On Energy Differences in Many Body Systems

The Mathematical Structure of the New-Tamm-Dancoff Procedure III

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Number- and operator-valued energy differences in von Neumann algebras are discussed by means of the Tomita-Takesaki theory. Small energy differences can be evaluated by the anti-commutator of a sort of relative entropy operator and the energy operator. The New-Tamm-Dancoff procedure is studied in terms of the standard form.

§ 1. Introduction

Given two nearby lying states of a many-body system, each one involving many one-particle contributions, it would be very inconvenient to express the difference of the energies of these states as a difference of absolute energy values. Small errors in the absolute values could drastically change the difference. In cases where the energies are infinite, their difference makes no sense at all.

At this point Dyson [1] proposed the "New Tamm-Dancoff formalism" (NTD). He modified an approximation procedure of Tamm [2] and Dancoff [3], the mathematical content of it being an approximative determination of the eigenvalues of a Schrödinger equation by the method of Ritz-Galerkin [4]. – In the framework of solid-state physics NTD has been discussed by Wahl and coworkers [5, 6, 7].

In the spirit of Dyson we here take NTD as an idea to look for a convenient reference state with respect to which energy differences should be calculated. In high energy physics the polarizable vacuum is such a reference state ("Dirac sea"). Referring to it avoids the infinite self-energy of this state. In solid-state physics, for example in the case of a semiconductor, the completely filled valence band can serve as a reference state ("Fermi sea"). Excitations with respect to the valence band produce already in low order such relevant features as polarons, excitons, ...

The theory of von Neumann algebras is a useful frame for a discussion of these physical problems. Here infinite energy constants can be circumvented by an appropriate choice of the representation of the algebra of observables. The emergence of inequivalent representations admits for posing well physical divergency problems.

There are some relations between NTD and the standard form of von Neumann algebras which have been used implicitly in the preceding studies [4–7]. In particular the difference Hamiltonian (10.8) in [7],

$$\mathbf{H} := h^{\Delta}(u^*, u) = h(i v^*, i v)\,, \tag{1}$$

arising in the structural analysis of NTD [4], is nothing but a standard implementation of the time evolution generator. Moreover the use of a generating vector ((7.7) in [7]) implies a faithful state which specifies a standard representation.

In the determination of the difference of the energy expectation values in two states φ, ψ we will employ the relative modular operator $(\Delta_{\Phi,\Psi})^{1/2}$ of the Tomita-Takesaki theory, and a related operator $R(\varphi/\psi)$ introduced in [8].

For concreteness we exhibit our method in the model of a semiconductor. We use the notation of [6] developed for many-body systems and applied in [7].

§ 2. Mathematical ingredients

Let M be a W^*-algebra and ψ a faithful element of M_{*+}, the set of positive normal linear functionals of M. Then the GNS-representation π_ψ of M with

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respect to ψ, $\pi_\psi(M) = \mathfrak{M}$, is a von Neumann algebra acting in a Hilbert space $\mathscr{H}$, $\mathfrak{M}$ being isomorphic to M. Let $\Psi \in \mathscr{H}$ be the cyclic and separating vector corresponding to the functional ψ:

$$\psi(x) = \langle \Psi, \pi_\psi(x)\, \Psi \rangle\,, \quad x \in M\,,$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product in $\mathscr{H}$. Let $\Phi \in \mathscr{H}$. Then the relative modular involution $\bar{S}_{\Phi,\Psi}$ is the closure of

$$S_{\Phi,\Psi}\, x\, \Psi := x^*\, \Phi\,, \quad x \in \mathfrak{M}\,, \tag{2}$$

and its polar decomposition defines the unitary involution $J_{\Phi,\Psi}$, and the "relative modular operator" $\Delta_{\Phi,\Psi}$:

$$\bar{S}_{\Phi,\Psi} =: J_{\Phi,\Psi}\, (\Delta_{\Phi,\Psi})^{1/2}\,. \tag{3}$$

$\Delta_{\Phi,\Psi}$ is positive and self-adjoint. If Φ coincides with Ψ, we put $\bar{S}_\Psi := \bar{S}_{\Psi,\Psi}$, $J := J_{\Psi,\Psi}$, and call $\Delta_\Psi := \Delta_{\Psi,\Psi}$ the modular operator. The "natural positive cone" $\mathscr{P} \subset \mathscr{H}$ is defined as

$$\mathscr{P} := \overline{\{x\, J\, x\, \Psi \mid x \in \mathfrak{M}\}}\,, \tag{4}$$

the bar denoting the norm-closure. If we choose another cyclic and separating vector $\Psi' \in \mathscr{H}$, we arrive at the same J and $\mathscr{P}$, i.e. J and $\mathscr{P}$ are universal. In the above situation, the quadruple $(\mathfrak{M}, \mathscr{H}, J, \mathscr{P})$ is called the "standard form" of the von Neumann algebra $\mathfrak{M}$. – Let $\mathfrak{M}'$ denote the commutant of $\mathfrak{M}$. One of the main properties of von Neumann algebras in standard form is the relation

$$J\, \mathfrak{M}\, J = \mathfrak{M}'\,. \tag{5}$$

There exists a homeomorphic bijection ξ,

$$\varphi \in \mathfrak{M}_{*+} \mapsto \xi(\varphi) =: \Phi \in \mathscr{P}\,, \tag{6a}$$

between the positive normal linear functionals of $\mathfrak{M}$ and the natural positive cone, such that

$$\varphi(x) = \langle \Phi, x\, \Phi \rangle\,, \quad x \in \mathfrak{M}\,. \tag{6b}$$

Let $\psi \in \mathfrak{M}_{*+}$ be faithful, and $\Psi \in \mathscr{P}$ the representing cyclic and separating vector. The modular automorphism group with respect to ψ is defined as

$$\sigma_t^\psi(x) := (\Delta_\psi)^{it}\, x\, (\Delta_\psi)^{-it}\,, \quad x \in \mathfrak{M}\,, \quad t \in \mathbb{R}\,. \tag{7}$$

Let φ be another faithful element of $\mathfrak{M}_{*+}$, and $\{\sigma_t^\varphi\}_{t \in \mathbb{R}}$ its modular automorphism group. Then there exists a family of unitary operators $(D\varphi : D\psi)_t$, $t \in \mathbb{R}$, strongly continuous in t, such that

$$(D\varphi : D\psi)_t\, \sigma_t^\psi(x)\, (D\varphi : D\psi)_t^* = \sigma_t^\varphi(x)\,, \quad x \in \mathfrak{M}\,, \quad t \in \mathbb{R}\,; \tag{8a}$$

$$(D\varphi : D\psi)_t \in \mathfrak{M}\,, \quad t \in \mathbb{R}\,; \tag{8b}$$

$$(D\varphi : D\psi)_t = (\Delta_{\Phi,\Psi})^{it}\, (\Delta_\Psi)^{-it}\,, \quad t \in \mathbb{R}\,. \tag{8c}$$

The (strong) time derivation of $(D\varphi : D\psi)_t$ at $t = 0$,

$$R(\varphi \mid \psi) := \lim_{t \to 0} \frac{i}{t} \{(D\varphi : D\psi)_t - \mathbb{1}\}\,, \tag{9}$$

defines in a Hilbert space $\mathscr{H}$ a self-adjoint operator, affiliated with $\mathfrak{M}$ [8].

The standard form has been established in [9, 10], and the unitary cocycle has been introduced by Connes [11]. A comprehensive treatment of this material can be found in [12, 13].

In the following we assume that a concrete physical system can be described by a (σ-finite) von Neumann algebra $\mathfrak{M}$ in standard form, and its states by the positive normal linear functionals on $\mathfrak{M}$.

§ 3. Difference of general energy expectation values

Given a von Neumann algebra $\mathfrak{M}$ in standard form $(\mathfrak{M}, \mathscr{H}, J, \mathscr{P})$, and a Hamiltonian H acting in the Hilbert space $\mathscr{H}$, we are interested in the difference of the energy expectation values

$$\omega_{\varphi,\psi}^H := \varphi(H) - \psi(H) \tag{10}$$

for states φ, ψ. If H is unbounded it may happen that Φ or Ψ do not belong to the domain of H, so that $\varphi(H)$ or $\psi(H)$ do not exist. Nevertheless $\omega_{\varphi,\psi}^H$ could eventually be defined even in such cases.

Let $H = \int_{-\infty}^{\infty} \lambda\, E^H(\mathrm{d}\lambda)$ be the spectral resolution of $H = H^*$. Define the bounded operators

$$H_\eta := \int_{-\eta}^{\eta} \lambda\, E^H(\mathrm{d}\lambda)\,, \quad \eta > 0\,, \tag{11}$$

such that $H = \lim_{\eta \to \infty} H_\eta$. If

$$\omega_{\varphi,\psi}^H := \lim_{\eta \to \infty} \{\varphi(H_\eta) - \psi(H_\eta)\} \tag{10'}$$

exists, the values $\pm\infty$ included, this definition is an extension of (10) to more general states φ, ψ, and Hamiltonians H.

Now we would like to evaluate the energy differences (10′) by one single expectation value:

* GNS = Gelfand Naimark Segal.

Proposition 1: For an arbitrary state $\varphi \in \mathfrak{M}_{*+}$ and a faithful $\psi \in \mathfrak{M}_{*+}$,

$$\omega^H_{\varphi,\psi} = \lim_{\eta \to \infty} \langle \Psi, \{(\Delta_{\Phi,\psi})^{1/2} H_\eta (\Delta_{\Phi,\psi})^{1/2} - H_\eta\} \Psi \rangle . \tag{12a}$$

For arbitrary $\varphi_1, \varphi_2 \in \mathfrak{M}_{*+}$,

$$\omega^H_{\varphi_1,\varphi_2} = \lim_{\eta \to \infty} \langle \Psi, \{(\Delta_{\Phi_1,\psi})^{1/2} H_\eta (\Delta_{\Phi_1,\psi})^{1/2} - (\Delta_{\Phi_2,\psi})^{1/2} H_\eta (\Delta_{\Phi_2,\psi})^{1/2}\} \Psi \rangle . \tag{12b}$$

Proof. The natural positive cone is pointwise invariant under J [12],

$$J\Omega = \Omega , \quad \Omega \in \mathscr{P} . \tag{13}$$

Now, for the representing vectors $\Phi, \Psi \in \mathscr{P}$ corresponding to φ, ψ definition (2) implies

$$\Phi = (\Delta_{\Phi,\psi})^{1/2} \Psi , \tag{14}$$

and for bounded operators acting in $\mathscr{H}$, $a \in \mathscr{B}(\mathscr{H})$, we have

$$\begin{aligned} \varphi(a) - \psi(a) &= \langle \Phi, a\Phi \rangle - \langle \Psi, a\Psi \rangle \\ &= \langle (\Delta_{\Phi,\psi})^{1/2} \Psi, a (\Delta_{\Phi,\psi})^{1/2} \Psi \rangle - \langle \Psi, a\Psi \rangle \\ &= \langle \Psi, \{(\Delta_{\Phi,\psi})^{1/2} a (\Delta_{\Phi,\psi})^{1/2} - a\} \Psi \rangle \end{aligned} \tag{15}$$

q.e.d.

If we linearize $(\Delta_{\Phi,\psi})^{1/2} = \exp(\log(\Delta_{\Phi,\psi})^{1/2})$, the R-operator becomes involved.

Definition 2. For a fixed faithful state $\psi \in \mathfrak{M}_{*+}$, we call a faithful $\varphi \in \mathfrak{M}_{*+}$ belonging to the "linear range of Φ" if

$$\| \log (\Delta_{\Phi,\psi})^{1/2} \Psi \| \ll \| \Psi \| , \tag{16a}$$

$$\| \Phi - (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi \| \ll \| \log (\Delta_{\Phi,\psi})^{1/2} \Psi \| . \tag{16b}$$

Proposition 3. Let $\varphi, \psi \in \mathfrak{M}_{*+}$ be faithful, and H bounded, $H \in \mathscr{B}(\mathscr{H})$. If φ is in the linear range of ψ, the energy difference is given in first (linear) order by

$$\omega^H_{\varphi,\psi} = -\tfrac{1}{2} \langle \Psi, [R, H]_+ \Psi \rangle , \tag{17}$$

where $[a, b]_+ := a b + b a$.

Proof. The vector Ψ is invariant under the group of unitaries $(\Delta_\psi)^{it}$, $t \in \mathbb{R}$,

$$(\Delta_\psi)^{it} \Psi = \Psi , \tag{18}$$

hence

$$\begin{aligned} &\log (\Delta_{\Phi,\psi})^{1/2} \Psi \\ &\quad = \lim_{t \to 0} \frac{i}{t} \left\{ -\frac{1}{2} (\Delta_{\Phi,\psi})^{it} + \frac{1}{2} \mathbb{1} \right\} \Psi \\ &\quad = \lim_{t \to 0} \frac{i}{t} \left\{ -\frac{1}{2} (\Delta_{\Phi,\psi})^{it} (\Delta_\psi)^{-it} + \frac{1}{2} \mathbb{1} \right\} \Psi \\ &\quad = -\frac{1}{2} R(\varphi \mid \psi) \Psi . \end{aligned}$$

$$\begin{aligned} &\langle \Phi, H\Phi \rangle \\ &\quad = \big\langle (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2} \Psi , \\ &\qquad H (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi \big\rangle \\ &\qquad + \big\langle \{\Phi - (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi\}, H\Phi \big\rangle \\ &\qquad + \big\langle (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi , \\ &\qquad\quad H \{\Phi - (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi\} \big\rangle \\ &\quad =: -\tfrac{1}{2} \langle \Psi, [RH + HR] \Psi \rangle + \langle \Psi, H\Psi \rangle + A . \end{aligned}$$

By the Cauchy-Schwarz inequality we have

$$\begin{aligned} |A| = |\{ &\big\langle \log (\Delta_{\Phi,\psi})^{1/2} \Psi, H \log (\Delta_{\Phi,\psi})^{1/2} \Psi \big\rangle \\ &+ \big\langle \{\Phi - (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi\}, H\Phi \big\rangle \\ &+ \big\langle (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi , \\ &\quad H \{\Phi - (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2} \Psi\} \big\rangle \}| \\ \leqq \| H \| \, \{ &\| \log (\Delta_{\Phi,\psi})^{1/2} \Psi \|^2 \\ &+ \| \Phi \| \, \| \Phi - (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi \| \\ &+ \| (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi \| \\ &\cdot \| \Phi - (\mathbb{1} + \log (\Delta_{\Phi,\psi})^{1/2}) \Psi \| \} \\ \ll \| H \| \, &\| \log (\Delta_{\Phi,\psi})^{1/2} \Psi \| \\ &\cdot \{ \| \Psi \| + \| \Phi \| + \| \Psi \| \\ &\quad + \| \log (\Delta_{\Phi,\psi})^{1/2} \Psi \| \} . \end{aligned}$$

Therefore, A is an order of magnitude smaller than $\langle \Psi, [R, H]_+ \Psi \rangle$, and we have

$$\langle \Phi, H\Phi \rangle - \langle \Psi, H\Psi \rangle = -\tfrac{1}{2} \langle \Psi, [R, H]_+ \Psi \rangle \quad \text{q.e.d.}$$

in first order.

Remark

Imposing additional conditions, Proposition 3 can be extended to unbounded Hamiltonians, and more general pairs of states. In particular

$$\langle \Psi, [R, H]_+ \Psi \rangle = \langle R\Psi, H\Psi \rangle + \langle H\Psi, R\Psi \rangle$$

exists (in the linear range where $\Psi \in \mathscr{D}(R)$) for $\Psi \in \mathscr{D}(H)$.

§ 4. Energy differences under an abstract thermodynamical aspect

In this paragraph we discuss the following three cases:

1. Evaluate the energy difference of two equilibrium states.
2. Given an arbitrary Hamiltonian H in a Hilbert space $\mathscr{H}$. Construct a reference state with energy expectation value zero.
3. Look for special pairs of states which make the "thermal" part of an energy operator vanish.

We adopt the point of view that there is inherent in each state an internal dynamics ruled by the modular automorphism group $\{\sigma_t^{\psi}\}_{t\in\mathbb{R}}$. So the specification of a state automatically implies the specification of the internal part of the dynamics. We identify $-\log \Delta_\psi$ with the internal energy "frozen" in the state ψ. This interpretation is supported by the fact that in the KMS-equilibrium (a concept which generalizes the canonical Gibbs ensemble – see [12]), where total energy and internal energy should coincide, the Hamiltonian is given by $-\log \Delta_\psi$, for $\beta = 1$ (see [14]). Therefore a general energy operator H for a system in a non-tracial state ψ should be given as

$$H_\eta = -\log \Delta_\psi + R_\eta, \quad R_\eta = R_\eta^* \in \mathfrak{M}, \quad \eta > 0. \tag{19}$$

The η-cut-off for R is introduced to handle domain questions ($\mathscr{D}(H_\eta) = \mathscr{D}(\log \Delta_\psi)$). Now R describes the mechanical part of the system under consideration, or – in a thermodynamical language – its free energy [14]. We have put $\beta = 1$, so the dimensions of energy and entropy are the same.

1. The operator of relative energy

Let $\varphi, \psi \in \mathfrak{M}_{*+}$ be faithful. Assume that the system goes (by an outer manipulation, disregarded here) from a KMS-equilibrium in the state ψ to a KMS-equilibrium in the state φ. Then the time evolution of the system is at first given by $\{\sigma_t^{\psi}\}_{t\in\mathbb{R}}$, and then by $\{\sigma_t^{\varphi}\}_{t\in\mathbb{R}}$. We are interested in the change of the energy operator with respect to $\mathfrak{M}$, described by the "difference evolution"

$$\alpha_t^{\mathrm{d}}(x) := \sigma_t^{\varphi}\{\sigma_{-t}^{\psi}(x)\}, \quad x \in \mathfrak{M}, \quad t \in \mathbb{R}. \tag{20a}$$

From a given time evolution

$$\alpha_t(x) = U_t\, x\, U_t^*, \quad x \in \mathfrak{M}, \quad t \in \mathbb{R}, \tag{21a}$$

where $U_t\colon \mathscr{H} \to \mathscr{H}$ is a family of unitaries, strongly continuous in $t \mapsto U_t$, $t \in \mathbb{R}$, we can recover the energy operator by the time derivation of U_t at $t = 0$:

$$i\,H := \frac{\mathrm{d}}{\mathrm{d}t}\, U_t \Big|_{t=0}. \tag{21b}$$

Applying the relations (8) to the difference evolution α^{d}, measuring σ^{φ} with respect to σ^{ψ}, we get

$$\alpha_t^{\mathrm{d}}(x) = (D\varphi : D\psi)_t\, x\, (D\varphi : D\psi)_t^*, \quad x \in \mathfrak{M}, \quad t \in \mathbb{R}. \tag{20b}$$

Therefore the change in the energy operator, with respect to $\mathfrak{M}$, results to be

$$-i\frac{\mathrm{d}}{\mathrm{d}t}(D\varphi : D\psi)_t \Big|_{t=0} = -R(\varphi/\psi). \tag{22}$$

2. The standard representation of $\mathscr{B}(\mathscr{H})$

Let an arbitrary Hamiltonian $H = H^*$ in a separable Hilbert space $\mathscr{H}$ be given. Now we assume that the reference state is not yet fixed a priori. We will construct a standard representation $\mathfrak{M}$ of $\mathscr{B}(\mathscr{H})$, the standard implementation $\mathbb{H}$ of H, and a state ψ of $\mathfrak{M}$ so that $\psi(\mathbb{H}) = 0$. Then the difference of the energy expectation values in an arbitrary faithful state $\varphi \in \mathfrak{M}_{*+}$ and in ψ is

$$\omega_{\varphi,\psi}^{\mathbb{H}} = \varphi(\mathbb{H}) - \psi(\mathbb{H}) = \varphi(\mathbb{H}). \tag{23}$$

Therefore the expectation value of an absolute energy, which is not observable a priori, can be interpreted as an energy difference.

Choose a complete set of linearly independent elements in the dense domain $\mathscr{D}(H)$ of H, and apply the Gram-Schmidt orthogonalization procedure to get an orthonormalized basis $\{\Psi_k\}_{k=1,2,\ldots}$ in $\mathscr{H}$, $\Psi_k \in \mathscr{D}(H)$. Define

$$\Phi = \sum_{k=1}^{\infty} \langle \Psi_k, \Phi\rangle\, \Psi_k \in \mathscr{H} \mapsto \Phi^c := \sum_{k=1}^{\infty} \langle \Phi, \Psi_k\rangle\, \Psi_k \in \mathscr{H}; \tag{24.1}$$

$$\mathscr{K} := \mathscr{H} \otimes \mathscr{H}; \tag{24.2}$$

$$J := \Phi_1 \otimes \Phi_2 \in \mathscr{K} \mapsto \Phi_2^c \otimes \Phi_1^c \in \mathscr{K}; \tag{24.3}$$

$$\mathfrak{M} := \{a \otimes \mathbb{1} \in \mathscr{B}(\mathscr{K}) \mid a \in \mathscr{B}(\mathscr{H})\}; \tag{24.4}$$

$$\Psi := \sum_{k=1}^{\infty} \mu_k\, \Psi_k \otimes \Psi_k \tag{24.5}$$

with a set of positive nonzero μ_k such that

$$\sum_{k=1}^{\infty} \mu_k^2 < \infty .$$

$$\mathscr{P} := \overline{\{ xJx\,\Psi \mid x \in \mathfrak{M} \}} \subseteq \mathscr{K} . \tag{24.6}$$

Proposition 4. (a) The operator J is the unitary modular conjugation for the vector Ψ which is cyclic and separating with respect to $\mathfrak{M}$. Hence $(\mathfrak{M}, \mathscr{K}, J, \mathscr{P})$ is a standard representation of $\mathscr{B}(\mathscr{H})$.

(b) $\mathbb{H} := H \otimes \mathbb{1} - J(H \otimes \mathbb{1})J$ is the standard representation of H.

(c) $\psi(\mathbb{H}) = 0$, where $\psi(x) := \langle \Psi, x\,\Psi \rangle$, $x \in \mathfrak{M}$.

In the proof of this proposition we need the following results.

Observation 1:

$$(\lambda\,\Phi + \Phi')^c = \bar{\lambda}\,\Phi^c + \Phi'^c, \quad \lambda \in \mathbb{C}, \quad \Phi, \Phi' \in H. \tag{25a}$$

The transposition with respect to the basis $\{\Psi_k\}_{k=1,2,\ldots}$ is defined as

$$\langle \Psi_l, a^T \Psi_{l'} \rangle := \langle \Psi_{l'}, a\,\Psi_l \rangle ,$$
$$a \in \mathscr{B}(\mathscr{H}), \quad l, l' = 1, 2, \ldots . \tag{26}$$

Observation 2:

$$(a\,\Psi_l)^c = a^{*T} \Psi_l, \quad a \in \mathscr{B}(\mathscr{H}) . \tag{25b}$$

Proof:

$$\begin{aligned}(a\,\Psi_l)^c &= \sum_k \langle a\,\Psi_l, \Psi_k \rangle\, \Psi_k \\ &= \sum_k \langle \Psi_l, a^*\,\Psi_k \rangle\, \Psi_k \\ &= \sum_k \langle \Psi_k, a^{*T} \Psi_l \rangle\, \Psi_k \\ &= a^{*T} \Psi_l . \qquad \text{q.e.d.}\end{aligned}$$

Observation 3:

$$(a\,\Phi)^c = a^{*T} \Phi^c, \quad a \in \mathscr{B}(\mathscr{H}), \quad \Phi \in \mathscr{H}. \tag{25c}$$

Proof:

$$\begin{aligned}(a\,\Phi)^c &= \sum_{k=1}^{\infty} \langle \Phi, \Psi_k \rangle\, (a\,\Psi_k)^c \\ &= a^{*T} \sum_{k=1}^{\infty} \langle \Phi, \Psi_k \rangle\, \Psi_k . \\ &= a^{*T} \Phi^c . \qquad \text{q.e.d.}\end{aligned}$$

Proof of Proposition 4:

(a)

(i)
$$\begin{aligned}&\langle J\,\Phi_1 \otimes \Phi_2, J\,\Omega_1 \otimes \Omega_2 \rangle \\ &= \langle \Phi_2^c \otimes \Phi_1^c, \Omega_2^c \otimes \Omega_1^c \rangle \\ &= \langle \Phi_2^c, \Omega_2^c \rangle \langle \Phi_1^c, \Omega_1^c \rangle \\ &= \sum_{k,k'=1}^{\infty} \overline{\langle \Psi_k, \Phi_2 \rangle}\, \overline{\langle \Psi_{k'}, \Omega_2 \rangle}\, \langle \Psi_k, \Psi_{k'} \rangle \\ &\quad \cdot \sum_{l,l'=1}^{\infty} \overline{\langle \Psi_l, \Phi_1 \rangle} \overline{\langle \Psi_{l'}, \Omega_1 \rangle}\, \langle \Psi_l, \Psi_{l'} \rangle \\ &= \langle \Omega_2, \Phi_2 \rangle \langle \Omega_1, \Phi_1 \rangle \\ &= \langle \Omega_1 \otimes \Omega_2, \Phi_1 \otimes \Phi_2 \rangle .\end{aligned}$$

(ii) $J^2 = \mathbb{1}$.

(iii)
$$\begin{aligned}J(a \otimes \mathbb{1}) J\,\Phi_1 \otimes \Phi_2 &= J(a \otimes \mathbb{1})\,\Phi_2^c \otimes \Phi_1^c \\ &= J\,a\,\Phi_2^c \otimes \Phi_1^c \\ &= \Phi_1 \otimes (a\,\Phi_2^c)^c \\ &= \Phi_1 \otimes a^{*T} (\Phi_2^c)^c \\ &= (\mathbb{1} \otimes a^{*T})\,\Phi_1 \otimes \Phi_2 ,\end{aligned}$$

where we used (25c). Therefore

$$J\,\mathfrak{M}\,J = \mathfrak{M}' = \{ \mathbb{1} \otimes a \in \mathscr{B}(\mathscr{H}) \mid a \in \mathscr{B}(\mathscr{H}) \} . \tag{27}$$

(iv) $J\,\Psi = \Psi$; $(\|\Psi\| < \infty \Rightarrow \Psi \in \mathscr{K})$.

(v)
$$\begin{aligned}&\langle (a \otimes \mathbb{1})\, J\,(a \otimes \mathbb{1})\,\Psi, \Psi \rangle \\ &= \Big\langle (a \otimes \mathbb{1})(\mathbb{1} \otimes a^{*T}) \sum_{k=1}^{\infty} \mu_k\, \Psi_k \otimes \Psi_k, \\ &\qquad \sum_{k'=1}^{\infty} \mu_{k'}\, \Psi_{k'} \otimes \Psi_{k'} \Big\rangle \\ &= \sum_{k,k'=1}^{\infty} \mu_k \mu_{k'} \langle \Psi_k \otimes a^{*T} \Psi_k, a^*\,\Psi_{k'} \otimes \Psi_{k'} \rangle \\ &= \sum_{k,k'=1}^{\infty} \mu_k \mu_{k'} \langle \Psi_k, a^*\,\Psi_{k'} \rangle \langle a^{*T} \Psi_k, \Psi_{k'} \rangle \\ &= \sum_{k,k'=1}^{\infty} \mu_k \mu_{k'} \langle \Psi_k, a^*\,\Psi_{k'} \rangle \overline{\langle \Psi_k, a^*\,\Psi_{k'} \rangle} \\ &\geqq 0 .\end{aligned}$$

(vi) Supposed $(a \otimes \mathbb{1})\,\Psi = \sum_k \mu_k (a\,\Psi_k) \otimes \Psi_k = 0$, $a \in \mathscr{B}(\mathscr{H})$. Since all μ_k are nonzero and positive, it follows that $(a\,\Psi_k) \otimes \Psi_k = 0$ for all k. But $\{\Psi_k\}$ is a basis, therefore $a = 0$. So Ψ is separating for $\mathfrak{M}$. Similarly it follows that Ψ is separating for $\mathfrak{M}'$,

hence cyclic for $\mathfrak{M}$ (and $\mathfrak{M}'$) (see Proposition 2.5.3 in [12]).

By Theorem 1.7 in [15] J is the unitary modular conjugation for a cyclic and separating vector Ψ if and only if (i) – (v) are satisfied.

(b)

(i)
$$\begin{aligned} & e^{i(H\otimes\mathbb{1})t - iJ(H\otimes\mathbb{1})Jt}(a\otimes\mathbb{1}) \\ & \cdot e^{-i(H\otimes\mathbb{1})t + iJ(H\otimes\mathbb{1})Jt} \\ & = e^{i(H\otimes\mathbb{1})t} J e^{-i(H\otimes\mathbb{1})t} J(a\otimes\mathbb{1}) \\ & \cdot e^{-i(H\otimes\mathbb{1})t} J e^{i(H\otimes\mathbb{1})t} J \\ & = e^{i(H\otimes\mathbb{1})t}(a\otimes\mathbb{1}) e^{-i(H\otimes\mathbb{1})t} \\ & = (e^{iHt} a e^{-iHt})\otimes\mathbb{1}, \quad a\otimes\mathbb{1}\in\mathfrak{M}. \end{aligned}$$

(ii) Given

$$\Psi_{a'} := (a\otimes\mathbb{1}) J(a\otimes\mathbb{1})\Psi \in \mathscr{P}, \quad a\otimes\mathbb{1}\in\mathfrak{M}.$$

$$\begin{aligned} & e^{itH\otimes\mathbb{1} - itJH\otimes\mathbb{1}J}(a\otimes\mathbb{1}) J(a\otimes\mathbb{1})\Psi \\ & = (e^{itH} a\otimes\mathbb{1}) J(e^{-itH} a\otimes\mathbb{1})\Psi \in \mathscr{P}. \end{aligned}$$

(iii)

$$J\mathbb{H}J = -\mathbb{H}. \tag{28a}$$

$$J e^{i\mathbb{H}t} J = e^{i\mathbb{H}t}. \tag{28b}$$

By Corollary 2.5.32 in [12],

$$(x\otimes\mathbb{1}) \mapsto e^{i\mathbb{H}t}(x\otimes\mathbb{1}) e^{-i\mathbb{H}t}, \quad x\otimes\mathbb{1}\in\mathfrak{M}, \quad t\in\mathbb{R}$$

implements canonically the automorphism

$$x \mapsto e^{iHt} x e^{-iHt}, \quad x\in\mathscr{B}(\mathscr{H}), \quad t\in\mathbb{R}$$

in the standard representation $\mathfrak{M}$ of $\mathscr{B}(\mathscr{H})$, i.e. $\mathbb{H}$ is the standard representation of H. Obviously $\mathbb{H}$ is self-adjoint.

(c)

$$\begin{aligned} \psi(\mathbb{H}) &= \lim_{\eta\to\infty} \psi(\mathbb{H}_\eta) \\ &= \lim_{\eta\to\infty} \langle\Psi, \{H_\eta\otimes\mathbb{1} - J H_\eta\otimes\mathbb{1} J\}\Psi\rangle \\ &= \lim_{\eta\to\infty} \{\langle\Psi, (H_\eta\otimes\mathbb{1})\Psi\rangle - \langle(H_\eta\otimes\mathbb{1})\Psi, \Psi\rangle\} \\ &= 0. \quad \text{q.e.d.} \end{aligned}$$

Remark:

If the Hamiltonian is given such that $D_H := e^{-H}$ is a trace class operator in $\mathscr{H}$, i.e. $\mathrm{tr}(D_H) < \infty$, then there exists a complete orthonormal basis $\{\Psi_k\}$ with $H\Psi_k = \lambda_k \Psi_k$. Then we can represent the state $a \mapsto \mathrm{tr}(D_H a)$, $a\in\mathscr{B}(\mathscr{H})$ by the cyclic and separating vector

$$\Psi_H := \sum_{k=1}^{\infty} e^{-\lambda_k/2} \Psi_k\otimes\Psi_k:$$

$$\begin{aligned} \psi_H(a) &:= \mathrm{tr}(D_H a) \\ &= \sum_{k=1}^{\infty} \langle\Psi_k, e^{-H} a \Psi_k\rangle \\ &= \sum_{k=1}^{\infty} e^{-\lambda_k} \langle\Psi_k\otimes\Psi_k, (a\otimes\mathbb{1})\Psi_k|\otimes\Psi_k\rangle \\ &= \sum_{k,k'=1}^{\infty} e^{-\lambda_k/2} e^{-\lambda_{k'}/2} \\ &\quad \cdot \langle\Psi_k\otimes\Psi_k, (a\otimes\mathbb{1})\Psi_{k'}\otimes\Psi_{k'}\rangle \\ &= \langle\Psi_H, (a\otimes\mathbb{1})\Psi_H\rangle, \quad a\in\mathscr{B}(\mathscr{H}). \end{aligned} \tag{29}$$

ψ_H satisfies the KMS-condition with respect to the evolution

$$a \mapsto e^{-iHt} a e^{iHt}, \quad a\in\mathscr{B}(\mathscr{H}), \quad t\in\mathbb{R} \tag{30}$$

as a state on $\mathscr{B}(\mathscr{H})$, and with respect to the evolution

$$\begin{aligned} & a\otimes\mathbb{1} \mapsto e^{-i\mathbb{H}t}(a\otimes\mathbb{1}) e^{i\mathbb{H}t}, \\ & a\otimes\mathbb{1}\in\mathfrak{M}, \quad t\in\mathbb{R} \end{aligned} \tag{31}$$

as a state on $\mathfrak{M}$. The modular operator for Ψ_H is given by

$$\Delta_{\Psi_H} = e^{-\mathbb{H}}. \tag{32}$$

Therefore, if $\mathrm{tr}(D_H) < \infty$, the KMS-equilibrium state ψ_H on the standard representation of $\mathscr{B}(\mathscr{H})$ is a natural reference state.

We must stress the fact that in this subsection we have constituted the energy by the time evolution and a standard normalization, not by the Hamiltonian! A given Hamiltonian H obviously defines a time evolution, but not vice versa.

For instance an additive constant in H will be cancelled in $\mathbb{H}$. (This can be used in the discussion of renormalization problems.) The uniqueness of the Hamiltonian can be introduced if one agrees on a canonical implementation of the time evolution, such as the standard implementation. – Notice that we use "Hamiltonian" in the case of a closed, reversible system with a time automorphism group, whereas "energy operator" is understood in a less restrictive sense.

3. Pairs of states invariant under a partial dynamics

We come back to the case of an arbitrary von Neumann algebra in standard form, where a faithful reference state $\psi \in \mathfrak{M}_{*+}$ and an energy operator H are given by (19), with a self-adjoint operator R affiliated with $\mathfrak{M}$. We are looking for a class of states with

$$\varphi(\log \Delta_\psi) = 0\,, \tag{33a}$$

so that

$$\begin{aligned}\omega^H_{\varphi,\psi} &= \lim_{\eta\to\infty} \{\varphi(-\log \Delta_\psi + R_\eta) \\ &\quad - \psi(-\log \Delta_\psi + R_\eta)\} \\ &= \lim_{\eta\to\infty} \{\varphi(R_\eta) - \psi(R_\eta)\}\,. \end{aligned} \tag{33b}$$

The following proposition answering this question is taken from Theorem 15.2 in [16] and Theorem 2 in [17].

Propositon 5. Let $\varphi \in \mathfrak{M}_{*+}$ be faithful. Then the following conditions are equivalent:

(i) $\varphi(\log \Delta_\psi) = 0$;

(ii) $\psi(\log \Delta_\Phi) = 0$;

(iii) $\varphi(\sigma^\psi_t(x)) = \varphi(x)\,, \quad x \in \mathfrak{M}\,, \quad t \in \mathbb{R}$;

(iv) $\psi(\sigma^\varphi_t(x)) = \psi(x)\,, \quad x \in \mathfrak{M}\,, \quad t \in \mathbb{R}$;

(v) $\sigma^\varphi_t(\sigma^\psi_s(x)) = \sigma^\psi_s(\sigma^\varphi_t(x))\,, \quad x \in \mathfrak{M}\,, \quad s, t \in \mathbb{R}$;

(vi) $|\varphi + i\psi| = |\varphi - i\psi|$
($|\omega|$ means the absolute value of $\omega \in \mathfrak{M}_*$);

(vii) $\varphi(x) = \langle h\Psi, x\, h\Psi\rangle, \quad x \in \mathfrak{M}$,
for some positive selfadjoint h affiliated with
$\mathfrak{M}_\psi := \{x \in \mathfrak{M} \mid \psi(x\,y) = \psi(y\,x)\,, \quad y \in \mathfrak{M}\}$
$= \{x \in \mathfrak{M} \mid \sigma^\psi_t(x) = x, t \in \mathbb{R}\}$;

(viii) $\psi(x) = \langle h\Phi, x\, h\Phi\rangle, \quad x \in \mathfrak{M}$,
for some positive selfadjoint h
affiliated with $\mathfrak{M}_\varphi$.

Proof:

(iii) $\Rightarrow$ (i), (iv) $\Rightarrow$ (ii):

$$\begin{aligned}\log(\Delta_\psi)\,\Phi &= -i\frac{\mathrm{d}}{\mathrm{d}t}(\Delta_\psi)^{it}\,\Phi\,|_{t=0} \\ &= -i\frac{\mathrm{d}}{\mathrm{d}t}\,\xi(\varphi\circ\sigma^\psi_t)\,|_{t=0} \\ &= -i\frac{\mathrm{d}}{\mathrm{d}t}\,\xi(\varphi) \\ &= 0\,.\end{aligned}$$

The second equation is known from the standard implementation of automorphisms (Corollary 2.5.3 in [12]).

(i) $\Rightarrow$ (iii), (ii) $\Rightarrow$ (iv): follows from the series expansion of the exponential function.

The other statements are covered by the above mentioned references. q.e.d.

§ 5. Standard form and New-Tamm-Dancoff procedure

So far we have discussed the problem of energy differences in von Neumann algebras which have been arbitrary, except in § 4.2. Now we establish the relations with the NTD method. Before we reproduce the results of the structural analysis of NTD from [4, 7, 18] we need a more specific set up.

A complex physical model usually starts with an assembly of a large but finite number of elementary objects. In solid state physics such elementary objects are the relevant electrons of a crystal constituted by the irreducible representations of the Galilei group, if one works in the Galilei-relativistic area. To have a definite frame of discussion we describe these objects by operators a_k labelled by numbers k of a set of modes, denoted Γ. Let a^*_k be the creation operator of an electron in the mode k acting on the antisymmetric Fock space $\mathcal{F}$, and a_k the corresponding destruction operator, such that

$$\begin{aligned}&[a_k, a^*_k]_+ = \delta_{kk'}\,\mathbb{1}\,, \\ &[a_k, a_{k'}]_+ = 0\,, \quad k, k' \in \Gamma\,.\end{aligned} \tag{34}$$

Let Ω_0 be the Fock vacuum,

$$a_k\,\Omega_0 = 0\,, \quad k \in \Gamma\,. \tag{35}$$

Denote the algebra of the canonical anticommutation relations (34) (CAR), acting on $\mathcal{F}$, by $\mathfrak{A}$.

For calculating energy differences with respect to an appropriate reference state, Dyson [1] originally introduced the NTD-coefficients

$$\varphi^D_{\Psi_0, X_0}(N' \mid N) = \langle \Psi_0, a^{*N'} a^N X_0\rangle\,, \quad N, N' \subseteqq \Gamma, \tag{36}$$

which distinguish the Fock space basis

$$a^{*N} a^{N'} \Psi_0\,. \tag{37}$$

The vector

$$\Psi_0 = a^{*N'}\,\Omega_0 \tag{38}$$

* X = capital greek chi.

describes the physical vacuum, and the vector χ_0 the actual state of the system. He proposed to use the difference equation ((6.1), (6.6) in [7])

$$\langle \Psi_0, [a^{*N'} a^N, H] X_0 \rangle = (E_{X_0} - E_{\Psi_0}) < \Psi_0, a^{*N'} a^N X_0 \rangle , \quad (39)$$

where H is the Hamiltonian, and E_{X_0}, E_{Ψ_0} eigenvalues of H for

$$X_0 / \| \chi_0 \| \quad \text{resp.} \quad \Psi_0 / \| \Psi_0 \| .$$

The analysis in [4, 7, 18] revealed the equivalence of (39) with (see (10.2) – (10.6) in [7])

$$e^{-u \cdot v} (H^{\Delta} \hat{\otimes} \mathbb{1} - \mathbb{1} \hat{\otimes} H_{iv^*}) (X^{\Delta} \hat{\otimes} \Psi_{iv^*}) = (E_{\chi_0} - E_{\Psi_0}) e^{-u \cdot v} (X^{\Delta} \hat{\otimes} \Psi_{iv^*}) . \quad (40)$$

In this product space formulation of NTD the CAR-algebra $\mathfrak{A}$ is replaced by a CAR-tensor-product $\mathfrak{A}_u \hat{\otimes} \mathfrak{A}_v$ of two copies of $\mathfrak{A}$, mutually distinguished by the u- resp. v-notation of their elements. The product Hilbert space is formed with the product of the Fock vacua of the single Fock spaces as

$$\mathscr{F}_u \hat{\otimes} \mathscr{F}_v := \overline{(\mathfrak{A}_u \hat{\otimes} \mathfrak{A}_v) (\Omega_u \otimes \Omega_v)} . \quad (41)$$

$\Psi_0 \leftrightarrow \Psi_0^{\Delta}$, and $X_0 \to (X_0)_{iv^*}$ are Hilbert space conjugations, up to unitary equivalence [6, 7].

$$e^{-u \cdot v} := \exp \left(- \sum_{k \in \Gamma} u_k v_k \right)$$

generates the so-called "Symanzik-transformation" ((10.2) in [7]).

If we isolate

$$\langle X_0 \otimes \Psi_0, \{H^T \otimes \mathbb{1} - \mathbb{1} \otimes H\} X_0 \otimes \Psi_0 \rangle = (E_{X_0} - E_{\Psi_0}) < X_0 \otimes \Psi_0, X_0 \otimes \Psi_0 \rangle \quad (42)$$

from (40) incorporating the antisymmetric character of the tensor product as well as the conjugations to the Symanzik transformation, and introducing the transposition conjugation instead of $H \to H^{\Delta}$, we can compare it directly with (12) which is shown as follows.

Assume the vector $\Psi_0 \in \mathscr{F}$ to be separating for $\mathfrak{A}$. Let D_{Ψ_0} and D_{X_0} be the density matrices of the states

$$x \in \mathfrak{A} \mapsto \psi_0(x) := \langle \Psi_0, x \Psi_0 \rangle ,$$
$$x \in \mathfrak{A} \mapsto \chi_0(x) := \langle X_0, x X_0 \rangle .$$

Let $\{\Psi_k\}$ be the orthonormal eigenbasis of D_{Ψ_0}, with corresponding eigenvalues μ_k^2. The vector

$$\Psi := \sum_{k=1}^{\infty} \mu_k \Psi_k \otimes \Psi_k \in \mathscr{F} \otimes \mathscr{F} \quad (43)$$

represents the state

$$\psi(x \otimes \mathbb{1}) := \langle \Psi, x \otimes \mathbb{1} \Psi \rangle , \quad x \in \mathfrak{A} \quad (44)$$

in the natural positive cone of the standard representation of $\mathfrak{A}$ (see § 4.2). Now we may rewrite (42) as

$$\psi \{ ((D_{X_0}^T)^{1/2} \otimes \mathbb{1}) (\mathbb{1} \otimes D_{\Psi_0}^{-1/2}) (H^T \otimes \mathbb{1}) \cdot ((D_{X_0}^T)^{1/2} \otimes \mathbb{1}) - (H^T \otimes \mathbb{1}) \} = (E_{X_0} - E_{\Psi_0}) \psi(\mathbb{1}) . \quad (45)$$

We have precisely arrived at (12) since (see [19])

$$\Delta_{\chi, \Psi} = D_{\chi} J D_{\Psi}^{-1} J , \quad (46)$$

where D_{χ}, D_{Ψ} are the density matrices of states χ resp. ψ with respect to the standard representation Hilbert space, and the standard representation construction of § 4.2 implies the identification

$$D_{\chi} = D_{\chi_0}^T \otimes \mathbb{1} , \quad J D_{\Psi} J = \mathbb{1} \otimes D_{\Psi_0} . \quad (47)$$

It seems that the non-unitary Symanzik transformation $\xi \in \mathscr{F}_u \hat{\otimes} \mathscr{F}_v \mapsto e^{-u \cdot v} \xi \in \mathscr{F}_u \hat{\otimes} \mathscr{F}_v$ is unphysically (see (11.2) in [7]) arising from a purely formal manipulation. Instead of (40) one should take (42) as a physically relevant difference equation.

The intention of the coefficients (36) is the choice of an appropriate basis. But this can be done by a unitary basis transformation. If the set of modes Γ is finite, the one-particle Hilbert space underlying the Fock space $\mathscr{F}$ is finite-dimensional too, and it does not matter which basis we choose. However if we produce idealizations by limit procedures, inequivalent representations of the canonical anticommutation relations emerge, and the choice of a basis does heavily matter. It has to be ruled by the specific physical idealization. – The question of transformations between two inequivalent representations opens another category.

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