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Galilei Invariant Molecular Dynamics

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Abstract. We construct a C^* -dynamical model for a chemical reaction. Galilei invariance of our nonrelativistic model is demonstrated by defining it directly on a Galilean space-time fibrebundle with C^* -algebra valued fibre, i.e. without reference to any coordinate system. The existence of equilibrium states in this model is established and some of their properties are discussed. PACS 05.30.Fk, 03.70.+k, 11.10.Cd, 11.15.Tk

1. Introduction

Galilei invariant quantum field theories provide a natural candidate for a comparison with relativistic models. Many of the properties typically attributed to relativistic field theories are actually a common feature of every theory with a zero mean-particle density and translation-invariant Hamiltonian [1]. Especially the Galilei invariant Lee model has attracted much attention [2-4]. More recently, Narnhofer and Thirring presented a Galilei invariant model [5,6] in the C*-algebraic approach to quantum field theory. The advantage of such a formulation is that the algebraic formulation of quantum statistical mechanics [7-10] and quantum ergodic theory [11-17] become applicable.

In chapter 3 we present a C*-dynamical model for a chemical reaction which was inspired by the Galilei invariant Lee model cited. We will consider molecules as the elementary objects. We show that our interaction defines a time-evolution in the Heisenberg picture¹. "Stability of matter" tells us that independent of the initial conditions the system does not heat up and collapse. The time development is well defined for arbitrary states and in principle one could tackle problems of nonequilibrium situations where the state changes globally with time and the time evolution can not be unitarily implemented in the GNS-representation corresponding to a state at a fixed time. But work in this direction seems difficult and much remains to be done. Mixing properties will be discussed elsewhere.

In chapter 2 the algebra of observables \mathcal{A} for our model is defined. We deal with three different species of fermions. Some remarks on the superselection structure are added. As usual, the algebra of local observables describes the possibilities of testing the system experimentally. Different methods for the construction of automorphisms are discussed.

It is one of the basic facts of quantum theory that space and time coordinates do not refer to an individual particle but refer to preparation and registration apparatuses. The 'classical' space-time structure is merely encoded in the net of local algebras. This aspect is worked out in the appendix, where the algebra of observables is equipped with the fibre-bundle structure induced by the structure of space-time. The symmetry group of 'nonrelativistic' space-time is of course the Galilei group [18,19]. In fact, the Galilei group provides the transition functions between different charts of the space-time manifold².

In chapter 4 we show that the time-evolution is Galilei invariant, i.e. it can be defined chart independently on the new bundle. While this might look extraordinary for the first sight, we feel that it is the natural, coordinate free formulation of Galilei invariance. That we are able to define a time-evolution in a coordinate-free way makes it evident that only the spatial relationship between the preparation and registration apparatuses are relevant.

Finally chapter 5 answers the question whether or not our model has ground and equilibrium states. The positive answer is based on a result by Powers and Sakai [26]. We point out that equilibrium states spontaneously break Galilei invariance and that even a local perturbation changes the number of parameters labelling different equilibrium states.

2. The Algebra of Observables

We want to describe molecular dynamics involving chemical reactions such as the dissociation of large molecules into two different smaller parts, for example a four atomic molecule which dissociates into two simple molecules:



¹ As in the model of Narnhofer and Thirring this is achieved by cutting of high relative momenta, thereby introducing a slightly non-local character of the interaction.

² The representation theory of the Galilei group on Hilbert spaces is well established [19]. Recently there has been some interest in more abstract aspects of this group [20-25]. Nevertheless the Banach space representations we construct in the appendix seem to have no counterpart in literature.

Since the difference between various isotopes are of no relevance for us we assume that all the particles are fermions. The relevant C^* -algebra is then the 3-fold tensor product of the usual CAR or Fermi algebra \mathcal{A}_F for one species of fermions. Uniqueness of this tensor product is guaranteed by the fact that the Fermi algebra \mathcal{A}_F is nuclear [8].

Definition. Let \mathcal{A} denote the unital C^* -algebra generated by annihilation and creation operators $a(f)$, $a^*(f)$, $b(f)$, $b^*(f)$, $c(f)$ and $c^*(f)$, where $f \in L^2(\mathbb{R}^3)$. These operators correspond to three different particle species with masses $m_a = m_b + m_c$ and obey anticommutation relations

$$\{a(f), a^*(g)\} = (f|g) \mathbf{1}, \quad \{a(f), a(g)\} = 0, \quad (1)$$

and similarly for b and c . Operators corresponding to particles of different species commute. Thus $\mathcal{A} = \mathcal{A}_a \otimes \mathcal{A}_b \otimes \mathcal{A}_c$; $\mathcal{A}_x \cong \mathcal{A}_F$, $x = a, b, c$.

If we are interested in obtaining a Galilei invariant quantum field theory exhibiting production processes, we have to include particles with mass values chosen in agreement with the mass conservation law. This was done in the definition of \mathcal{A} . As noticed by Bargmann [18], the mass operator \mathbf{M} , appearing as an element of the centre of the extended Galilei group Lie algebra, gives rise to a superselection rule. In fact, as long as we have no chemical reactions the superselection sectors are labelled by three charges, corresponding to the three different total masses $\mathbf{M} = \mathbf{M}_a + \mathbf{M}_b + \mathbf{M}_c$. The corresponding equilibrium states are labeled by three distinct chemical potentials. A chemical interaction will change the superselection structure. Besides the total mass only one more parameter will survive. If the particles are charged, then this parameter turns out to be the total charge.

The Lie algebra of the extended Galilei group (see Appendix) tells us that gauge transformations have to commute with time translation. We might therefore think of the gauge group as representing inner symmetries. In addition we expect gauge-dependent quantities to be unobservable. Nevertheless a chemical reaction, corresponding to an operator of the form a^*bc , has to be observable. This suggests the following choice for the action of gauge transformations on \mathcal{A} .

Definition. The action of the gauge group $U(1)$ on \mathcal{A} is given by the continuous, faithful representation $\lambda \in S^1 \rightarrow \gamma_\lambda$ of $U(1)$ into the $*$ -automorphism group of \mathcal{A} , defined by their action on the generating elements of \mathcal{A} ,

$$(a(f), b(f), c(f)) \rightarrow (e^{im_a \lambda} a(f), e^{im_b \lambda} b(f), e^{im_c \lambda} c(f)), \quad (2)$$

and linear extension. The fixed-point algebra under the action of $U(1)$ is called the *observable algebra*.

We list three different procedures for the construction of automorphisms γ of \mathcal{A} . Their common feature is that $\gamma(a(f))$, $\gamma(b(f))$ and $\gamma(c(f))$ are specified on a total set \mathcal{T} of functions $f \in \mathcal{T} \subset L^2(\mathbb{R}^3)$. Then this definition is extended to the whole generating system of \mathcal{A} by setting $\gamma(\mathbf{1}) := \mathbf{1}$ and $\gamma(a^*(f)) := (\gamma(a(f)))^*$ and similarly for b and c . If now γ respects the defining relations among the generators, it can be extended to a $*$ -isomorphism of \mathcal{A} (again denoted by γ), because of the uniqueness of the CAR-algebra [8] and the involved tensor products.

(i) . Coherent states

$$f_{q,p}(x) := \pi^{-\frac{3}{4}} e^{-\frac{1}{2}(x-q)^2 + ip(x-q)} \in L^2(\mathbb{R}^3, d^3x), \quad z = (q, p) \in T^*(\mathbb{R}^3), \quad (3)$$

explicitly relate to the classical picture. We may think of $a_z := a(f_z)$ as an operator destroying a particle centred at $z = (q, p)$ in phase space. This correspondence between the classical and the quantum picture allows us to lift group representations from ordinary phase space $T^*(\mathbb{R}^3)$ to groups of automorphisms of \mathcal{A} . For example, the *kinematical* automorphisms

$$\gamma_g^{Kin}(t)(a_z) := e^{im_a \lambda + im_a \frac{v^2}{2}(t-s) + im_a v Rq} a_{Rq+vt+a-sv, Rp+m_a v} \quad (4)$$

$g = (\lambda, s, a, v, R)$, define a representation of the extended Galilei group G^1 in $Aut(\mathcal{A})$. (The phase-factor was chosen in agreement with the cocycle relation of the Galilei group extension.)

- (ii) . The standard procedure to lift unitary representations of groups from the quantum mechanical one-particle space to quasifree automorphisms of the algebra was introduced by Bogoliubov [8]. Since the kinematical automorphisms are quasifree we could as well use representations of the Galilei group in coordinate-space [19]:

$$f(x) \rightarrow e^{im\lambda + im\frac{v^2}{2}(t-s) + imv \cdot (x-a)} f(R^{-1}(x - a - vt + vs)), \quad f \in L^2(\mathbf{R}^3), \quad (5)$$

for a construction of these automorphisms. The free time evolution $\tau_t^\circ(a(f)) := a(e^{-i\frac{\Delta}{2m}t}f)$ provides another example.

- (iii) . Each hermitian element $b = b^*$ of \mathcal{A} defines a so-called inner automorphism:

$$\gamma_g^b := e^{-ibg} a e^{ibg} \quad b = b^* \in \mathcal{A}, \quad a \in \mathcal{A} \quad (6)$$

Since \mathcal{A} is a Banach space, we are allowed to consider limits. The limit $\gamma_g^b := \lim_{n \rightarrow \infty} \gamma_g^{b_n}$ might exist even when $\{b_n\}_{n \in \mathbf{N}}$ does not converge in \mathcal{A} . Such automorphisms are called outer automorphisms.

3. A Thermodynamical System with Chemical Reactions

While the Narnhofer-Thirring model is concerned with pair interactions, of similar molecules with (regularised) Van der Waal's interaction for example, the present interaction only includes vertex functions that model the restructuring of the electrons once the molecules have got so close to one another that their electron clouds overlap.

We construct the interacting time-evolution in three steps, as proposed by Guenin [27]:

- (i) . We "cut-off" the interaction in such a way that v_n exists as an element in \mathcal{A} , thereby destroying Galilei invariance.
- (ii) . We define inner automorphisms τ^n corresponding to the "cut-off" interaction v_n .
- (iii) . We construct the interacting time-evolution as a limit of inner automorphisms by releasing the cut-offs and thereby restoring Galilei invariance.

Two atomic molecules are idealised as point particles at a fixed distance \hat{q} and with equal momentum. The spatial orientation of the molecular axis should be of secondary importance and is therefore neglected.

Definition. Let $\tau_s := s - \lim_{n \rightarrow \infty} \tau_s^n$ — where $s - \lim$ denotes the strong (=pointwise) limit in $\mathcal{B}(\mathcal{A})$ — of the following automorphisms τ_s^n :

$$\tau_s^n(a) := \tau_s^\circ(a) + \sum_{k=1}^{\infty} \frac{i^k}{k!} \int_{[0,s]^k} d(t_1 \dots t_k) [\tau_{t_k}^\circ(v_n), [\dots, [\tau_{t_1}^\circ(v_n), \tau_s^\circ(a)] \dots]] \quad (7)$$

where

$$v_n = \int_{|q_i|, |p_i| \leq n} d^3 q_1 d^3 q_2 d^3 q_3 d^3 p_1 d^3 p_2 d^3 p_3 \int_{|\hat{q}| = \text{const}} d^2 O V(|q_1 - q_2|, |q_1 - q_3|, |\frac{p_1}{m_a} - \frac{p_2}{m_b}|, |\frac{p_1}{m_a} - \frac{p_3}{m_c}|, \vartheta_q, \vartheta_p) \times \left(a_{q_1, p_1}^* a_{q_1 + \hat{q}, p_1}^* b_{q_2, p_2} b_{q_2 + \hat{q}, p_2} c_{q_3, p_3} c_{q_3 + \hat{q}, p_3} + c_{q_3 + \hat{q}, p_3}^* c_{q_3, p_3}^* b_{q_2 + \hat{q}, p_2}^* b_{q_2, p_2}^* a_{q_1 + \hat{q}, p_1} a_{q_1, p_1} \right). \quad (8)$$

ϑ_q denotes the angle between $(q_1 - q_2)$ and $(q_1 - q_3)$ and ϑ_p between $(\frac{p_1}{m_a} - \frac{p_2}{m_b})$ and $(\frac{p_1}{m_a} - \frac{p_3}{m_c})$. The vertex $V(|q|, |q'|, |p|, |p'|, \vartheta_q, \vartheta_p)$ is assumed to be in $L^1(\mathbf{R}^{12}, d^3 q d^3 q' d^3 p d^3 p') \cap C(\mathbf{R}^{12})$, thus all Bochner-integrals exist.

We have symmetrized our description, for example the creation operator of a molecule of type a centred around q, p was taken to be

$$a_{q,p}^* = \int_{|\hat{q}|=const} dO a_{q+\hat{q},p}^* \quad (9)$$

where dO denotes the surface integral over the sphere $|\hat{q}| = const$.

The vertex function V should be strictly localised in a region of order of the atomic distances \hat{q} . The momentum dependence of the vertex function is unknown, but we have only required integrability and this seems to be a decent assumption. We have made no restrictions on the angular dependence of the position and the momentum distributions since V will certainly depend on ϑ_q and ϑ_p .

Furthermore, our six-particle vertex will not allow dissociation with very high relative momenta of the molecules. However, there will be no limit on the momentum cut-off and one can expect that for stable systems where high momenta do not occur in a reasonable subset of states, our interaction gives a physically acceptable description.

One can interpret the presented model alternatively as one involving particle creation and annihilation. In any case, it exists strictly on the C^* -algebraic level, without any renormalization or restriction to any representation. The interaction is constructed so that there are two conservation laws: the number of a -particles plus the number of b -particles is conserved, and the number of b particles minus the number of c -particles.

Before we enter the proof of the existence of the limits used to define the time evolution we mention that the interaction is stable for both signs of the coupling constant. It was argued in [14] that this is necessary, if the interaction defines a strongly continuous automorphism. Furthermore it automatically ensures a reasonable thermodynamical behaviour of the system by guaranteeing that the energy is an extensive quantity, which is a basic assumption in phenomenological thermodynamics.

Lemma 3.1. *The interaction is stable³, i.e., there exists a positive real number $c \in \mathbb{R}^+$, such that*

$$h_n := h_n^\circ + v_n > -c((N_a)_n + (N_b)_n), \quad (10)$$

where $(h_a^\circ)_n = \frac{1}{2m_a} \int_{|q|,|p| \leq n} d^3q d^3p a^*(\nabla f_{q,p}) a(\nabla f_{q,p})$ and $(N_a)_n = \int_{|q|,|p| \leq n} d^3q d^3p a_{q,p}^* a_{q,p}$ and similar for b, c .

Proof. We first show that $x + x^* \leq \sqrt{2}(x^*x + xx^*)^{1/2}$. From $(x - x^*)^*(x - x^*) \geq 0$ we infer

$$x^*x + xx^* \geq x^2 + (x^*)^2. \quad (11)$$

Thus $2(x^*x + xx^*) \geq (x + x^*)^2$. We recall that operators corresponding to different particles commute. Thus

$$\begin{aligned} v_n &= \int_{|q_i|,|p_i| \leq n} d^3q_1 \dots d^3p_3 \int_{|\hat{q}|=const} dO V(\dots) \left(a_{q_1,p_1}^* a_{q_1+\hat{q},p_1}^* b_{q_2,p_2} b_{q_2+\hat{q},p_2} c_{q_3,p_3} c_{q_3+\hat{q},p_3} + \text{herm.conj.} \right) \\ &\leq \sqrt{2} \int_{|q_i|,|p_i| \leq n} d^3q_1 \dots d^3p_3 \int_{|\hat{q}|=const} dO V(|q_1 - q_2|, |q_1 - q_3|, \left| \frac{p_1}{m_a} - \frac{p_2}{m_b} \right|, \left| \frac{p_1}{m_a} - \frac{p_3}{m_c} \right|, \vartheta_q, \vartheta_p) \times \\ &\quad \times \left(c_{q_3+\hat{q},p_3}^* c_{q_3,p_3}^* b_{q_2+\hat{q},p_2}^* b_{q_2,p_2}^* a_{q_1+\hat{q},p_1} a_{q_1,p_1} a_{q_1,p_1}^* a_{q_1+\hat{q},p_1}^* b_{q_2,p_2} b_{q_2+\hat{q},p_2} c_{q_3,p_3} c_{q_3+\hat{q},p_3} \right. \\ &\quad \left. + a_{q_1,p_1}^* a_{q_1+\hat{q},p_1}^* b_{q_2,p_2} b_{q_2+\hat{q},p_2} c_{q_3,p_3} c_{q_3+\hat{q},p_3} c_{q_3+\hat{q},p_3}^* c_{q_3,p_3}^* b_{q_2+\hat{q},p_2}^* b_{q_2,p_2}^* a_{q_1+\hat{q},p_1} a_{q_1,p_1} \right)^{1/2}. \end{aligned} \quad (12)$$

³ This result evolved from discussions with E. Lieb, D. Buchholz, H. Narnhofer and R. Verch.

Next we apply the operator inequality

$$abb^*a^* \leq aa^* \|b\| \|b^*\| \quad (13)$$

and use the operator monotony of the square root. Once more it is crucial that operators corresponding to different particles commute. We find

$$\begin{aligned} v_n &\leq \sqrt{2} \int_{|q_i|, |p_i| \leq n} d^3 q_1 \dots d^3 p_3 \int_{|\hat{q}| = \text{const}} dO V(|q_1 - q_2|, |q_1 - q_3|, \dots, \vartheta_q, \vartheta_p) \left(b_{q_2, p_2}^* b_{q_2, p_2} + a_{q_1, p_1}^* a_{q_1, p_1} \right)^{1/2} \\ &\leq \sqrt{2} \ 4\pi |\hat{q}|^2 \sup_{q_2, p_2} \int_{|q_i|, |p_i| \leq n} d^3 q_2 \dots d^3 p_3 V(|q_1 - q_2|, |q_1 - q_3|, \dots, \vartheta_q, \vartheta_p) \int_{|q_2|, |p_2| \leq n} d^3 q_2 d^3 p_2 b_{q_2, p_2}^* b_{q_2, p_2} \\ &\quad + \sqrt{2} \ 4\pi |\hat{q}|^2 \sup_{q_1, p_1} \int_{|q_i|, |p_i| \leq n} d^3 q_2 \dots d^3 p_3 V(|q_1 - q_2|, |q_1 - q_3|, \dots, \vartheta_q, \vartheta_p) \int_{|q_1|, |p_1| \leq n} d^3 q_1 d^3 p_1 a_{q_1, p_1}^* a_{q_1, p_1} \\ &\leq \sqrt{2} \ 4\pi |\hat{q}|^2 m_a^6 \|V\|_1 \left(\int_{|q_2|, |p_2| \leq n} d^3 q_2 d^3 p_2 b_{q_2, p_2}^* b_{q_2, p_2} + \int_{|q_1|, |p_1| \leq n} d^3 q_1 d^3 p_1 a_{q_1, p_1}^* a_{q_1, p_1} \right) \end{aligned} \quad (14)$$

In the last two inequalities we used the fact that $P_a = a_{q_2, p_2}^* a_{q_2, p_2}$ and $P_b = b_{q_1, p_1}^* b_{q_1, p_1}$ are commuting projection operators and therefore $(P_a + P_b)^{1/2} \leq P_a + P_b$. Thus $v_n < 4\pi |\hat{q}|^2 m_a^6 \|V\|_1 ((N_a)_n + (N_b)_n)$ and similarly for a and c . \square

Stability for the opposite sign follows by the same line of arguments.

Theorem 3.2. τ is well defined (as a strongly continuous one-parameter group of automorphism of \mathcal{A} .)

Proof. We show that the perturbation formula (7) for $\tau_t^n(a_z)$ converges for all $z \in T^*(\mathbf{R}^3)$ as $n \rightarrow \infty$. We proceed in three steps.

(i) *The number of graphs does not increase too fast.* The strategy is to rewrite commutators in terms of anticommutators. The first order in the coupling constant is

$$\begin{aligned} &\int_0^t dt_1 \int_{|q_i|, |p_i| \leq n} d^3 q_1 \dots d^3 p_3 \int_{|\hat{q}| = \text{const}} dO V(|q_1 - q_2|, |q_1 - q_3|, |\frac{p_1}{m_a} - \frac{p_2}{m_b}|, |\frac{p_1}{m_a} - \frac{p_3}{m_c}|, \vartheta_q, \vartheta_p) \times \\ &\quad \times [\tau_{t_1}^\circ (a_{q_1, p_1}^* a_{q_1 + \hat{q}, p_1}^* b_{q_2, p_2} b_{q_2 + \hat{q}, p_2} c_{q_3, p_3} c_{q_3 + \hat{q}, p_3} + c_{q_3, p_3}^* c_{q_3 + \hat{q}, p_3}^* b_{q_2, p_2}^* b_{q_2 + \hat{q}, p_2}^* a_{q_1, p_1} a_{q_1 + \hat{q}, p_1}), \tau_t^\circ(a_{z'})] \end{aligned} \quad (15)$$

As one can see from this expression, every new order in the coupling constant introduces two products of six creation and annihilation operators. Given a fixed creation operator (resp. annihilation operator) only one of these two terms has a nonvanishing commutator. For example, in the first order we find:

$$\begin{aligned} &[\tau_{t_1}^\circ (a_{q_1, p_1}^* a_{q_1 + \hat{q}, p_1}^* b_{q_2, p_2} b_{q_2 + \hat{q}, p_2} c_{q_3, p_3} c_{q_3 + \hat{q}, p_3} + c_{q_3, p_3}^* c_{q_3 + \hat{q}, p_3}^* b_{q_2, p_2}^* b_{q_2 + \hat{q}, p_2}^* a_{q_1, p_1} a_{q_1 + \hat{q}, p_1}), \tau_t^\circ(a_{z'})] \\ &= [\tau_{t_1}^\circ (a_{q_1, p_1}^* a_{q_1 + \hat{q}, p_1}^*), \tau_t^\circ(a_{z'})] \tau_{t_1}^\circ (b_{q_2, p_2} b_{q_2 + \hat{q}, p_2} c_{q_3, p_3} c_{q_3 + \hat{q}, p_3}) \\ &= \{ \tau_{t_1}^\circ (a_{q_1, p_1}^*), \tau_t^\circ(a_{z'}) \} \tau_{t_1}^\circ (a_{q_1 + \hat{q}, p_1}^* b_{q_2, p_2} b_{q_2 + \hat{q}, p_2} c_{q_3, p_3} c_{q_3 + \hat{q}, p_3}) \\ &\quad + \{ \tau_{t_1}^\circ (a_{q_1 + \hat{q}, p_1}^*), \tau_t^\circ(a_{z'}) \} \tau_{t_1}^\circ (a_{q_1, p_1}^* b_{q_2, p_2} b_{q_2 + \hat{q}, p_2} c_{q_3, p_3} c_{q_3 + \hat{q}, p_3}) \end{aligned} \quad (16)$$

Thus we are left with two products of five (=4+1) creation and annihilation operators. If we expand the next commutator into anticommutators each of the 4+1 creation and annihilation operators has two non vanishing anticommutators with the interaction. Therefore in second order we have to compute bounds for

2.(4 + 1).2 terms of length $2 \times 4 + 1$. By the same line of arguments the number of nonvanishing terms in third order is given by $2 \times (4 + 1) \times 2 \times (8 + 1) \times 2$. For arbitrary order k we get

$$\frac{2.(4 + 1).2.(2.4 + 1)...2.(k.4 + 1).2}{1.2.3...k} = 2^{k+1} \cdot (4 + 1) \cdot (4 + \frac{1}{2}) \dots (4 + \frac{1}{k}) \leq 2 \times (2 \times 5)^k \quad (17)$$

(ii) The time-evolution can be written as a series of absolutely convergent summands.

$$\|\tau_t^n(a)\| \leq \|\tau_t^\circ(a)\| + \sum_{k=1}^{\infty} \left\| \lim_{m \rightarrow \infty} \frac{1}{k!} \int_{[0,t]^k} d(t_1 \dots t_k) [\tau_{t_k}^\circ(v_m), [\dots, [\tau_{t_1}^\circ(v_m), \tau_t^\circ(a)] \dots]] \right\| \quad \forall n \in \mathbf{N} \quad (18)$$

The idea is to use the fact that the spreading of free coherent wave functions f_z does not depend on the footpoint $z \in T^*(\mathbf{R}^3)$:

$$\int d^6 z' \|\{\tau_t^\circ(a^*(f_z)), \tau_{t'}^\circ(a(f_{z'}))\}\| = \int d^6 z' |(e^{i\mathbf{H}_0 t} f_z | e^{-i\mathbf{H}_0 t'} f_{z'})| = 2^3 (1 + (t - t')^2)^{3/4} \quad \forall z \in T^*(\mathbf{R}^3). \quad (19)$$

Explicitly the norm of the first order term of $\tau_t^n(a_{z'})$,

$$\left\| \int_0^t dt_1 \int_{|q_i|, |p_i| \leq n} d^3 q_1 \dots d^3 p_3 \int_{|\hat{q}| = \text{const}} dO \ V(|q_1 - q_2|, |q_1 - q_3|, |\frac{p_1}{m_a} - \frac{p_2}{m_b}|, |\frac{p_1}{m_a} - \frac{p_3}{m_c}|, \vartheta_q, \vartheta_p) \times \right. \\ \left. \times [\tau_{t_1}^\circ(a_{q_1, p_1}^* a_{q_1 + \hat{q}, p_1}^* b_{q_2, p_2} b_{q_2 + \hat{q}, p_2} c_{q_3, p_3} c_{q_3 + \hat{q}, p_3} + c_{q_3, p_3}^* c_{q_3 + \hat{q}, p_3}^* b_{q_2, p_2}^* b_{q_2 + \hat{q}, p_2}^* a_{q_1, p_1} a_{q_1 + \hat{q}, p_1}), \tau_t^\circ(a_{z'})] \right\| \quad (20)$$

is bounded uniformly in n by

$$\leq \int d^3 q_1 \dots d^3 p_3 \int_{|\hat{q}| = \text{const}} dO \ |V(|q_1 - q_2|, |q_1 - q_3|, |\frac{p_1}{m_a} - \frac{p_2}{m_b}|, |\frac{p_1}{m_a} - \frac{p_3}{m_c}|, \vartheta_q, \vartheta_p)| \\ \times \|\tau_{t_1}^\circ(a_{q_1, p_1}^*) \tau_{t_1}^\circ(a_{q_1 + \hat{q}, p_1}^*), \tau_t^\circ(a_{z'})\| \|\tau_{t_1}^\circ(b_{q_2, p_2})\| \|\tau_{t_1}^\circ(b_{q_2 + \hat{q}, p_2})\| \|\tau_{t_1}^\circ(c_{q_3, p_3})\| \|\tau_{t_1}^\circ(c_{q_3 + \hat{q}, p_3})\| \\ \leq \int_0^t dt_1 \int d^3 q_1 \dots d^3 p_3 \int_{|\hat{q}| = \text{const}} dO \ |V(|q_1 - q_2|, |q_1 - q_3|, |\frac{p_1}{m_a} - \frac{p_2}{m_b}|, |\frac{p_1}{m_a} - \frac{p_3}{m_c}|, \vartheta_q, \vartheta_p)| \\ \times \left(\|\tau_{t_1}^\circ(a_{q_1, p_1}^*)\| \|\{\tau_{t_1}^\circ(a_{q_1 + \hat{q}, p_1}^*), \tau_t^\circ(a_{z'})\}\| + \|\{\tau_{t_1}^\circ(a_{q_1, p_1}^*), \tau_t^\circ(a_{z'})\}\| \|\tau_{t_1}^\circ(a_{q_1 + \hat{q}, p_1}^*)\| \right) \\ \leq 2 \sup_{q_1, p_1} \int d^3 q_2 \dots d^3 p_3 \ |V(|q_1 - q_2|, \dots, |\frac{p_1}{m_a} - \frac{p_3}{m_c}|, \vartheta_q, \vartheta_p)| \times 4\pi |\hat{q}|^2 \int d^6 z_1 \int_0^t dt_1 |(e^{i\mathbf{H}_0 t_1} f_{z_1} | e^{-i\mathbf{H}_0 t} f_{z'})| \\ \leq 8\pi |\hat{q}|^2 \ m_a^6 \|V\|_1 \ |t| \ 2^3 (1 + t^2)^{3/4} \quad (21)$$

Higher orders can be treated in a similar manner. Thus

$$\|\tau_t(a_z')\| \leq 1 + 2 \sum_{k=1}^{\infty} \frac{10^k}{k!} \left(4\pi |\hat{q}|^2 m_a^6 \|V\|_1 |t| 2^3 (1 + t^2)^{3/4} \right)^k \quad (22)$$

and we have established the convergence of $\lim \tau_t^n(a_{z'})$ for $|t| < t_0$ with

$$4\pi |\hat{q}|^2 m_a^6 \|V\|_1 |t_0| 2^3 (1 + t_0^2)^{3/4} = 10^{-1}. \quad (23)$$

(iii) The coherent states $f_{q,p}$ form a total set in $L^2(\mathbf{R}^3)$, thus τ_t can be extended to arbitrary $a(f)$, $f \in L^2(\mathbf{R}^3)$. $\tau_t(b(f))$ and $\tau_t(c(f))$ are constructed in exactly the same manner and so $\lim_{n \rightarrow \infty} \tau_t^n(a)$, $a \in \mathcal{A}$ exists for t small enough by the Banach-Steinhaus theorem. It even defines a *-isomorphism, as can be seen from the (anti-)commutator relations, e.g., $\{\tau_t(a(f)), \tau_t(a^*(g))\} = \{a(f), a^*(g)\}$. Thus $\forall a \in \mathcal{A}$, $\|\tau_t(a)\| = \|a\|$. This allows us to define τ_t for arbitrary $t \in \mathbf{R}$:

$$\tau_t(a) := \tau_{t_1}(\tau_{t_2}(\dots(\tau_{t_r}(a))\dots)) \quad \forall a \in \mathcal{A}, \quad t = t_1 + t_2 + \dots + t_r \in \mathbf{R}, \quad |t_i| < t_0. \quad (24)$$

□

4. Galilei Invariance of the Time Evolution

In nonrelativistic models we deal with nets of local observables $(I \times \mathcal{O}) \rightarrow (I, \mathcal{A}(\mathcal{O}))$, I an open interval, \mathcal{O} an open region in \mathbf{R}^3 , and $\mathcal{A}(\mathcal{O})$ the C^* -algebra corresponding to the respective region. We now³ equip

$$(\mathbf{R}, \mathcal{A}) := \bigcup_{(I, \mathcal{O}) \subset \mathbf{R}^4} (I, \mathcal{A}(\mathcal{O})), \quad (25)$$

with the bundle structure induced from the space-time structure.

Definition. Let $\hat{g}, \hat{h} \in G_o^1 := \{\lambda, s, a, v, R\} \in G^1 | s = 0\}$. Furthermore consider the transition functions

$$\begin{aligned} \Psi_{\hat{g}, \hat{h}} : \mathbf{R} &\rightarrow \text{Aut}(\mathcal{A}) \\ t &\rightarrow \gamma_{\hat{g}^{-1}}^{Kin}(t) \circ \gamma_{\hat{h}}^{Kin}(t). \end{aligned} \quad (26)$$

We define the *Galilean field algebra bundle* to be the fibre bundle

$$\mathcal{M}_{\mathcal{A}} := \left(\bigcup_{\hat{g} \in G_o^1} \{\hat{g}\} \times \mathbf{R} \times \mathcal{A} \right) / \sim, \quad (27)$$

where the equivalence relation \sim is given by $[\hat{g}, t, a] \sim [\hat{h}, t', a'] : \Leftrightarrow t = t'$ and $a' = \Psi_{\hat{h}, \hat{g}}(t) a$.

The set of transition functions $\{\Psi_{\hat{g}, \hat{h}}\}_{\hat{g}, \hat{h} \in G_o^1}$ satisfies the necessary cocycle condition $\Psi_{\hat{g}, \hat{g}} = \gamma_{\hat{g}^{-1} \circ \hat{g}}^{Kin} = id_{\mathcal{A}}$ and $\Psi_{\hat{g}, \hat{h}} \circ \Psi_{\hat{h}, \hat{f}} = \gamma_{\hat{g}^{-1}}^{Kin} \circ \gamma_{\hat{h}}^{Kin} \circ \gamma_{\hat{h}^{-1}}^{Kin} \circ \gamma_{\hat{f}}^{Kin} = \gamma_{\hat{g}^{-1} \circ \hat{h} \circ \hat{h}^{-1} \circ \hat{f}}^{Kin} = \Psi_{\hat{g}, \hat{f}}$, so $\mathcal{M}_{\mathcal{A}}$ is well defined.

Our intention is to show Galilei invariance of the time-evolution by defining it chart-independent on the Galilean field algebra bundle. We will need the following result.

Theorem 4.1. *Let $\hat{g} = (\lambda, s, a, v, R)$ and $g = (\lambda', s', a', v', R')$. The composition law of the automorphisms γ_g is given by*

$$\gamma_g(t + s') \circ \gamma_{g'}(t)(a) = \gamma_{g \circ g'}(t)(a_z), \quad (28)$$

where $g, g' \in G^1$ and $a \in \mathcal{A}$.

Remark. It can be verified by restricting γ_g , $g \in G^1$, to one parameter subgroups, that Theorem 4.1 reproduces the relations used by Narnhofer and Thirring [6] to characterise Galilei invariance. We will see in a moment that this leads to a chart independent description.

Proof. Let denote $g = (0, s, 0, 0, \mathbb{1}) \circ \hat{g} = (\hat{\lambda}, s, \hat{a}, \hat{v}, \hat{R})$. A straight forward computation yields

$$\begin{aligned} \gamma_g(t + s') \circ \gamma_{g'}(t)(a) &= \tau_s \circ \left(\tau_{s'} \circ \gamma_{\hat{g} \circ \hat{g}'}^{Kin}(t)(a) + \lim_{n \rightarrow \infty} \sum_{k=1}^{\infty} \frac{i}{k!} \int_{[0, s']^k} d(t_1 \dots t_k) [\tau_{t_k} \circ \gamma_{(\hat{\lambda} + \frac{1}{2} v^2 t_k, 0, a + vt_k, v, R)}^{Kin}(t + s' - t_k)(v_n), \right. \\ &\quad \left. [\dots, [\tau_{t_k} \circ \gamma_{(\hat{\lambda} + \frac{1}{2} v^2 t_k, 0, a + vt_1, v, R)}^{Kin}(t + s' - t_1)(v_n), \tau_{s'} \circ \gamma_{\hat{g} \circ \hat{g}'}^{Kin}(t)(a)] \dots] \right) \end{aligned} \quad (29)$$

Thus it remains to show that the spatial symmetry gets restored, $\lim_{n \rightarrow \infty} \|[v_n - \gamma_{\hat{g}}^{Kin}(v_n), a]\| = 0$, for all $a \in \mathcal{A}$. This can be seen as follows:

³ For further details we refer the reader to the appendix.

$$\begin{aligned}
\gamma_{\hat{g}}^{Kin}(t)(v_n) &= \int_{\substack{|R^{-1}q_i - a - vt| \leq n \\ |R^{-1}p_i - m_i v| \leq n}} d^3 z_1 d^3 z_2 d^3 z_3 \int dOV(|R^{-1}q_1 - a - vt - R^{-1}q_2 + a + vt|, \dots, |\frac{R^{-1}p_1}{m_a} - v - \frac{R^{-1}p_3}{m_c} + v|, \vartheta_q, \vartheta_p) \\
&\quad \times \left(a_{z_1}^* a_{z_1 + \hat{q}}^* b_{z_2} b_{z_2 + \hat{q}} c_{z_3} c_{z_3 + \hat{q}} + c_{z_3}^* c_{z_3 + \hat{q}}^* b_{z_2}^* b_{z_2 + \hat{q}}^* a_{z_1} a_{z_1 + \hat{q}} \right) \\
&= \int_{\substack{|R^{-1}q_i - a - vt| \leq n \\ |R^{-1}p_i - m_i v| \leq n}} d^3 z_1 d^3 z_2 d^3 z_3 \int_{|\hat{q}|=const} dOV(|q_1 - q_2|, \dots, \vartheta_p) \left(a_{z_1}^* a_{z_1 + \hat{q}}^* b_{z_2} b_{z_2 + \hat{q}} c_{z_3} c_{z_3 + \hat{q}} + c_{z_3}^* c_{z_3 + \hat{q}}^* b_{z_2}^* b_{z_2 + \hat{q}}^* a_{z_1} a_{z_1 + \hat{q}} \right)
\end{aligned} \tag{30}$$

and the change of integration boundaries vanishes in the limit n to infinity. Due to the strong continuity of τ° this implies

$$\begin{aligned}
s - \lim_{n \rightarrow \infty} \sum_{k=1}^{\infty} \frac{i}{k!} \int_{[0,s]^k} d(t_1 \dots t_k) [\tau_{t_k}^\circ \circ \gamma_{\hat{g}}^{Kin}(v_n), [\dots, [\tau_{t_1}^\circ \circ \gamma_{\hat{g}}^{Kin}(v_n), \tau_s^\circ(\cdot)] \dots]] \\
= s - \lim_{n \rightarrow \infty} \sum_{k=1}^{\infty} \frac{i}{k!} \int_{[0,s]^k} d(t_1 \dots t_k) [\tau_{t_k}^\circ(v_n), [\dots, [\tau_{t_1}^\circ(v_n), \tau_s^\circ(\cdot)] \dots]], \tag{31}
\end{aligned}$$

and consequently (28) holds. \square

Together with the kinematical automorphisms γ^{Kin} the time evolution provides a representation of the extended Galilei group G^1 as bundle isomorphisms on \mathcal{M}_A :

Theorem 4.2. *Let $\hat{g} = (\hat{\lambda}, 0, \hat{a}, \hat{v}, \hat{R})$ and $g = (\lambda, s, a, v, R)$. The interacting time-evolution $\Pi : G^1 \rightarrow Iso(\mathcal{M}_A)$:*

$$\begin{aligned}
g \rightarrow i_g : \mathcal{M}_A &\rightarrow \mathcal{M}_A \\
[\hat{g}, t, a] &\rightarrow [(\hat{\lambda}, s, \hat{a}, \hat{v}, \hat{R}) \circ g^{-1}, t + s, \tau_s \circ \gamma_{(\hat{\lambda}, 0, \hat{a}, \hat{v}, \hat{R})}^{Kin}(t)(a)]
\end{aligned} \tag{32}$$

defines a representation of G^1 as fibre bundle-isomorphisms on \mathcal{M}_A .

Proof. Let $\gamma_g(t) = \tau_s \circ \gamma_{(\lambda, 0, a, v, R)}^{Kin}(t)$ and $g = (\lambda, s, a, v, R)$.

(i) i_g is well defined, $\gamma_g(t)(a') = (\gamma_g(t)(a))'$. Let $[\hat{g}, t, a] \sim [\hat{g}', t', a']$ then (by definition) $t = t'$ and $a' = \Psi_{\hat{g}', \hat{g}}(t)(a)$, therefore $t + s = t' + s$. Furthermore

$$\begin{aligned}
\gamma_g(t)(a') &= \gamma_g(t)(\Psi_{\hat{g}', \hat{g}}(t)(a)) = (\gamma_g \circ \gamma_{\hat{g}'^{-1}} \circ \gamma_{\hat{g}})(t)(a) = (\gamma_{(\hat{g}' \circ g^{-1})^{-1}} \circ \gamma_{\hat{g} \circ g^{-1}})(t + s) \circ \gamma_g(t)(a) \\
&= (\gamma_{((0, s, 0, 0, 1) \circ \hat{g}' \circ g^{-1})^{-1}} \circ \gamma_{(0, s, 0, 0, 1) \circ \hat{g} \circ g^{-1}})(t + s) \circ \gamma_g(t)(a) \\
&= \Psi_{(\hat{\lambda}', s, \hat{a}', \hat{v}', \hat{R}') \circ g^{-1}, (\hat{\lambda}, s, \hat{a}, \hat{v}, \hat{R}) \circ g^{-1}}(t + s) \circ \gamma_g(t)(a) = (\gamma_g(t)(a))'
\end{aligned} \tag{33}$$

(ii) The group multiplication law holds.

$$\begin{aligned}
i_g \circ i_{g'}([\hat{g}, t, a_z]) &= i_g([\hat{\lambda}, s', \hat{a}, \hat{v}, \hat{R}) \circ g'^{-1}, t + s', \gamma_{g'}^\circ(t)(a_z)]) \\
&= ([(\hat{\lambda}, s' + s, \hat{a}, \hat{v}, \hat{R}) \circ g'^{-1} \circ g^{-1}, t + s' + s, \gamma_g(t + s') \circ \gamma_{g'}^\circ(t)(a_z)]) \\
&= ([(\hat{\lambda}, s + s', \hat{a}, \hat{v}, \hat{R}) \circ (g \circ g')^{-1}, t + (s' + s), \gamma_{g \circ g'}(t)(a_z)]) = i_{g \circ g'}([\hat{g}, t, a_z])
\end{aligned} \tag{34}$$

\square

Corollary 4.3. τ_s defines a Galilei invariant time evolution.

Proof. The restriction of Π to the time component, $\Pi|_{time} : \mathbb{R} \rightarrow Iso(\mathcal{M}_A)$:

$$\begin{aligned} g &\rightarrow i_g : \mathcal{M}_A &\rightarrow \mathcal{M}_A \\ &[\hat{g}, t, a] &\rightarrow [\hat{g}, t + s, \tau_s(a)] \end{aligned} \quad (35)$$

defines the time evolution independent of the chart. \square

5. Equilibrium and Ground States

True (pure phase) equilibrium states are distinguished by strict invariance under time translations and stability against local perturbations. If we add some technical assumptions, then these requirements are equivalent [28-30] to a characterising property first found by Kubo, Martin and Schwinger [31-32]. A state ω over \mathcal{A} is defined to be a (τ, β) -KMS state, if

$$\omega(ab) = \omega(b\tau_{i\beta}(a)) \quad (36)$$

for all a, b in a norm dense, τ -invariant $*$ -subalgebra of \mathcal{A}_τ , where \mathcal{A}_τ denotes the set of analytic elements for τ . The GNS-representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ associated with an equilibrium state ω_β connects our state-independent results with the more common equilibrium formalism.

While the laws of physics have to be Galilei invariant, the corresponding equilibrium states are not [33]. The following proposition tells us that the breakdown of Galilei invariance is unavoidable. Any symmetry not commuting with time translations can not leave a KMS state invariant. This is a consequence of the Tomita-Takesaki theory, first noticed by Narnhofer [34], see also [35]:

Proposition 5.1. (Narnhofer) Let \mathcal{A} be a simple C^* -algebra, ω_β be a (τ, β) -KMS state and $\gamma_g \in Aut(\mathcal{A})$, $g \in G$, a representation of a symmetry group G of the state, i.e.,

$$\omega_\beta(\gamma_g(\cdot)) = \omega_\beta(\cdot), \quad \forall g \in G. \quad (37)$$

Then γ_g commutes with the time evolution,

$$\gamma_g \circ \tau_t = \tau_t \circ \gamma_g, \quad (38)$$

for all $t \in \mathbb{R}$, $g \in G$.

Proof. Because of the invariance, the symmetry group can be unitarily implemented in the GNS representation $(\mathcal{H}_\beta, \pi_\beta, \Omega_\beta)$ of the KMS state ω_β , i.e.,

$$e^{-ig\Gamma} \pi_\omega(a) \Omega_\beta := \pi_\omega(\gamma_g(a)) \Omega_\beta, \quad a \in \mathcal{A}, \quad (39)$$

densely defines a selfadjoint generator Γ a group of unitary operators $\{U(g)\}_{g \in G}$ associated with γ . Consequently we find

$$\begin{aligned} (\Omega_\beta | \pi_\beta(a) e^{-ig\Gamma} e^{-\beta \mathbf{H}_\beta} \pi_\beta(b) | \Omega_\beta) &= (\Omega_\beta | \pi_\beta(b) e^{ig\Gamma} \pi_\beta(a) | \Omega_\beta) \\ &= (\Omega_\beta | \pi_\beta(a) e^{-\beta \mathbf{H}_\beta} e^{-ig\Gamma} \pi_\beta(b) | \Omega_\beta), \quad a, b \in \mathcal{A}. \end{aligned} \quad (40)$$

Thus the generator of the time evolution, \mathbf{H}_β , and the generator of the symmetry, Γ , associated to ω_β , commute. This entails the commutativity of γ with the time translation τ_t of \mathcal{A} which is essentially identical to the modular automorphism:

$$\pi_\beta(\tau_t(\gamma_g(a))) = \pi_\beta(\gamma_g(\tau_t(a))), \quad a \in \pi_\beta(\mathcal{A})'', \quad (41)$$

and since any representation of a simple algebra is faithful, $\gamma_g(\tau_t(a)) = \tau_t(\gamma_g(a))$. \square

In other words, the KMS condition distinguishes a rest frame. If we want to describe a KMS state from a different inertial frame, we have to use the following covariant KMS condition,

$$\omega(ab) = \omega(b\kappa_{i\beta}(a)) \quad (42)$$

where $\{\kappa_t\}_{t \in \mathbb{R}} \subset \{\gamma_g\}_{g \in G}$ denotes a one parameter group of automorphism corresponding to the central element $U = \mathbf{H} - \mathbf{P}^2/2m$ of the extended Galilei group (see appendix).

After these model independent considerations it is time to establish the existence of equilibrium states for our model. The free time evolution respects the tensor product structure of \mathcal{A} ,

$$\tau^\circ(a \otimes b \otimes c) = \tau^\circ(a \otimes \mathbf{1} \otimes \mathbf{1}) \otimes \tau^\circ(\mathbf{1} \otimes b \otimes \mathbf{1}) \otimes \tau^\circ(\mathbf{1} \otimes \mathbf{1} \otimes c); \quad \forall a \in \mathcal{A}_a, b \in \mathcal{A}_b, c \in \mathcal{A}_c. \quad (43)$$

The unique $(\tau^\circ, \beta, \mu_a, \mu_b, \mu_c)$ -KMS state [8], where $\beta = 1/kT$ is the inverse temperature and μ_a, μ_b, μ_c are the chemical potentials for the different species, is given by

$$\omega_\beta^\circ(abc) = \omega_{\beta, \mu_a}^\circ(a) \omega_{\beta, \mu_b}^\circ(b) \omega_{\beta, \mu_c}^\circ(c) \quad \forall a \in \mathcal{A}_a, b \in \mathcal{A}_b, c \in \mathcal{A}_c; \quad (44)$$

with

$$\omega_{\beta, \mu_a}^\circ(a_{z_1}^* \dots a_{z_n}^* a_{z_{n+1}} \dots a_{z_{n+k}}) = \delta_{i,j} \text{Det}(f_{z_i} | \frac{e^{-(\frac{k^2\beta}{2m_a} - \mu_a)}}{1 + e^{-(\frac{k^2\beta}{2m_a} - \mu_a)}} f_{z_{n+j}}) \quad (45)$$

and similar for b and c . In order to see how the three chemical potentials enter one has to examine the role of the $U(1)$ gauge invariance more closely [36-37].

Even if we allow chemical reactions only in a local region, the situation changes dramatically: The tensor product structure is destroyed and we lose control over the relative particles densities. The chemical reaction itself will adjust the equilibrium relative densities, depending on the temperature. Nevertheless the existence of equilibrium states follows from standard results (c.f. [8], Prop. 5.4.1 and Cor. 5.4.5):

Proposition 5.2. *Let ω_β° denote the unique $(\tau^\circ, \beta, \mu_a, \mu_b, \mu_c)$ -KMS state. For each $n \in \mathbb{N}$ and $\beta \in \mathbb{R}$ there exists a unique (τ^n, β) -KMS state ω_β^n defined by*

$$\omega_\beta^n(a) := \frac{\omega_\beta^\circ(\Gamma_{i\beta/2}^n * a \Gamma_{i\beta/2}^n)}{\omega_\beta^\circ(\Gamma_{i\beta/2}^n * \Gamma_{i\beta/2}^n)} \quad (46)$$

where $\Gamma_t^n \in \mathcal{A}$ is a one-parameter family of unitary elements, determined by

$$\Gamma_t^n := \mathbf{1} + \sum_{k>0} i^k \int_0^t ds_1 \int_0^{s_1} ds_2 \dots \int_0^{s_k} ds_k \tau_{s_k}^\circ(v_n) \dots \tau_{s_1}^\circ(v_n) \quad (47)$$

which satisfies the co-cycle relation $\Gamma_{t+s}^n = \Gamma_t^n \tau_t^\circ(\Gamma_s^n)$.

For each initial choice of (μ_a, μ_b, μ_c) there exists exactly one KMS state when we switch on the interaction. The reverse is of course false. Different initial states can lead to the same interacting KMS state.

By another standard result (c.f. [8]) our system allows equilibrium states.

Theorem 5.3. *Let ω_β^n denote the unique (τ^n, β) -KMS state and assume that $\lim_{n \rightarrow \infty} \tau^n$ exists with respect to the strong topology on the automorphism group. Then weak* limit points of ω_β^n exist and each weak* limit point is a (τ, β) -KMS state.*

Proof. Let ω_β denote one of the weak* limit points of ω_β^n . The unit ball in \mathcal{A}_F^* is weak* compact, thus there exists a subsequence $\{\omega_{\beta,\mu}^n\}_{n \in \mathbb{N}}$ converging to ω_β . We have to show that ω_β is (τ, β, μ) -KMS states. A priori we can not be sure that the intersection of the sets of analytic elements for the different automorphisms is dense. This problem is avoided by using a different formulation of the KMS condition ([8], 5.3.12) emphasising the properties of analyticity. Let \mathcal{D} denote the set of infinitely differentiable functions with compact support in \mathbb{R} . If $\tilde{f} \in \mathcal{D}$ then the inverse Fourier transform f is an entire analytic function and

$$\begin{aligned} \int_{-\infty}^{\infty} dt f(t) \omega_{\beta,\mu}^n(a\tau_t(b)) &= \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} dt f(t) \omega_{\beta,\mu}^n(a\tau_t^n(b)) = \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} dt f(t + i\beta) \omega_{\beta,\mu}^n(\tau_t^n(b)a) \\ &= \int_{-\infty}^{\infty} dt f(t + i\beta) \omega_{\beta,\mu}(\tau_t(b)a) = \int_{-\infty}^{\infty} dt f(t) \omega_{\beta,\mu}(\tau_{t-i\beta}(b)a); \quad \forall a, b \in \mathcal{A}_\tau \end{aligned} \quad (48)$$

Now choose $\tilde{f}_k \in \mathcal{D}$ such that $0 \leq \tilde{f}_k \leq 1$, $\tilde{f}_k(x) = 1$ if $|x| \leq k$ and $\tilde{f}_k(x) = 0$ if $|x| \geq k+1$. Since $\tilde{f}_k \xrightarrow{w^*} 1 \in \mathcal{D}'$, it follows that $f_k \xrightarrow{w^*} \delta$. Thus, for any bounded, continuous function g ,

$$\lim_{k \rightarrow \infty} \int_{-\infty}^{\infty} dt f_k(t) g(t) = g(0) \quad (49)$$

and hence $\omega_{\beta,\mu}^n(ab) = \omega_{\beta,\mu}(\tau_{-i\beta}(b)a)$; $\forall a, b \in \mathcal{A}_\tau$. \square

Uniqueness for all temperatures can no longer be expected since phase transitions might occur. There is no uniform convergence $\lim_{n \rightarrow \infty} \sup_{\|a\|=1} \|\tau_t^n(a) - \tau_t(a)\| = 0$. Consequently also the representations given by the KMS state ω_β^0 and ω_β will not be quasi-equivalent, which means that there will be no weakly continuous isomorphism between the corresponding von Neumann algebras. ω_β^0 is space translation-invariant and the extremal translation-invariant components of ω_β will not admit another normal translation-invariant state.

For the ground state, formally corresponding to $\beta = \infty$ the whole modular structure is lacking and one has to use autocorrelation lower bounds [8]. This was done by Powers and Sakai [26], who also gave the first proof of the existence of KMS states for approximately inner automorphisms.

6. Appendix

In non-relativistic classical as well as quantum physics it is a basic assumption that the laws of nature have a Galilei invariant meaning, i.e., they are independent of the actual time, the position, the orientation and the centre of mass momentum of the described physical system. Two descriptions of a series of physical events are equivalent if they can be connected by a coordinate transformation induced by an element $g = (s, a, v, R) \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}^3 \times O(3, \mathbb{R})$ of the proper Galilei group G :

$$x' = Rx + vt + a \quad t' = t + s \quad (50)$$

Starting from an arbitrary coordinate system we can label equivalent frames by the corresponding group element $g \in G$. Space-time, ore more precisely, the space-time manifold \mathcal{M}_G , is constructed by gluing different frames together and then identifying equivalent points in different charts. While in Aristotelian physics both, space and time, were absolute, every event defined by an instant of time and a location in space, in Galilean physics space becomes relative: the space-like distance of two space-time points with different time components has no a priori meaning. Time remains absolute and gives rise to a (fibre-bundle) projection $p_G: \mathcal{M}_G \rightarrow \mathbb{R}$, providing a universal synchronisation prescription for watches [38-39]. Once the watches are synchronised in different charts, the group connecting equivalent charts is reduced to the *isochronous* Galilei group $G_\circ := \{(s, a, v, R) \in G \mid s = 0\}$. This is the starting-point for our construction of the space-time fibre bundle. Equivalent points in the charts \tilde{g} and $\tilde{h} \in G_\circ$ are identified by transition functions $\psi_{\tilde{g}, \tilde{h}}(t)$ acting in the fibre \mathbb{R}^3 (=space) and depending on the basispoint $t \in \mathbb{R}$ (=time).

Definition. Let $\tilde{g}, \tilde{h} \in G_o$ and E_3 denote the Euclidean group in three dimensions. Furthermore, consider the following transition functions

$$\begin{aligned} \psi_{\tilde{g}, \tilde{h}} : \mathbf{R} &\rightarrow E_3 \\ t &\rightarrow e_{\tilde{g}}(t)^{-1} \circ e_{\tilde{h}}(t) \end{aligned} \quad (51)$$

where $e_{\tilde{g}}(t) x := Rx + vt + a$. *Galilean space-time* is defined to be the fibrebundle $(\mathcal{M}_G, p_G, \mathbf{R})$ with fibre \mathbf{R}^3 , the space-time manifold $\mathcal{M}_G := (\bigcup_{\tilde{g} \in G_o} \{\tilde{g}\} \times \mathbf{R} \times \mathbf{R}^3) / \sim$ which is described by the equivalence relations $[\tilde{g}, t, x] \sim [\tilde{h}, t', x'] : \Leftrightarrow t = t'$ and $x' = \psi_{\tilde{h}, \tilde{g}}(t) x$; the bundle projection is given by $p_G([\tilde{g}, t, x]) = t$.

Although \mathcal{M}_G is split up into space and time components in every (uniformly moving) coordinate system $\tilde{g} : \mathcal{M}_G \rightarrow \mathbf{R} \times \mathbf{R}^3$, there is no canonical projection from $\mathcal{M}_G \rightarrow \mathbf{R}^3$. \mathcal{M}_G is trivializable, but not canonically trivial. By definition, the set $\{\psi_{\tilde{g}, \tilde{h}}\}_{\tilde{g}, \tilde{h} \in G_o}$ fulfils the cocycle conditions $\psi_{\tilde{g}, \tilde{h}} \circ \psi_{\tilde{h}, \tilde{f}} = \psi_{\tilde{g}, \tilde{f}}$ and $\psi_{\tilde{g}, \tilde{g}} = id$ on \mathbf{R}^3 , the required compatibility condition for the construction of fibrebundles [40].

The Galilei group was analysed in detail by Lévy-Leblond [19]. We collect a view facts relevant for a discussion of the present model. Each element of the Galilei group G can be written as a product of a *time translation* $(s, 0, 0, \mathbf{1})$, a *space translation* $(0, a, 0, \mathbf{1})$, a *pure Galilei transformation* $(0, 0, v, \mathbf{1})$ and a *rotation* $(0, 0, 0, R_\theta)$ with generators $\mathbf{H}, \mathbf{P}, \mathbf{X}, \mathbf{J}$ respectively:

$$\begin{aligned} (s, a, v, R_\theta) &= (s, 0, 0, \mathbf{1}) \circ (0, a, 0, \mathbf{1}) \circ (0, 0, v, \mathbf{1}) \circ (0, 0, 0, R_\theta) \\ &= e^{-i\mathbf{H}s} e^{-i\mathbf{P}a} e^{-i\mathbf{X}mv} e^{-i\mathbf{J}\theta}. \end{aligned} \quad (52)$$

θ denotes the three rotation angles. So far space and momentum translations commute, as can be seen from the group multiplication law. In classical mechanics the observables form an abelian algebra of functions over phase space $T^*(\mathbf{R}^{3N})$. The generators $\mathbf{P}, \mathbf{X}, \mathbf{J}$ and \mathbf{H} are identified with the momentum, position, angular momentum and energy of the physical system.

In quantum theory this scheme is generalised by releasing the commutativity of space and time translations. Since Galilei invariance should not be affected by gauge transformations, a central extension of the Galilei group seems appropriate. $U(1)$, the gauge group of classical electromagnetism, is the minimal choice.

Definition. Let $m \in \mathbf{R}$. The *extended Galilei group* (G^m, \circ) is the eleven parameter group $g = (\lambda, s, a, v, R) \in S^1 \times \mathbf{R} \times \mathbf{R}^3 \times \mathbf{R}^3 \times O(3, \mathbf{R})$ with the group multiplication \circ defined by

$$(\lambda, s, a, v, R) \circ (\lambda', s', a', v', R') = (\lambda + \lambda' + \frac{m}{2}(v^2 s' + v.Ra'), s + s', a + Ra' + vs', v + Rv', RR') \quad (53)$$

Let \mathbf{M} denote the generator of the gauge transformations. Then the Lie algebra of the extended Galilei group G^m is characterised by the relations:

$$\begin{aligned} [\mathbf{J}_i, \mathbf{J}_j] &= \epsilon_{ijk} \mathbf{J}_k & [\mathbf{J}_i, \mathbf{H}] &= 0 & [\mathbf{P}_i, \mathbf{P}_j] &= 0 & (54) \\ [\mathbf{J}_i, \mathbf{X}_j] &= \epsilon_{ijk} \mathbf{X}_k & [\mathbf{J}_i, \mathbf{M}] &= 0 & [\mathbf{P}_i, \mathbf{H}] &= 0 \\ [\mathbf{J}_i, \mathbf{P}_j] &= \epsilon_{ijk} \mathbf{P}_k & [\mathbf{X}_i, \mathbf{X}_j] &= 0 & [\mathbf{P}_i, \mathbf{M}] &= 0 \\ [\mathbf{X}_i, \mathbf{P}_j] &= i\delta_{ij} & [\mathbf{X}_i, \mathbf{M}] &= 0 & [\mathbf{H}, \mathbf{M}] &= 0 \\ [m\mathbf{X}_i, \mathbf{H}] &= i\mathbf{P}_i \end{aligned}$$

As argued, the extension is central, so \mathbf{M} commutes with all other Lie algebra elements. But it is nontrivial, so \mathbf{M} appears in some Lie bracket. The total mass \mathbf{M} , the internal energy $\mathbf{U} := \mathbf{H} - \mathbf{P}^2/2m$ and the spin, i.e., the internal angular momentum $\mathbf{S}^2 := (\mathbf{J} - \mathbf{X} \times \mathbf{P})^2 = s(s+1)$ generate the three dimensional centre of the group and are therefore chart independent properties associated with a particle.

As pointed out in [19], the difference between Galilei and Poincare invariance is that, if we add an interaction \mathbf{V} to the Hamiltonian $\mathbf{H} = \mathbf{H}_o + \mathbf{V}$, the commutation relations are not modified in the Galilean case, provided that \mathbf{V} commutes with $(\mathbf{P}, \mathbf{J}, \mathbf{K}, \mathbf{M})$, while in the relativistic case any modification of the Hamiltonian requires a subsequent modification of other elements of the Lie algebra, since the Hamiltonian appears in the commutator of the generators of space translations and pure Lorentz transformations.

All the quantities usually considered as physically relevant, namely the energy, momentum, position angular momentum and mass, appear as generators of the (extended) Galilei group. The problem is that for systems with an infinite number of particles quantities like the Hamiltonian or even the particle number are not well defined without reference to a representation of \mathcal{A} . We therefore present a representation of the Lie algebra of G^m as an algebra of derivations acting on \mathcal{A} .

Proposition 6.1. *Each $\gamma_g(t)$, $g \in G^m$ can be written as a product of derivable automorphisms, $\gamma_g(t) = \gamma_{(\lambda,0,0,0,1)} \circ \gamma_{(0,s,0,0,1)} \circ \gamma_{(0,0,a,0,1)} \circ \gamma_{(0,0,0,v,1)}(t) \circ \gamma_{(0,0,0,0,\mathcal{R}_\theta)}$. The corresponding derivations δ_m , δ_h , δ_p , δ_x and δ_j generate a representation of the Lie group of G^m on a common dense set \mathcal{D} ,*

$$\begin{aligned} [\delta_{j_i} \circ \delta_{j_j}] &= \epsilon_{ijk} \delta_{jk} & [\delta_{j_i}, \delta_m] &= 0 & [\delta_{p_i}, \delta_{p_j}] &= 0 \\ [\delta_{j_i}, \delta_{x_j}] &= \epsilon_{ijk} \delta_{x_k} & [\delta_{j_i}, \delta_h] &= 0 & [\delta_{p_i}, \delta_h] &= 0 \\ [\delta_{j_i}, \delta_{p_j}] &= \epsilon_{ijk} \delta_{p_k} & [\delta_{x_i}, \delta_{x_j}] &= 0 & [\delta_{p_i}, \delta_m] &= 0 \\ [\delta_{x_i}, \delta_{p_j}] &= i \delta_{ij} & [\delta_{x_i}, \delta_m] &= 0 & [\delta_h, \delta_m] &= 0 \\ [\delta_{x_i}, \delta_h] &= \frac{i}{m} \delta_{p_i} \end{aligned} \quad (55)$$

where the Lie-bracket is defined by $[\delta, \delta'](a) := \delta(\delta'(a)) - \delta'(\delta(a))$.

Proof. Let $\mathcal{D} = \{b_n | b \in \mathcal{A}\}$, with

$$b_n := \left(\frac{n}{\pi}\right)^{7/2} \int \gamma_{(0,0,s,a,v,\mathbb{1})}(b) e^{-n(s^2+a^2+v^2)} ds d^3a d^3v, \quad b \in \mathcal{A}. \quad (56)$$

It follows ([7], 2.5.22.) that each b_n is an entire analytic element for γ_g , i.e., there exists a derivation δ_{γ_g} , such that

$$\gamma_g(b_n) = \sum_{k \geq 0} \frac{g^k \delta_{\gamma_g}^k(b_n)}{k!} \quad \text{and} \quad \sum_{k \geq 0} \frac{|g|^k}{k!} \|\delta_{\gamma_g}^k(b_n)\| < +\infty \quad (57)$$

for some open neighbourhood U of the identity in G . $\|b_n\| \leq \|b\|$ for all n , and $b_n \rightarrow b$ in the norm topology as $n \rightarrow \infty$. The multiplication table (55) can be established by direct computation. \square

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