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A uniqueness result for quasi-free KMS states*

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Abstract. We introduce the concept of 'KMS one-particle structure', in terms of which the construction of a class of thermal states for linear Bose systems may be reduced to second quantization. For such structures, we prove a uniqueness result which strengthens earlier work of Rocca, Sirugue and Testard. We elucidate these structures further by introducing a certain doubling procedure. The results here together with those in a companion paper on the purification of KMS states are preparatory for a third paper about constructing linear quantum fields on black holes.

§1. Introduction

This paper settles some mathematical questions concerning thermal equilibrium (i.e. KMS [1–4]) states on linear (i.e. 'quasi-free') Bose systems. While such matters were much studied in the early '70's ([5–7], see also the early paper [8]), it seems that some important things were left unsaid and the purpose of the present work is to fill some of the gaps.

Our discussion centres around the concept, which we introduce, of 'KMS one-particle structure' in terms of which the construction of a class of KMS states for a large family of linear Bose systems may essentially be reduced to second quantization. Our main result is a uniqueness result for these structures. This strengthens (at the technical level) a part of some earlier work of Rocca, Sirugue and Testard [7]). Finally, we explain how the structure of our quasi-free KMS states is more fully revealed by a certain doubling procedure. This doubling procedure will be discussed further in a more general context in a companion paper [9]. Essential use will be made of both these papers in a third paper [10] which concerns some aspects of quantum field theory in curved space-time related to the Hawking effect, and which constituted the immediate motivation for the present work.

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§2. Preliminaries

In this section, we establish our notation and also recall some basic facts about the quantization of linear systems, emphasizing the structure of the ground state representation. We also review some basic facts about the second quantization process.

§2.1

A general linear dynamical system $(D, \sigma, \mathcal{T}(t))$ consists of a linear phase-space D equipped with a linear symplectic form σ – together with a one-parameter group $\mathcal{T}(t)$ of linear symplectic transformations on (D, σ) describing time evolution:

$$\sigma(\mathcal{T}(t)\Phi_1, \mathcal{T}(t)\Phi_2) = \sigma(\Phi_1, \Phi_2) \quad \forall \Phi_1, \Phi_2 \in D \tag{2.1}$$

In the algebraic approach to quantum field theory on such linear systems (see e.g. [11]), one constructs the Weyl algebra $\mathcal{W}$ over (D, σ) generated by Weyl operators $W(\Phi)$ satisfying

$$W(\Phi_1) W(\Phi_2) = \exp(-i\sigma(\Phi_1, \Phi_2)/2) W(\Phi_1 + \Phi_2) \tag{2.2}$$

(for further details, which we shall not however require here, see e.g. [12]) and describes the quantum time-evolution by an automorphism group $\alpha(t)$ fixed by

$$\alpha(t) W(\Phi) = W(\mathcal{T}(t)\Phi) \tag{2.3}$$

Recall that to define a state on the Weyl algebra, it suffices to specify its expectation values on the $W(\Phi)$'s.

§2.2.

We now discuss the construction of a ground state for such systems:

In the case that D were given as a complex Hilbert space $\mathcal{H}$, $\sigma(\cdot, \cdot)$ arose as $2\,\mathrm{Im}\,\langle \cdot \mid \cdot \rangle$, and $\mathcal{T}(t)$ arose as e^{-ith} for some *strictly positive*[1]) one-particle Hamiltonian h, a ground state would be defined by

$$\omega_0(W(\Phi)) = \exp(-\tfrac{1}{2} \|\Phi\|^2_{\mathcal{H}}) \tag{2.4}$$

and the corresponding ground state representation by the Fock representation. (see §2.3 below). One may extend this procedure to systems which admit a 'ground one-particle structure' $(K, \mathcal{H}, e^{-ith})$.

Definition 1a. A ground one-particle structure $(K, \mathcal{H}, e^{-ith})$ over $(D, \sigma, \mathcal{T}(t))$ consists of a complex Hilbert space $\mathcal{H}$, a map $K: D \to \mathcal{H}$ and a strongly continuous unitary group e^{-ith} on $\mathcal{H}$ s.t.

(i) K is real-linear and symplectic, i.e. satisfies

$$2\,\mathrm{Im}\,\langle K\Phi_1 \mid K\Phi_2 \rangle = \sigma(\Phi_1, \Phi_2)$$

(ii) KD is dense in $\mathcal{H}$

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[1]) i.e. positive, self-adjoint and with no zero eigenvalue.

(iii) $K\mathcal{T}(t) = e^{-ith} K$ where h is strictly positive.

One then obtains a ground state[2]) via:

$$\omega_0(W(\Phi)) = \exp\left(-\tfrac{1}{2}\|K\Phi\|^2_{\mathcal{H}}\right) \tag{2.5}$$

(corresponding to the representation $W(\Phi) \mapsto W^{\mathcal{F}}(K\Phi)$ – see §2.3 below). Moreover, it is known that when such a ground one-particle structure exists, it is unique up to unitary equivalence in the following sense ([14], re-proved here in §4).

Theorem 1a. *Given two ground one-particle structures* $(K_i, \mathcal{H}_i, \exp(-ith_i))$ $i = 1, 2$, *over a given linear dynamical system* $(D, \mathcal{T}(t))$, *then there exists a unique unitary* $U: \mathcal{H}_1 \to \mathcal{H}_2$ s.t.
(i) $UK_1 = K_2$ *on* D
(ii) $U \exp(-ith_1) = \exp(-ith_2)\, U$ *on* $\mathcal{H}_1$.

As we shall explain in the next chapter, one of our main aims here will be to prove an analogue theorem to Theorem 1a (Theorem 1b of §3) for the concept (which we shall introduce) of *KMS one-particle structure.*

§2.3. *Second quantization*

We briefly recall for completeness some basic facts about the Fock representation $W(x) \mapsto W^{\mathcal{F}}(x)$ (In the discussion above, $x = K\Phi$) of the Weyl algebra over $(\mathcal{H}, 2\,\mathrm{Im}\langle\cdot \mid \cdot\rangle)$ for some one-particle Hilbert space $\mathcal{H}$. (i.e. about Segal's 'abstract free Bose field' [15, 16]) The representation space $\mathcal{F}(\mathcal{H})$ may be realized as $\mathbb{C} \oplus \mathcal{H} \oplus (\mathcal{H} \otimes_s \mathcal{H}) \oplus \cdots$ $W(x) = \exp\overline{[a^+(x) - a^+(x)^*]}$ with $a^+(x)$, $x \in \mathcal{H}$ the usual creation operators satisfying $[a^+(x)^*, a^+(x)] = \langle x \mid y\rangle$, $a^+(x)^*\Omega = 0$, etc. Here Ω is the cyclic vector $\mathbb{1} \oplus 0 \oplus 0 \oplus \cdots$ and we have

$$\langle \Omega \mid W^{\mathcal{F}}(x)\Omega\rangle = \exp\left(-\tfrac{1}{2}\|x\|^2_{\mathcal{H}}\right)$$

justifying the remarks after equations (2.4) (2.5) above. Corresponding to $\mathcal{T}(t)$ and e^{-ith} in the discussion above, the second quantized time-evolution is given by $\Gamma(e^{-ith})$ where for an arbitrary operator A on $\mathcal{H}$, $\Gamma(A)$ on $\mathcal{F}(\mathcal{H})$ is $\mathbb{1} \oplus A \oplus (A \otimes A) \oplus \cdots$. We have

$$W^{\mathcal{F}}(e^{-ith}x) = \Gamma(e^{-ith})\, W^{\mathcal{F}}(x)\, \Gamma(e^{-ith})^{-1}$$

(and such a formula holds more generally for unitary or anti-unitary operators U on $\mathcal{H}$). We may also write $\Gamma(e^{-ith}) = \exp(-it\, d\Gamma(h))$ and $d\Gamma(h)$ is then the second quantized Hamiltonian. More properties of the Fock representation will be taken up in [9].

§3. KMS one-particle structures

Our main aim is to give an account of the structure of Gibbs states on linear systems in the same spirit as the account we gave in §2.2 for the structure of

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[2]) not necessarily unique because of the possibility of replacing ω_0 by ω_0' with $\omega_0'(W(\Phi)) = \omega_0(W(\Phi))e^{i\chi(\Phi)}$ where χ is a linear functional on D satisfying

$\chi(\mathcal{T}(t)\Phi) = \chi(\Phi)$ (see [13]) ground states. We shall also make precise the relationship between these two types of state.

§3.1

As our starting point, we take the standard heuristic expression (in the notation of §2) for a Gibbs state with inverse temperature $\beta = (kT)^{-1}$:

$$\omega_\beta(W(\Phi)) = Z^{-1} \operatorname{tr}(e^{-\beta H} W(\Phi)) \tag{3.1}$$

Here $Z = \operatorname{tr} e^{-\beta H}$, and, if we assume a ground one-particle structure exists, we may set $H = d\Gamma(h)$ and $W(\Phi) = W^{\mathcal{F}}(K\Phi)$. As is well-known, we cannot expect to give this expression any rigorous mathematical sense as a trace in the vacuum sector. Nevertheless, one can argue convincingly for it being assigned the value (see §A1)

$$\omega_\beta(W(\Phi)) = \exp\left[-\tfrac{1}{2}\left\langle K\Phi \,\middle|\, \coth\left(\frac{\beta h}{2}\right) K\Phi\right\rangle_{\mathcal{H}}\right] \tag{3.2}$$

If we now assume that a ground one-particle structure exists satisfying the 'regularity condition' $KD \subset \mathcal{D}(h^{-1/2})$, then the formula (3.2) makes good mathematical sense, with $\coth(\beta h/2)$ interpreted in the sense of quadratic forms [17] (see §A2 for details) and defines a well-defined state on the Weyl algebra. (One may also easily check that it satisfied the KMS condition [1–4].) The question arises as to what extent ω_β is unique.[3]) As in the case of the ground state ω_0, we shall establish a uniqueness result at the one-particle level, and our first task is to isolate a suitable version of the one-particle structure concept in the case of finite temperature. To motivate our definition, let us continue to assume the condition $KD \subset \mathcal{D}(h^{-1/2})$ and let us also assume the existence of a preferred complex conjugation C on $\mathcal{H}$ satisfying

$$Ce^{-ith} = e^{ith}C \tag{3.3}$$

Then, observe that the ω_β of (3.2) may be written as

$$\omega_\beta(W(\Phi)) = \exp(-\tfrac{1}{2}\|K^\beta\Phi\|^2_{\tilde{\mathcal{H}}}) \tag{3.4}$$

where we define $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H}$ and K^β by

$$K^\beta : D \to \mathcal{H} \oplus \mathcal{H}$$
$$\Phi \mapsto C sh Z^\beta K\Phi \oplus ch Z^\beta K\Phi$$

where Z^β is defined implicitly through

$$\tanh Z^\beta = \exp(-\beta h/2) \tag{3.5}$$

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[3]) It is clearly not always unique amongst the set of all KMS states with the same β because of the possibility (related to Bose condensation) of replacing ω_β by ω'_β with $\omega'_\beta(W(\Phi)) = \omega_\beta(W(\Phi))e^{i\chi(\Phi)}$ where χ is a linear functional on D satisfying $\chi(\mathcal{T}(t)\Phi) = \chi(\Phi)$ (cf. footnote 2). See also [7].

The formula (3.4) generalizes a construction used by Araki and Woods [8] in their treatment of the non-relativistic free Bose gas (cf. their case of 'No macroscopic occupation of the ground state'). Now, define $\exp(-it\tilde{h})$ on $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H}$ to be

$$\begin{pmatrix} \exp(ith) & 0 \\ 0 & \exp(-ith) \end{pmatrix}$$

We shall call the triple $(K^\beta, \tilde{\mathcal{H}}, \exp(-it\tilde{h}))$ the *standard KMS one-particle structure over* $(D, \sigma, \mathcal{T}(t))$ (with inverse temperature β). We now isolate what we claim are the essential features (see §A2) in the following definition.

Definition 1b. A KMS one-particle structure $(K^\beta, \tilde{\mathcal{H}}, \exp(-it\tilde{h}))$ over a linear dynamical system $(D, \sigma, \mathcal{T}(t))$ consists of a complex Hilbert space $\tilde{\mathcal{H}}$, a map $K^\beta : D \to \tilde{H}$ and a strongly continuous unitary group $\exp(-it\tilde{h})$ on $\tilde{\mathcal{H}}$ s.t.

(i) K^β is real-linear and symplectic – i.e. $2 \operatorname{Im} \langle K^\beta \Phi_1 \mid K^\beta \Phi_2 \rangle = \sigma(\Phi_1, \Phi_2)$

(ii) $K^\beta D + iK^\beta D$ is dense in $\tilde{\mathcal{H}}$

(iii) (a) $K^\beta \mathcal{T}(t) = \exp(-it\tilde{h}) K^\beta$ on D

(b) $\tilde{h}$ has no zero eigenvalues

(c) $\exp(-it\tilde{h})$ satisfies the 'one-particle KMS condition' namely $\forall x, y \in K^\beta D, \forall t \in \mathbb{R}$:

$$\langle \exp(-it\tilde{h})x \mid y \rangle_{\tilde{\mathcal{H}}} = \langle \exp(-\beta\tilde{h}/2)y \mid \exp(-it\tilde{h}) \exp(-\beta\tilde{h}/2)x \rangle_{\tilde{\mathcal{H}}}$$

Note that the concept of KMS one-particle structure differs essentially from that of ground one-particle structure in that the Hilbert space $\tilde{\mathcal{H}}$ is 'twice as big' as $\mathcal{H}$. This is reflected both in condition (ii) where – in the KMS case – $K^\beta D + iK^\beta D$ is dense, while in the ground case, KD alone is dense, and in condition (iii) where, in the KMS case, $\tilde{h}$ has symmetric spectrum, in contrast to the positive spectrum of the ground case. We shall return to this point in §4. At the second quantized level, it is of course related to the fact that GNS representations of KMS states are only cyclic, while those of ground states are (often) irreducible (see [9]).

That this is a suitable definition is justified by the uniqueness theorem (which we prove in §4):

Theorem 1b. *Given two KMS one particle structures* $(K_i^\beta, \tilde{\mathcal{H}}_i, \exp(-it\tilde{h}_i))$ $i = 1, 2$ *(for the same* β*) for some given linear dynamical system, then there exists a unique unitary* $U : \tilde{\mathcal{H}}_1 \to \tilde{\mathcal{H}}_2$ *s.t.*

(i) $UK_1^\beta = K_2^\beta$ *on* D

(ii) $U \exp(-it\tilde{h}_1) = \exp(-it\tilde{h}_2) U$ *on* $\tilde{\mathcal{H}}_1$

Theorem 1b corresponds to a result which is already known for quasi-free Fermion fields (where in fact there is the stronger result of uniqueness of KMS states – see Rocca, Sirugue and Testard [18] and Araki [19]). For Bosons, a similar result to ours may be extracted from the work of Rocca, Sirugue and Testard [7] who essentially prove uniqueness of KMS states over linear systems up to the freedom mentioned in footnote 3. (See also Araki and Shiraishi [5] and Araki [6] which are closely related although they do not appear to consider the uniqueness question.) However, rather strong technical conditions are required in

[7] and our approach appears capable of settling uniqueness problems which arise in applications (such as [10]), which cannot be settled with the methods and results of [7].[4])

§4. Uniqueness of ground and KMS one-particle structures

The aim of this section is to prove Theorem 1b. Since it appears to require almost no extra space, we begin by recalling the proof of Theorem 1a ([14], see also [13]) in a form suitable for generalization.

Proof of Theorem 1a. Consider the map $T = K_2 \circ K_1^{-1}$ between the (dense) subspaces K_1D and K_2D in $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. Since K_1 and K_2 are each symplectic, we have

$$\operatorname{Im}\langle Tx \mid Ty\rangle_{\mathcal{H}_2} = \operatorname{Im}\langle x \mid y\rangle_{\mathcal{H}_1} \quad \forall x, y \in K_1D \tag{4.1}$$

Now, for fixed $x, y \in K_1D$, consider the function

$$f_{x,y} : t \mapsto \langle \exp(-ith_2)Tx \mid Ty\rangle_{\mathcal{H}_2} - \langle \exp(-ith_1)x \mid y\rangle_{\mathcal{H}_1}$$

Since h_1, h_2 are positive, this extends by a standard argument (see e.g. [2]) to a function of complex t which is bounded and continuous in the region $\operatorname{Im} t \leqslant 0$ and holomorphic in $\operatorname{Im} t < 0$. Furthermore, for t real, we calculate

$$\begin{aligned}\operatorname{Im} f_{x,y}(t) &= \operatorname{Im}[\langle TK_1\mathcal{T}(t)K_1^{-1}x \mid Ty\rangle_{\mathcal{H}_2} - \langle K_1\mathcal{T}(t)K_1^{-1}x \mid y\rangle_{\mathcal{H}_1}] \\ &= 0 \text{ (by (4.1) above)}\end{aligned}$$

Hence, by the Schwarz reflection principle, $f_{x,y}(t)$ extends to a bounded holomorphic function in the entire complex plane and it thus has a constant value by Liouville's theorem. Finally, the fact that h_1, h_2 have no zero eigenvalues guarantees that this constant value is zero. A proof of this which will generalize to the KMS case is to look at $\lim_{t\to\infty} 1/t \int_0^t \langle \exp(-it'h_1)x \mid y\rangle \, dt'$ (and similarly for h_2) for real t, and notice that by von-Neumann's ergodic theorem [17] this tends to zero. In particular we get for $t = 0$

$$\langle Tx \mid Ty\rangle_{\mathcal{H}_2} = \langle x \mid y\rangle_{\mathcal{H}_1} \quad \forall x, y \in K_1D$$

It results by the following lemma that T extends to a unique unitary U.

Lemma 5.1. *Given two complex Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$ with real-linear subspaces M_1, M_2 s.t. $M_1 + iM_1$ is dense in $\mathcal{H}_1$, $M_2 + iM_2$ is dense in $\mathcal{H}_2$ and given a (one-one) onto real-linear map $T : M_1 \to M_2$ s.t. $\langle Tx \mid Ty\rangle_{\mathcal{H}_2} = \langle x \mid y\rangle_{\mathcal{H}_1}$ $\forall x, y \in M_1$. Then T extends to a unique unitary.*

Proof. Define U on the dense complex-linear set $M_1 + iM_1$ by $U(x + iy) = Tx + iTy$. With this definition, U is complex-linear. We must still check it is

[4]) One difficulty with [7] is its assumption 'E3'. For the problem in [10], it is difficult to check this assumption and in fact it is presumably false. (The connection between the present paper and [7] may be made only in a restricted class of cases for which the exponent $\langle K\Phi \mid \coth(\beta h/2)K\Phi\rangle$ in expressions such as (3.2) may be written as $\sigma(\Phi, X\Phi)$ for some X (in the notation of [7], $X^{-1} = D^{\beta}$) which maps $D \to D$. This appears for example to be untrue in our application in [10].

well-defined. We clearly need to show $Tx + iTy = 0 \Rightarrow x = y = 0$. This follows since $\|T(x+iy)\|^2 = \|(x+iy)\|^2$. In fact: Given x_a, y_a, x_b, $y_b \in M_1$, we have

$$\begin{aligned}\langle Tx_a + iTy_a \mid Tx_b + iTy_b\rangle &= \langle Tx_a \mid Tx_b\rangle + \langle iTy_a \mid Tx_b\rangle \\ &\quad + \langle Tx_a \mid iTy_b\rangle + \langle iTy_a \mid iTy_b\rangle \\ &= \langle x_a \mid x_b\rangle - i\langle y_a \mid x_b\rangle + i\langle x_a \mid y_b\rangle + \langle y_a \mid y_b\rangle \\ &= \langle x_a + iy_a \mid x_b + iy_b\rangle\end{aligned}$$

which also shows U is inner-product preserving. Finally, since it has dense range, it must extend to a unitary. For uniqueness note that any U' which extends T must have $\forall x,\ y \in M_1$,

$$U'(x+iy) = U'x + iU'y = Tx + iTy$$

and so coincides with U on a dense set. $\square$

Note that this lemma does not require KD to be dense and that we have nowhere used this assumption in the proof of Theorem 1a. The above proof is thus easily adaptable to the proof of Theorem 1b. (See definitions and statements in §2.)

Proof of Theorem 1b. We proceed exactly as in Theorem 1a, defining $T = \tilde{K}_2 \circ \tilde{K}_1^{-1}$ (we drop the superscript β) between K_1D and K_2D in $\tilde{\mathscr{H}}_1$ and $\tilde{H}_2$ (of course K_iD are not assumed dense now). Again we have

$$\operatorname{Im} \langle Tx \mid Ty\rangle_{\tilde{\mathscr{H}}_2} = \operatorname{Im} \langle x \mid y\rangle_{\mathscr{H}_2} \quad \forall x,\ y \in K_1D$$

As before, define a function

$$f_{x,y} : t \mapsto \langle \exp(-it\tilde{h}_2)Tx \mid Ty\rangle_{\tilde{\mathscr{H}}_2} - \langle \exp(-it\tilde{h}_1)x \mid y\rangle_{\tilde{\mathscr{H}}_1}$$

Now, by the one-particle KMS condition, $f_{x,y}(t)$ extends by a standard argument (see e.g. [2]) to a function of complex t which is bounded and continuous on the strip $-i\beta \leq \operatorname{Im} t \leq 0$ and holomorphic in $-i\beta < \operatorname{Im} t < 0$. Furthermore,

$$\begin{aligned}f_{x,y}(t - i\beta) &= \langle Ty \mid \exp(-it\tilde{h}_2)Tx\rangle_{\tilde{\mathscr{H}}_2} - \langle y \mid \exp(-it\tilde{h}_1)x\rangle_{\tilde{\mathscr{H}}_1} \\ &= \overline{f_{x,y}(t)}.\end{aligned}$$

Again, for t real, we find $\operatorname{Im} f_{x,y}(t) = 0$ so that we actually have $f_{x,y}(t - i\beta) = f_{x,y}(t)$ and also by the Schwarz reflection principle, we can extend $f_{x,y}$ to the region $-i\beta \leq \operatorname{Im} t \leq i\beta$ (bounded, continuous in the full region and analytic in the interior). It will also clearly satisfy $f_{x,y}(t + i\beta) = f_{x,y}(t) = f_{x,y}(t - i\beta)$ and have zero imaginary part on $\operatorname{Im} t = \pm i\beta$. We can thus extend it again etc. getting finally a bounded holomorphic function (periodic in $i\beta$) in the entire complex plane. Again, by Liouville's theorem, this will be a constant function, and again, since $\tilde{h}_1$, $\tilde{h}_2$ have no zero eigenvalues we conclude by von-Neumann's ergodic theorem that $f_{x,y}(t) = 0$. Taking $t = 0$, we see that

$$\langle Tx \mid Ty\rangle_{\tilde{\mathscr{H}}_2} = \langle x \mid y\rangle_{\tilde{\mathscr{H}}_1} \quad \forall x,\ y \in D$$

The theorem then follows by Lemma 4.1. $\square$

§5. Double dynamical systems and double KMS one-particle structures

As mentioned in §3, the one-particle Hilbert space $\tilde{\mathscr{H}}$ is 'twice as big' in the KMS case as in the ground case. This suggests that the structure of K^{β} would be more fully revealed if we extended its domain by 'doubling things up' at the classical level. This is indeed the case as we now show:

§5.1. *Standard example of a double linear dynamical system*

Let $(D, \sigma, \mathscr{T}(t))$ be a linear dynamical system as in §§2, 3 and suppose it admits an antisymplectic involution T which reverses the sense of time-evolution:

$$
\begin{aligned}
&T: D \to D, \qquad T^2 = 1 \\
&\sigma(T\Phi, T\Psi) = -\sigma(\Phi, \Psi) \quad \forall \Phi, \Psi \in D \\
&T\mathscr{T}(t) = \mathscr{T}(-t)T
\end{aligned}
\tag{5.1}
$$

Let D^R, D^L each be a copy of D and let $\tilde{D}$ be the vector sum $D^L \oplus D^R$. $\tilde{D}$ inherits a symplectic form $\tilde{\sigma}$ according to

$$\tilde{\sigma}(\Phi_1 \oplus \Psi_1, \Phi_2 \oplus \Psi_2) = \sigma(\Phi_1, \Phi_2) + \sigma(\Psi_1, \Psi_2) \quad \forall \Phi_1, \Phi_2 \in D^L; \qquad \Psi_1, \Psi_2 \in D^R$$

Define the doubled time-evolution $\tilde{\mathscr{T}}(t)$ by

$$\tilde{\mathscr{T}}(t)(\Phi \oplus \Psi) = (\mathscr{T}(-t)\Phi \oplus \mathscr{T}(t)\Psi)$$

and define the doubled involution

$$\mathscr{I}(\Phi \oplus \Psi) = (T\Psi \oplus T\Phi)$$

Before continuing, we summarize the essential features in the

Definition 2. A double (classical) linear dynamical system $(\tilde{D}, \tilde{\sigma}, \tilde{\mathscr{T}}(t), \mathscr{I})$ consists of a linear dynamical system $(\tilde{D}, \tilde{\sigma}, \tilde{\mathscr{T}}(t))$ and an antisymplectic involution $\mathscr{I}$ s.t.

(a) $[\tilde{\mathscr{T}}(t), \mathscr{I}] = 0$

(b) $\tilde{D}$ consists of the sum of two independent subspaces:

$\tilde{D} = D^L + D^R$ s.t.

(i) $\sigma(\Phi^L, \Phi^R) = 0 \quad \forall \Phi^L \in D^L, \qquad \Phi^R \in D^R$

(ii) $\mathscr{T}(t): D^L \to D^L, \qquad D^R \to D^R$

(iii) $\mathscr{I}D^L = D^R$ (and $\mathscr{I}D^R = D^L$)

We shall say such a double system extends a $(D, \sigma, \mathscr{T}(t))$, whenever we can (and do!) identify $(D^R, \tilde{\sigma} \restriction_{D^R}, \tilde{\mathscr{T}}(t) \restriction_{D^R})$ with $(D, \sigma, \mathscr{T}(t))$.

§5.2. *Standard example of a double KMS one-particle structure*

Suppose that the $(D, \sigma, \mathscr{T}(t))$ of §5.1 admits a regular ground one-particle structure $(K, \mathscr{H}, e^{-ith})$ (i.e. one satisfying $KD \subset \mathscr{D}(h^{-1/2})$) and suppose further that the classical symmetry T is implemented at the one-particle level by a complex conjugation C s.t. $CK = KT$ on D. We then automatically have $Ce^{-ith} = e^{ith}C$. Writing $\Phi \oplus \Psi \in \tilde{D}$ as a column vector, and defining $\tilde{H} = \mathscr{H} \oplus \mathscr{H}$ we may now fill out the definition of K^β as promised by defining

$$K^\beta\begin{pmatrix}\Phi\\ \Psi\end{pmatrix}=\begin{pmatrix} chZ^\beta & shZ^\beta C\\ shZ^\beta C & chZ^\beta\end{pmatrix}\begin{pmatrix}-K\Phi\\ K\Psi\end{pmatrix}$$

(cf. definition after equation (3.4), see §3 and §A2 for definition of Z^β and well-definedness.)

If we now recall from §3 the definition

$$\exp(-i\tilde{h}t)=\begin{pmatrix} e^{iht} & 0\\ 0 & e^{-iht}\end{pmatrix}$$

and define the anti-unitary involution j on $\mathscr{H}$ by

$$j=\begin{pmatrix} 0 & -C\\ -C & 0\end{pmatrix}$$

then one may easily check (see again §A2 for property 2 below) that $(\tilde{K}^\beta, \tilde{H}, \exp(-i\tilde{h}t), j)$ satisfies the

Definition 3. Given some $\beta>0$, a double KMS one-particle structure $(\tilde{K}^\beta, \tilde{\mathscr{H}}, \exp(-it\tilde{h}), j)$ over some $(\tilde{D}, \tilde{\sigma}, \tilde{\mathscr{T}}(t), \mathscr{I})$ consists of a complex Hilbert space $\tilde{\mathscr{H}}$, a map $\tilde{K}^\beta:\tilde{D}\to\tilde{\mathscr{H}}$, a strongly continuous unitary group $\exp(-it\tilde{h})$ on $\tilde{\mathscr{H}}$ and a complex conjugation j. s.t.

(1) $\tilde{K}^\beta:\tilde{D}\to\tilde{\mathscr{H}}$, is real-linear, symplectic
(2) $K^\beta D^R+iK^\beta D^R$ is dense in $\tilde{\mathscr{H}}$
(and similarly for $L\leftrightarrow R$)
(3) $\tilde{K}^\beta\tilde{\mathscr{T}}(t)=\exp(-it\tilde{h})\tilde{K}^\beta$
(4) $\tilde{h}$ has no zero eigenvalues
(5) $\tilde{K}^\beta\mathscr{I}=j\tilde{K}^\beta$
(6) $\tilde{K}^\beta D^R+i\tilde{K}^\beta D^R\subset\mathscr{D}(\exp(-\beta\tilde{h}/2))$, $\tilde{K}^\beta D^L+i\tilde{K}^\beta D^L\subset\mathscr{D}(\exp(+\beta\tilde{h}/2))$ and $\exp(-\beta\tilde{h}/2)x=-jx\ \forall x\in\tilde{K}^\beta D^R$, $\exp(\beta\tilde{h}/2)y=-jy\ \forall y\in\tilde{K}^\beta D^L$

Note that the $(\tilde{K}^\beta, \tilde{\mathscr{H}}, \exp(-it\tilde{h}))$ of such a definition – when restricted to $(D^R, \sigma, \mathscr{T}(t))$ is a KMS one-particle structure in the sense of §3. To check the 'one-particle KMS condition', we note that it easily follows from our definitions that $[\exp(-it\tilde{h}), j]=0$ on $\tilde{K}^\beta\tilde{D}$, and calculate $\forall x, y\in\tilde{K}^\beta D^R$

$$\begin{aligned}\langle\exp(-it\tilde{h})x\mid y\rangle&=\langle jy\mid j\exp(-it\tilde{h})x\rangle\\&=\langle jy\,|\exp(-it\tilde{h})|\,jx\rangle\\&=\langle\exp(-\beta\tilde{h}/2)\,y\mid\exp(-it\tilde{h})\exp(-\beta\tilde{h}/2)x\rangle\end{aligned}$$

§5.3.

Finally, our uniqueness theorem extends to give

Theorem 2. *Given a double linear dynamical system $(\tilde{D}, \tilde{\sigma}, \tilde{\mathscr{T}}(t), \mathscr{I})$ for which are given two double KMS one-particle structures $(\tilde{K}_i^\beta, \tilde{\mathscr{H}}_i, \exp(-it\tilde{h}_i), j_i)$ $i=1,2$, for some given $\beta>0$, then there exists a unique unitary $U:\tilde{\mathscr{H}}_1\to\tilde{\mathscr{H}}_2$* s.t.

A) $U\tilde{K}_1^\beta=\tilde{K}_2^\beta$ *on* $\tilde{D}$
B) $U\exp(-it\tilde{h}_1)=\exp(-it\tilde{h}_2)U$ *on* $\tilde{\mathscr{H}}_1$
C) $Uj_1=j_2U$ *on* $\tilde{\mathscr{H}}_1$.

Proof. By Theorem 1b, we conclude the existence of some $U^R : \tilde{\mathcal{H}}_1 \to \tilde{\mathcal{H}}_2$ which satisfies A) restricted to D^R and B) on all of $\tilde{\mathcal{H}}_1$. (Similarly, we could conclude the existence of a U^L with corresponding properties for D^L. We shall see below that $U^L = U^R$.) From B), we conclude

$$U^R : \mathcal{D}(\exp(-\beta\tilde{h}_1/2)) \to \mathcal{D}(\exp(-\beta\tilde{h}_2/2))$$

and

$$U^R \exp(-\beta\tilde{h}_1/2) = \exp(-\beta\tilde{h}_2/2) U^R$$

on

$$\mathcal{D}(\exp(-\beta\tilde{h}_1/2))$$

In particular, this is true on $\tilde{K}_1^\beta D^R$ which, by construction, is mapped by U^R onto $\tilde{K}_2^\beta D^R$. Applying Property (6), we recover $U^R j_1 = j_2 U^R$ on $\tilde{K}_1^\beta D^R$ and hence on the dense set $\tilde{K}_1^\beta D^R + i\tilde{K}_1^\beta D^R$ and hence on all of $\tilde{\mathcal{H}}_1$ since U^R, j_1, j_2 are bounded. This gives C). It remains to show that A) holds on D^L. For this, we use the following argument: $U^R j_1 \tilde{K}_1^\beta = j_1 U^R \tilde{K}_1^\beta$ on $D^R \Rightarrow U^R \tilde{K}_1^\beta \mathcal{J} = j_1 \tilde{K}_2^\beta = \tilde{K}_2^\beta \mathcal{J}$ on D^R. I.e. $U^R \tilde{K}_1^\beta = \tilde{K}_2^\beta$ on D^L since $\mathcal{J} D^R = D^L$. □

One can show quite generally a number of properties which justify the naturalness of the above developments. For example, it follows from Definitions 2 and 3 that $\tilde{K}^\beta \tilde{D}$ is necessarily dense in $\tilde{\mathcal{H}}$ (and thus that U in Theorem 2 is actually the closure of $\tilde{K}_2^\beta \circ (\tilde{K}_1^\beta)^{-1}$ on $\tilde{K}_1^\beta \tilde{D}$.) Rather than prove these things here, we postpone discussion of such things to the companion paper [9] where we shall emphasize the meaning of doubling in the wider context of KMS states on general (i.e. not necessarily linear) quantum systems.

Appendices

§A1. *Heuristic derivation of a class of KMS states for linear systems*[5])

We sketch a heuristic derivation for the formula (3.2). We proceed as if the one-particle Hamiltonian h has discrete spectrum $h\psi_i = h_i\psi_1$ and write (adopting Dirac notation)

$$h = \sum_i h_i |\psi_i\rangle\langle\psi_i| \quad \text{on} \quad \mathcal{H} = \bigoplus_i \mathcal{H}_i$$

(with each $\mathcal{H}_i \approx \mathbb{C}$).

It is convenient to realize our representation space for the second quantized theory (Fock s ace) in infinite tensor product form adapted to the spectrum of $h : \mathcal{F}(\mathcal{H}_i) = \otimes_i \mathcal{F}(\mathcal{H}_i)$ where each $\mathcal{F}(\mathcal{H}_i) \approx \ell_2)$. Here, one may think of the incomplete tensor product [20] associated with the vacuum vector $\Omega = \otimes_i \Omega_i$. The Weyl operator is represented by $W^{\mathcal{F}}(K\Phi)$ (see §2) which in this version of Fock space clearly becomes

$$\exp\left(\sum_i (\langle\psi_i \mid k\Phi\rangle a_i^+ - \langle k\Phi \mid \psi_i\rangle a_i)\right)$$

[5]) This appendix is a mild generalization of Appendix 1 in [8]. We include it here for the sake of completeness.

where a_i^+, a_i are the creation and annihilation operators on $\mathcal{F}(\mathcal{H}_i)$, so that $[a_i, a_i^+] = 1$, $a_i\Omega_i = 0$. Finally, the second quantized Hamiltonian is clearly given by $d\Gamma(h) = \sum_i h_i a_i^+ a_i$.

By the usual Gibbs prescription

$$\omega_\beta(W(\Phi)) = Z^{-1} \operatorname{tr}(e^{-\beta d\Gamma(h)} W^{\mathcal{F}}(K\Phi))$$
$$= Z^{-1} \operatorname{tr}\left(\exp\left[-\beta \sum_i h_i a_i^+ a_i\right] \exp\left[\sum_i \alpha_i a_i^+ - \sum_i \bar{\alpha}_i a_i\right]\right)$$

where

$$\alpha_i = \langle \psi_i \mid K\Phi \rangle, \qquad \bar{\alpha}_i = \langle K\Phi \mid \psi_i \rangle$$

and

$$Z = \operatorname{tr} e^{-\beta d\Gamma(h)} = \operatorname{tr}\left(\exp\left[-\beta \sum_i h_i a_i^+ a_i\right]\right).$$

Here the trace is to be taken over all vectors $\otimes_i |n_i\rangle$ in Fock space. Ignoring mathematical rigour, we may rearrange this formula to give an infinite product of terms – each of which corresponds to a Gibbs state on a single degree of freedom:

$$\omega_\beta(W(\Phi)) = \prod_i Z_i^{-1} \operatorname{tr}(\exp[-\beta h_i a_i^+ a_i] \exp[\alpha_i a_i^+ - \alpha_i a_i])$$

with $Z_i = \operatorname{tr}(\exp[\beta h_i a_i^+ a_i])$. Z_i is of course just $\sum_{n=0}^\infty e^{-n\beta h_i} = (1 - e^{-\beta h_i})^{-1}$. The other trace (using the cyclicity of the trace and the Baker–Hausdorff formula) is equal to

$$\exp(-|\alpha_i|^2/2) \sum_{n=0} \exp(-n\beta h_i)\langle n| \exp(\alpha_i a^+) \exp(-\alpha_i a) |n\rangle$$

which, on using $a_i |n\rangle = n^{1/2} |n-1\rangle$ and a straightforward calculation

$$= \exp(-|\alpha_i|^2/2 \sum_{m=0}^\infty (-)^k \frac{|\alpha_i|^{2m}}{(m!)^2} \sum_{n=m}^\infty n(n-1)\cdots(n-m+1)e^{-n\beta h}$$

The sum over k is evaluated by

$$\sum_{n=m}^\infty n(n-1)\cdots(n-m+1)x^n = \left(\frac{d}{dx}\right)^m \sum_{n=0}^\infty x^n$$
$$= x^m m!(1-x)^{-m-1}$$

So our trace becomes

$$[1 - \exp(-\beta h_i)]^{-1} \exp(-|\alpha_i|^2/2) \sum_{m=0}^\infty (-)^m \frac{|\alpha_i|^{2m}}{m!} \left(\frac{\exp(-\beta h_i)}{1 - \exp(-\beta h_i)}\right)$$

Cancelling the first term with Z_i^{-1}, summing the series over m and taking the infinite product, we get finally

$$\omega_\beta(W(\Phi)) = \exp\left[-\sum_i \frac{|\alpha_i|^2}{2} \coth\left(\frac{\beta h_i}{2}\right)\right]$$

On recalling $h\psi_i = h_i\psi_i$ and $|\alpha_i|^2 = \langle K\Phi \mid \psi_i \rangle\langle \psi_i \mid K\Phi \rangle$ we see this is equal to (3.2) which we now take to be the correct formula even in the case of non-discrete spectrum.

§A2. *Some details omitted from* §§3, 5

In §3, the operators

$$shZ^{\beta} = \exp(-\beta h/2)(1-\exp(-\beta h))^{-1/2} \quad \text{and} \quad chZ^{\beta} = (1-\exp(-\beta h))^{-1/2},$$

are each defined by the spectral theorem and, using the simple estimates on positive numbers x

$$\exp(-\beta x/2)(1-\exp(-\beta x))^{-1/2} \leq C(\max(1, x^{-1/2})$$
$$(1-\exp(-\beta x))^{-1/2} \leq C(\max(1, x^{-1/2})$$

we see that $\mathscr{D}(h^{-1/2}) \subset \mathscr{D}(shZ^{\beta})$, $\mathscr{D}(chZ^{\beta})$.

Similarly, one can check, regarding equation (3.2) that $\mathscr{D}(h^{-1/2})$ is contained in the quadratic form domain $\mathscr{Q}(\coth(\beta h/2))$ (use $\coth(\beta h/2) = ch^2Z^{\beta} + sh^2Z^{\beta}$). The regularity condition $KD \subset \mathscr{D}(h^{-1/2})$ thus suffices as claimed in the text.

In checking that the standard KMS one-particle structure $(K^{\beta}, \tilde{\mathscr{H}}, \exp(-it\tilde{h}))$ satisfies Definition 1b, (i) and (iii) are easily checked by straightforward calculations. We now check (ii) that $K^{\beta}D + iK^{\beta}D$ is dense in $\mathscr{H} \oplus \mathscr{H}$. Using the relation $shZ^{\beta} = \exp(-\beta\tilde{h}/2)chZ^{\beta}$ it suffices by the following argument to prove $chZ^{\beta}K^{\beta}D$ is a (real-linear) dense set in $\mathscr{H}$. For, given $\alpha \oplus \beta$ in the sense set $\mathscr{D}(\exp(\beta\tilde{h}/2)) \oplus \mathscr{H}$, we may then find sequences Φ_i, $\Psi_i \in D$ s.t.

$$chZ^{\beta}K^{\beta}\Phi_i \to \tfrac{1}{2}(\exp(\beta\tilde{h}/2)C\alpha + \beta)$$

and

$$chZ^{\beta}K^{\beta}\Psi_i \to \frac{i}{2}(\exp(\beta\tilde{h}/2)C\alpha - \beta),$$

so that

$$(shZ^{\beta}CK^{\beta}\Phi_i \oplus chZ^{\beta}K^{\beta}\Phi_i) + i(shZ^{\beta}CK^{\beta}\Psi_i \oplus chZ^{\beta}K^{\beta}\Psi_i) \to \alpha \oplus \beta.$$

To prove that $chZ^{\beta}K^{\beta}D$ is dense, note that ran (chZ^{β}) on its full domain is dense since chZ^{β} clearly has no zero eigenvalues. The result now follows on showing that $K^{\beta}D$ is a core for chZ^{β}. For this, one may use the convenient

Lemma (Rigotti [21]). *Let K be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Let f be a real Borel function bounded on the compacts. If $\Delta \subset D(f(K))$ is a dense subspace invariant for the group e^{-itK}, then Δ is a core for $f(K)$.*

(We shall need this lemma again in [9]. For the proof, see Theorem 4 of [21].) In applying this lemma here to $\Delta = K^{\beta}D$, take $f(x) = (1-e^{-\beta x})^{-1/2}$, and $K = \tilde{h}$; and use the fact that $K^{\beta}D$ is invariant for $\exp(-it\tilde{h})$.

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