} \widetilde{\rho}(q_1,\ldots,q_n) =\ & z e^{-\beta W_{q_1}(q_2,\ldots,\rho_n)} \sum_{h=0}^{\infty} \int \frac{dy_1\ldots dy_h}{h!} \cdot \\ & \prod_{i=1}^{h} (e^{-\beta\varphi(q_1-y_i)} - 1)\widetilde{\rho}(q_2,\ldots,q_n,y_1,\ldots,y_h), \end{aligned} \tag{7.4}$$

and, viceversa, if z is small enough and φ is a stable potential, the Maxwellian state with position correlation functions satisfying (7.4) is a KMS *state (here $\widetilde{\rho}(\emptyset) = 1$).*

In other words ([10]), if ξ is small enough, the family of the correlation functions of an invariant flowless Maxwellian KMS state is uniquely determined by the density $\widetilde{\rho}(q)$ and defines a state which is the thermodynamic limit of finite volume Gibbs' states.

([8]) C.B. Morrey, Comm. Pure and Appl. Math., **8**, 279 (1955).
([9]) M. Duneau, D. Iagolnitzer and G. Soulliard: *Comm. Math. Phys.*, **35**, 307 (1974). Notice that the truncation used in formula (7.2) can be easily established for low density systems along the same lines.
([10]) D. Ruelle: *Statistical Mechanics* (New York, N.Y., 1969), p. 72, 93.

Proof. See ([8]), a self contained proof of the direct statement (essentially identical to the one in ([8])) is given in the Appendix: an independent proof of the converse statement can be found in ([7]).

8. – Conclusions

We have investigated some properties of the static KMS boundary condition: the discussion in this paper is outlined under some very strong assumptions. It would be interesting to see which are the minimal assumptions under which the above results can be obtained. There are several directions of research which would be of particular interest:

1) How the smoothness conditions on φ could be released. For instance how to take into account hard cores,

2) how the smoothness conditions on ρ could be released to obtain Theorem 2 and/or Theorem 1.

Another line of research is to study the dynamical KMS condition and to use it to imitate the stability theorem of ref. ([11]): under some strong assumptions of clustering and asymptotic Abelianess the analogous result of ([8]) has been proved ([12]).

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Appendix A.

Proof of Morrey's theorem

We sketch the essential steps:

1) Assume

a) $|\widetilde{\rho}_n(q_1, ..., q_n)| \le \xi^n$;

b) $\widetilde{\rho}_n$ are Euclidean invariant;

c) $\widetilde{\rho}_n$ are exponentially clustering, i.e.

$$\left|\widetilde{\rho}^T(q_1, ..., q_n)\right| \le (\xi C)^n exp[-\kappa\,|q_1 - q_n|],$$

where $C > 0$ and $\kappa > 0$.

2) Solve (6.2) using the Wronskian method

([11]) R. Haag, D. Kastler and E. Trych-Pohlmeyer: *Comm. Math. Phys*, **38**, 173 (1974).

([12]) M. Aizenman, G. Gallavotti, S. Goldstein and J. Lebowitz: *Comm. Math. Phys.*: **48**, 1 (1976).

$$\rho(q_1,...,q_n) = (e^{[-\beta(W_{q_1}(q_2,...,q_n) - W_{q_0}(q_2,...,q_n))]}\rho(q_0,q_2,...,q_n)) +$$
$$+ \int_{q_0}^{q_1} d\bar{q}_1 \int_{R^d} dy_1 \frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial\bar{q}_1}$$
$$\cdot\, e^{[-\beta(W_{q_1}(q_2,...,q_n) - W_{\bar{q}_1}(q_2,...,q_n))]}\rho(\bar{q}_1,q_2,...,q_n,y_1)$$

where $\int_{q_0}^{q_1} d\bar{q}_1$ symbolically denotes integration along a straight line $\overrightarrow{q_0 q_1}$ connecting q_0 with q_1 and $\partial/\partial\bar{q}_1$ denotes differentiation along $\overrightarrow{q_1 q_0}$; q_0 is arbitrary.

3) Notice that by symmetry

$$\int_{R^d} dy_1 \int_{q_0}^{q_1} \frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial\bar{q}_1}\rho(\bar{q}_1 y_1)d\bar{q}_1 \equiv 0.$$

4) Combining 3) and 2), and interchanging the integrations we obtain

$$\rho(q_1,...,q_n) = (e^{[-\beta(W_{q_1}(q_2,...,q_n) - W_{q_0}(q_2,...,q_n))]}\rho(q_0,q_2,...,q_n)) +$$
$$+ e^{[-\beta W_{q_1}(q_2,...,q_n)]}\int_{R^d} dy_1 \int_{q_0}^{q_1} d\bar{q}_1 \frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial\bar{q}_1}\cdot$$
$$\cdot\, (e^{[\beta W_{\bar{q}_1}(q_2,...,q_n)]}\rho(\bar{q}_1,q_2,...,q_n,y_1) - \rho(\bar{q}_1 y_1)\rho(q_2,...,q_n)).$$

5) Notice that the double integral in 4) is absolutely convergent, uniformly in q_0 by our assumed cluster property and by finiteness of the range of φ. Hence we can take the limit as $q_0 \to \infty$:

$$\rho(q_1,...,q_n) = \rho e^{[-\beta W_{q_1}(q_2,...,q_n)]}\,\rho(q_2,...,q_n) +$$
$$+ e^{[-\beta W_{q_1}(q_2,...,q_n)]}\int_{R^d} dy_1 \int_{-\infty}^{q_1} d\bar{q}_1 \frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial\bar{q}_1}\cdot$$
$$\cdot\, \big(e^{[\beta W_{\bar{q}_1}(q_2,...,q_n)]}\rho(\bar{q}_1,q_2,....,q_n,y_1) - \rho(q_2,...,q_n)\rho(\bar{q}_1,y_1)\big)$$

[Note added by GG: the symbol $\int_{-\infty}^{q_1}$ indicates that the point q_0 is sent to infinity on the half line connecting q_1 to $-\infty$ in the direction of the x-axis (say). The integrals $\int_{-\infty}^{q_1}$ here and in the following are intended performed along such half line.]

6) Put

$$\gamma = \int_{R^d} dy_1 \int_{-\infty}^{q_1} \rho(\bar{q}_1 y_1)\frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial\bar{q}_1}d\bar{q}_1,$$

and notice that by the assumed symmetry

$$\gamma = \int_{S(q_1)} dy_1 \int_{-\infty}^{q_1} \rho(\bar{q}_1 y_1)\frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial\bar{q}_1}d\bar{q}_1,$$

where $S(q_1)$ is the sphere with radius equal to the range of φ and centered in q_1.
[*Note added by GG: it is* $\gamma = -\beta \int_{S(q_1)} \frac{d^d y_1 d^d q'}{\omega_d |q'|^{d-1}} \rho(q', y_1) \partial_{q'} \varphi(q' - y_1)$*, where* ω_d *is the surface of the* $(d-1)$*-dimensional unit ball*].
Also

$$|\gamma| \le A\xi^2,$$

where A could be taken $3\int_{\mathbb{R}^d} |\varphi(y)|dy$ if φ were a monotonic function of $|q|$ and, more generally,

$$A < \left(\int |\varphi(y)|dy \right) \cdot 2 \cdot \left(\left(\text{number of times } \frac{\partial \varphi}{\partial |q|} \text{ changes sign} \right) + 1 \right);$$

for more complicated interactions A could be obviously bounded in terms of the integral of $|\partial_q \varphi|$ and the range of the potential φ.

7) If $z = \rho - \gamma, |z| \le \xi + A\xi^2$, we find

$$\begin{aligned}\rho(q_1, ..., q_n) &= z e^{[-\beta W_{q_1}(q_2,\ldots,q_n)]} \rho(q_2, ..., q_n) + e^{[-\beta W_{q_1}(q_2,\ldots,q_n)]} \cdot \\ &\cdot \int_{R^d} dy_1 \int_{-\infty}^{q_1} d\overline{q}_1 \rho(\overline{q}_1 q_2, ..., q_n, y_1) e^{[\beta W_{\overline{q}_1}(q_2,\ldots,q_n)]} \frac{\partial(-\beta\varphi(\overline{q}_1 - y_1))}{\partial \overline{q}_1},\end{aligned}$$

where the integrations are no longer interchangeable. [*Note added by GG: unless use is made of the cancellation in 6) which implies that the points in the integrals have to be in a ball around* q_1 *of radius* $2(N+1)$ *times the radius of the potential: as done in step 8).*]

8) Iterating 7) N times we find

$$\begin{aligned}&\rho(q_1, ..., q_n) = z\, e^{[-\beta W_{q_1}(q_2,\ldots,q_n)]} \sum_{h=0}^{N} \int_{(R^d)^h} \frac{dy_1 ... dy_h}{h!} \\ &\cdot \prod_{i=1}^{h} (e^{[-\beta\varphi(q_1 - y_i)]} - 1) \rho(q_2, ..., q_n, y_1, ..., y_h) + \\ &+ e^{[-\beta W_{q_1}(q_2,\ldots,q_n)]} \int_{R^d} dy_1 \int_{-\infty}^{q_1} d\overline{q}_1 \int_{R^d} dy_2 \int_{-\infty}^{\overline{q}_1} d\overline{q}_2 ... \int_{R^d} dy_{N+1} \int_{-\infty}^{\overline{q}_N} d\overline{q}_{N+1} \cdot \\ &\cdot \prod_{j=1}^{N+!} \left\{ \frac{\partial}{\partial \overline{q}_j} (e^{[-\beta\varphi(\overline{q}_j - y_j)]} - 1) \right\} \cdot \\ &\cdot e^{[\beta W_{\overline{q}_{N+1}}(q_2,\ldots,q_n,y_1,\ldots,y_{N+1})]} \rho(\overline{q}_{N+1}, q_2, ..., q_n, y_1, ..., y_{N+1}),\end{aligned}$$

and the above integrations cannot be interchanged.

9) The last integral can be bounded in a similar way as in 6), using the cluster property, by

$$\widetilde{A}^N \xi^N,$$

where $\widetilde{A}$ is a suitable number depending on $\beta, C, \kappa, \max|\varphi|$, but not on ξ. So if ξ is small enough, the theorem follows by taking $N \to \infty$.

Appendix B.

Proof of Theorem 1

The calculation is lengthy: therefore we introduce shorthand notations. An infinite configuration will be X; if h, g are two observables, we shall write

$$g(X) = \sum_{S \subset X} \gamma(S), \qquad h(X) = \sum_{S \subset X} \eta(S),$$

where the sums run over the finite subconfigurations of X. Simple algebra leads to

$$\begin{aligned} h(X)g(X) &= \sum_{S \subset X} \Psi_{h,g}(S) \\ \{h,g\}(X) &= \sum_{S \subset X} \Phi_{h,g}(S) \end{aligned}$$

where

$$\begin{aligned} \Psi_{h,g}(S) &= \sum_{R \subset S} \sum_{\substack{V,W \subset S/R \\ V \cap W = \emptyset \\ V \cup W = S/R}} \eta(R \cup V)\gamma(R \cup W), \\ \Phi_{h,g}(S) &= \sum_{R \subset S} \sum_{\substack{V,W \subset S/R \\ V \cap W = \emptyset \\ R \cup V \cup W = S}} \{\eta(R \cup V), \gamma(R \cup W)\} \end{aligned}$$

We abbreviate $R \cup S$ in RS. Put

$$\int \cdot \, dX = \sum_{n=0}^{\infty} \cdot \frac{dx_1 \ldots dx_n}{n!}.$$

The following well known combinatorial identity will be of great help:

$$\int G(X)\big(\sum_{T \subset X} F(T)\big) \, dX \; = \int dT_1 \, dT_2 \, G(T_1 T_2) F(T_1).$$

Then

$$\int hg \, d\rho = \int \rho(VWR)\eta(RV)\gamma(RW) dRdVdW, \tag{B.1}$$

$$\int \{h,g\} \, d\rho = \int \rho(VWR)\{\eta(RV), \gamma(RW)\} dRdVdW, \tag{B.2}$$

If $H(X) = \sum_i p_i^2/2 + \sum_{i<j} \varphi(q_i - q_j)$ is a formal Hamiltonian, $H(X) = T(X) + V(X)$, we see using (B.1),(B.2) that

$$\int g\,\{h, T\}\,d\rho = \int \gamma(RV)\Big(\sum_{q_j \in RW} \frac{\partial \eta(RW)}{\partial \mathbf{q}_j} \cdot \mathbf{p}_j\Big)\,\rho(RVW)\,dR\,dV\,dW.$$

When the sum runs over the positional coordinates of RW and p_j is the velocity corresponding to q_j, $\frac{\partial}{\partial \mathbf{q}_j} \cdot \mathbf{p}_j$ means scalar product of $\mathbf{p}_j$ with the gradient $\frac{\partial}{\partial \mathbf{q}_j}$.

Also, if $W_q(q'_1, \ldots, q'_n)$ is also written $W_q(q'_1, p'_1, \ldots, q'_n, p'_n)$

$$\begin{aligned}\int g\,\{h, V\} d\rho = &\int \gamma(RV)\Big[\sum_{q_\tau \in RW}\Big(-\frac{\partial \eta(RW)}{\partial \mathbf{p}_\tau}\frac{\partial W_{q_\tau}(RW)}{\partial \mathbf{q}_\tau}\Big)\Big]\rho(RVW) dR dV dW\\ + &\int \gamma(RV)\Big(\sum_{\substack{\mathbf{q}_\tau \in RW\\ \mathbf{q}_\theta \in RW/(\mathbf{q}_\tau, \mathbf{p}_\tau)}} -\frac{\partial \eta(RW/q_\theta p_\theta)}{\partial \mathbf{p}_\tau}\frac{\partial \varphi(q_\tau - q_\theta)}{\partial \mathbf{q}_\tau}\Big)\rho(RVW) dR dV dW\end{aligned}$$

with the natural meaning of the symbols.

So the condition $\rho(\{h, g\}) = \beta\,\rho(g\{h, H\})$ becomes

$$\begin{aligned}&\int \rho(VWR)\,\{\eta(RW), \gamma(RV)\}\,dRdVdW =\\ &-\beta \int \gamma(RV)\Big(\sum_{q_\tau \in RW} \frac{\partial \eta(RW)}{\partial \mathbf{q}_\tau} \cdot \mathbf{p}_\tau\Big)\rho(VWR)\,dRdVdW +\\ &+\beta \int \Big(\sum_{q_\tau \in RW} -\frac{\partial \eta(RW)}{\partial \mathbf{p}_\tau} \cdot \frac{\partial W_{q_\tau}(RW)}{\partial \mathbf{q}_\tau}\Big)\rho(VWR)\,dRdVdW +\\ &+\beta \int \Big(\sum_{\substack{q_\tau \in RW\\ q_\theta \in RW/(q_\tau, p_\tau)}} -\frac{\partial \eta(RW/q_\theta p_\theta)}{\partial \mathbf{p}_\tau} \cdot \frac{\partial \varphi(q_\tau - q_\theta)}{\partial \mathbf{q}_\tau}\Big)\rho(VWR)\,dRdVdW\end{aligned} \tag{B.3}$$

Choose η to be momentum independent; the arbitrariness of γ then implies

$$0 = \int \sum_{R \subset T}\Big(\sum_{q \in R}\Big(-\frac{\partial \rho(TW)}{\partial \mathbf{p}} \cdot \frac{\partial \eta(RW)}{\partial \mathbf{q}}\Big) - \beta \sum_{q \in RW} \frac{\partial \eta(RW)}{\partial \mathbf{q}} \cdot \mathbf{p}\,\rho(TW)\Big)dW.$$

Choose $\eta^{(m)} \equiv 0$ for $m \neq 1$; then $W = \emptyset$ is the only term that contributes to the integration (because ρ is flowless) and the above equation becomes

$$\sum_{q_r \in T}\Big(-\frac{\partial \rho(T)}{\partial \mathbf{p}_r} \cdot \frac{\partial \eta^{(1)}(q_r)}{\partial \mathbf{q}_r} - \beta\,\rho(T)\,\mathbf{p}_r \cdot \frac{\partial \eta^{(1)}(q_r)}{\partial \mathbf{q}_r}\Big) = 0$$

and the arbitrariness of $\eta^{(1)}$ implies

$$-\frac{\partial\rho(p_1q_1,\ldots,p_t,q_t)}{\partial\mathbf{p}_i}-\beta\,\mathbf{p}_i\,\rho(p_1q_1,\ldots,p_tq_t)=0,\qquad\forall\, i=1,\ldots t,$$

or

$$\rho(p_1q_1,\ldots,p_t,q_t)=\prod_{i=1}^{t}\Big(\frac{e^{-\beta p_i^2/2}}{\sqrt{2\pi/\beta}}\Big)\,\widetilde{\rho}(q_1,\ldots,q_t). \tag{B.4}$$

Choose next γ to be momentum independent with support in Λ and $\eta^{(m)}\equiv 0$ except when $m=1$; choose $\eta^{(1)}(pq)=\eta^{(1)}(p)\chi_{\Lambda+\varepsilon}(q)$, where $\chi_{\Lambda+\varepsilon}(q)$ is a C^s–function, positive and ≤ 1 such that $\chi_{\Lambda+\varepsilon}(q)=1$ if $q\in\Lambda$, $\chi_{\Lambda+\varepsilon}(q)\equiv 0$ if $q\notin\Lambda$ and (distance of q from $\partial\Lambda)>\varepsilon$.

We insert the above choices of η and γ in (B.3) together with the relation (B.4); then we integrate by parts to free the η's and γ's from derivatives. If $G(p)=\frac{e^{-\beta p^2/2}}{\sqrt{2\pi/\beta}}$ and T,R,V,W *etc.* denote now only positional configurations, we obtain the following expression (for $T\subset\Lambda$):

$$\begin{aligned}
&-\sum_{t\in T}\int \mathbf{p}_t\cdot\frac{\partial\widetilde{\rho}(T)}{\partial\mathbf{q}_t}\,\eta^{(1)}(p_t)\chi_{\Lambda+\varepsilon}(q_t)G(p_t)dp_t=\\
&=+\beta\sum_{t\in T}\int \mathbf{p}_t\cdot\frac{\partial\varphi(q_t-q)}{\partial\mathbf{q}_t}\,\widetilde{\rho}(Tq)\eta^{(1)}(\mathbf{p}_t)\chi_{\Lambda+\varepsilon}(q_t)G(p_t)dq_tdp_t+\\
&+\beta\sum_{t\in T}\int \mathbf{p}_t\cdot\frac{\partial W_{q_t}(T)}{\partial\mathbf{q}_t}\widetilde{\rho}(T)\eta^{(1)}(p_t)\chi_{\Lambda+\varepsilon}(q_t)G(p_t)dq_tdp_t,
\end{aligned}$$

or, because of the arbitrariness of η,

$$\begin{aligned}
\frac{\partial}{\partial\mathbf{q}_1}\widetilde{\rho}(q_1,\ldots,q_n)=&-\beta\widetilde{\rho}(q_1,\ldots,q_n)\frac{\partial W_{q_1}(q_2,\ldots,q_n)}{\partial\mathbf{q}_1}\\
&-\beta\int\widetilde{\rho}(q_1,\ldots,q_n,q)\frac{\partial\varphi(q_1-q)}{\partial\mathbf{q}_1}dq.
\end{aligned}\tag{B.5}$$

It is easy to see that this equation together with (B.4) implies $\rho(\{h,g\})=\beta\,\rho(\eta\{g,H\})$ under only the assumptions of C^1–smoothness and uniform boundedness of $\widetilde{\rho}(q_1,\ldots,q_n)$ of the form $|\widetilde{\rho}(q_1,\ldots,q_n)|\le\xi^n$ for some $\xi>0$.

• RIASSUNTO

Si discutono alcune proprietà della condizione KMS classica e si trovano alcune condizioni sufficienti per la sua equivalenza alle equazioni di Kirkwood-Salzburg.