Quantum Chaos and Dynamical Entropy

Fabio Benatti* Thomas Hudetz† Andreas Knauf‡

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Abstract

We review the notion of dynamical entropy by Connes, Narnhofer and Thirring and relate it to Quantum Chaos. A particle in a periodic potential is used as an example. This is worked out in the classical and the quantum mechanical framework, for the single particle as well as for the corresponding gas.

The comparison does not only support the general assertion that quantum mechanics is qualitatively less chaotic than classical mechanics. More specifically, the same dynamical mechanism by which a periodic potential leads to a positive dynamical entropy of the classical particle may *reduce* the dynamical entropy of the quantum gas in comparison to free motion.

*Dipartimento di Fisica teorica, Università di Trieste, Strada Costiera 11, Italy. e-mail: benatti@trieste.infn.it

†Institut für Mathematik, Strudlhofgasse 4, A-1090 Wien, Austria, e-mail: hudetz@pap.univie.ac.at. Supported by 'Österreichische Forschungsgemeinschaft' (1995/96) and 'Austrian Science Foundation' (FWF; Dec. 1996/Febr. 1997).

‡Max-Planck-Institute for Mathematics in the Sciences, Inselstr. 22–26, D-04103 Leipzig, Germany. e-mail: knauf@mis.mpg.de

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1 Introduction

In his 1990 book ‘Chaos in Classical and Quantum Mechanics’ Gutzwiller wrote

> ‘While the idea of an entropy is of great help in understanding classical mechanics, nobody has been able to define its analog in quantum mechanics; therein lies the great unresolved mystery of quantum chaos.’ [20]

Here entropy of a system of classical mechanics means its Kolmogorov-Sinai (KS) metric entropy. Since this quantity is a measure of the loss of information per time unit about the dynamical system, it is also called dynamical entropy.

In 1987 Connes, Narnhofer and Thirring described in [13] a generalization of that dynamical entropy to quantum systems (henceforth abbreviated as CNT entropy). Since then, this quantum dynamical entropy has been applied to infinite particle systems of statistical mechanics, and its general mathematical properties were studied.

However, the above citation suggests that it could be useful to study in some depth the dynamical entropy of *finite* quantum systems which exhibit ‘quantum chaos’.

In classical mechanics the KS entropy can be regarded as an order parameter which is (strictly) positive if the system is chaotic, and thus may even be used to define what chaotic means.

Now for many years physicists looked for order parameters indicating (and defining!) the occurrence of quantum chaos. We prove in Prop. 3.4 that CNT entropy is not such an order parameter, and argue that there is no other order parameter for finite localized quantum systems. Thus we support the operational definition of a quantum chaotic system as one whose semiclassical limit $\hbar \searrow 0$ leads to a classical system with positive dynamical entropy. So quantum chaos is an emergent phenomenon which can only be seen in the semiclassical limit.

Entropy measures information (or ignorance). Thus it is a probabilistic notion. But unlike the classical theory, quantum statistical mechanics is *not* a probabilistic theory.

Since information about a system is gained by measuring it and since a measurement may change the state of a quantum system, one has to be careful if one wants to define a physically relevant notion of quantum dynamical entropy.

In our opinion, CNT entropy describes a property of the quantum system which is as little as possible influenced by the repeated measurements necessary to define it. We have to emphasize that the more recent work by Alicki, Fannes, and coauthors, beginning with [2], explores a different approach to a physically relevant quantum dynamical entropy, with which we will not be concerned in this paper.

One purpose of our paper is to give a pedagogical introduction into quantum dynamical entropy in the sense of Connes, Narnhofer and Thirring, starting from the more familiar notion of classical dynamical entropy.

To our opinion the notion of quantum dynamical entropy has not yet really become popular within the mathematical physics community, not to speak of theoretical physics. We see two reasons for this deplorable fact:

- As mentioned above, it does not help to discern quantum chaos for finitely many particles.

- The very notion of CNT entropy is involved, and it is quite complicated to estimate its basic functional. Thus it could up to now only be applied to systems of statistical mechanics which are relatively simple from a physical point of view (e.g. space translations).

Conceptually speaking, we think that what is needed is the development of techniques which allow to *localize* in configuration space and, more far-fetched, to *microlocalize* in phase space.

In the theory of partial differential equations the pseudodifferential calculus has been developed in the last decades and applied to the Schrödinger equation (see Robert [42] for a general introduction and Helffer [21], and [30] for reviews on the application to quantum chaos).

In recent years, there have been successful attempts to apply this calculus to problems of statistical mechanics.

Our paper is also aimed to promote the development of such localization techniques for CNT entropy, in order to widen its field of potential applications.

In order to describe in which sense CNT entropy generalizes KS entropy one needs a common framework for classical and quantum mechanics. This is given by the C^*–dynamical systems, which are discussed in Sect. 2.

In Sect. 3 the notion of CNT entropy is introduced and explained. Prop. 3.4 says that in a situation typical for finitely many particles (algebra of bounded operators on a Hilbert space, time evolution implemented by unitaries, state represented by a density matrix) the CNT entropy equals zero.

Classically *topological entropy* is the supremum over all phase space probability measures of the (metric) KS entropy. Sect. 4 is devoted to a brief introduction to the approach, developed by one of the present authors [23, 24], to a physically relevant non–commutative generalization of topological entropy, which approach had been formally inspired by the CNT entropy theory. Again, we have to emphasize that there are alternative approaches, by Thomsen and by Voiculescu, to topological entropy for non–commutative operator algebras [49, 47].

In Sect. 5 we work out in detail the example of a particle in a periodic potential (crystal). We shortly describe the main results.

Periodic Potentials

One Particle (Classical). The notion of measure theoretic entropy is not directly applicable to the description of a classical particle in a periodic potential, since Liouville measure is invariant under lattice translation and thus infinite. However one may divide by the lattice $\mathcal{L}$ and thus consider motion on the configuration torus $\mathbb{T} = \mathbb{R}^n/\mathcal{L}$, using Liouville measure.

In that case the KS entropy is zero if the potential is separable, and should be positive in the generic case. If the potential is smooth, it is of order $1/\sqrt{E}$ as the energy E of the particle goes to infinity (Prop. 5.6).

Classical topological entropy has a generalization, due to Bowen, to non–compact phase spaces. So it is directly applicable to the motion in the crystal but coincides with the topological entropy of the motion on the configuration torus. The topological entropy of smooth potentials has an E–independent upper bound, and for ≥ 3 freedoms there exist smooth potentials with a similar E–independent lower bound (Prop. 5.5).

As a special class of examples we analyze planar periodic potentials with attractive singularities of Coulombic $(-1/r)$ form. For these potentials the motion is diffusive above a threshold energy. In the high energy limit the topological entropy is a smooth increasing function asymptotic to $c\sqrt{E}$ (Prop. 5.8).

One Particle (Quantal). In the quantum case the motion in periodic potentials is ballistic, but for the Coulombic case the speed is known to vanish in the semiclassical limit $\hbar \searrow 0$ as a consequence of quantum chaos, see Prop. 5.11.

The CNT entropy is undefined for the motion in configuration space and zero for motion on the configuration torus.

Classical Gas. Although second quantization (or Poisson construction, as it is called in the case of classical dynamical systems, see Def. 5.12) is a purely functorial construction, the consideration of a gas of non–interacting particles sheds new light on the single–particle dynamics.

Classically the unbounded system is now described by a *probability* measure. As noted by Goldstein, the total entropy of an ideal gas is infinite. This was a motivation for him to introduce space time entropy which, as he showed, equals entropy density. This is a finite quantity for the motion in a periodic potential, since it equals the entropy per particle multiplied by the density of particles (Thm. 5.14).

However, if one considers only a *bounded* configuration space region B, then for large energies and smooth potentials the local entropy associated with that region is infinite, since every incoming particle carries an infinite amount of information.

For energies below the delocalization threshold that entropy is finite (Thm. 5.14).

Above an energy threshold, the gas of classical particles in a Coulombic periodic potential forms a space-time $\mathbb{K}$-system with strictly positive entropy densities (Prop. 5.15). Thus it has extremely good ergodic properties.

Fermi Gas. In Sect. 5.4 we consider a noninteracting Fermi gas in $\mathbb{R}^n$ with a lattice-invariant quasi-free state.

We prove that for a *shift* by a lattice vector v the local CNT entropy in region B is finite and for large B asymptotically proportional to the surface area of ∂B in the v direction times the speed $|v|$ (Thm. 5.19). Here adapt the method of the paper [39] by Park and Shin to our situation, which is only invariant under lattice translations, not under general space translations. We simplify their estimate for the entropy defect. At the same time we obtain a more localized estimate which shows that entropy defect is only due to the boundary of the region of observation.

The finiteness of local CNT entropy is a consequence of coarse–graining of phase space with cells of volume $(2\pi\hbar)^n$. So each particle carries only a finite amount of information.

In a forthcoming paper we will apply these techniques to the motion of the noninteracting quantum electron gas in a periodic potential. This needs phase space microlocalization, and we indicate in an appendix the usefulness of local algebras of Wannier functions in this context.

The growth of the local CNT entropy with the surface area instead with the volume is a clear sign of the fact that quantum chaos is less chaotic than classical chaos. For it is not the dynamics of the particles in the bulk, but the information carried by the electron entering the region, that leads to that growth of entropy.

In the case of the Coulombic potential the abovementioned vanishing of speed in the semiclassical limit has the curious consequence that, apart from a 'kinematical factor' $(2\pi\hbar)^{-n}$ corresponding to coarse-graining of phase space, the local CNT entropy associated with B *decreases* as Planck's constant goes to zero. The physical reason is simply that less particles enter B per unit time.

Perspectives

- At a first glance the vanishing of the CNT entropy (density) is somewhat disappointing, seen from the point of view of quantum chaology. On the other hand, it fits well with many other observations made in that field.

  The obvious answer is *not* to perform the large time limit but to ask in which sense and up to which time the quantum time evolution imitates the classical one.

  Mathematically, for this study *semiclassical techniques* are used (e.g. Egorov's theorem on the convergence of quantum to classical time evolution). We think that the analysis leading to the notion of CNT entropy can also be useful in that context.

- The connection between the CNT definition of the multi-algebra entropy (Def. 3.2) and *quantum information theory* should be studied further. The latter is a rapidly growing field with new experimental and theoretical content. As has been shown recently in [7] the basic quantum generalization of Shannon information is directly related to the CNT one-algebra entropy 3.1.

- We mention that our use of Wannier functions resembles techniques in *wavelet analysis*. Namely, the Wannier functions of a given band are related by lattice translations and orthonormal. Moreover, going to sublattices and subbands, as we do, is similar to the dilations used in the case of wavelets.

- Concerning infinite particle systems, an obvious question is whether the introduction of an interaction between the electrons leads to a positive configuration space density of quantum dynamical entropy.

  This question is probably out of reach of presently available techniques. However it is a challenging problem to develop some intuition.

  The case of *Fermi liquids* is of particular interest, since there the one-particle concept of the Fermi surface is still important, and since their mathematical understanding has progressed much in recent years.

Notation. Whenever it is clear from the context which measure μ we use (Lebesgue, Liouville, counting etc.), we denote $\mu(S)$ by $|S|$.

2 C*-Dynamical Systems

Instead of using a Hilbert space picture, we develop our considerations about the dynamical properties of quantum systems in the language of the algebra $\mathcal{A}$ of observables. This makes it easier to compare with classical dynamical systems, where $\mathcal{A}$ is an Abelian algebra. Anyhow, one cannot observe everything in statistical mechanics, so that the quantum algebra of observables need not be $\mathcal{A} = B(\mathbb{H})$, the bounded operators on some Hilbert space $\mathbb{H}$.

On $\mathcal{A}$ the (discrete or continuous) time evolution $\sigma^t : \mathcal{A} \to \mathcal{A}$ (with $t \in \mathbb{Z}$ resp. $\mathbb{R}$) acts as a group of automorphisms.

We have then two possibilities: either we focus on the C*-dynamical system $(\mathcal{A}, \sigma)$, independently of any reference state, or we fix a time-invariant ($\omega \circ \sigma^t =$

ω) state ω and concentrate on the triple $(\mathcal{A}, \sigma, \omega)$. In the first instance we will speak of (non–commutative) 'topological', in the second of state-dependent properties.

The algebra $\mathcal{A}$ may be a C* or a von Neumann algebra.

- In quantum mechanics of *finitely many particles* $\mathcal{A}$ is typically the algebra $B(\mathbb{H})$ (both a C* and a von Neumann algebra) of all bounded linear operators on some (separable) Hilbert space $\mathbb{H}$. The dynamics is usually defined by a one–parameter group $\{\hat{U}_t\}$ of unitaries generated by a Hamiltonian $\hat{H}$, such that $\sigma_t : \mathcal{A} \to \mathcal{A}$ is given by

$$\sigma_t(\hat{X}) = \hat{U}_t^* \hat{X} \hat{U}_t\,, \quad \hat{U}_t := \exp\left(-i\,\hat{H}\,t\right)\,, \qquad (\hat{X} \in B(\mathbb{H})). \tag{1}$$

  Typical invariant states ω on $B(\mathbb{H})$ are given by density matrices $\hat{\rho} \in B(\mathbb{H})$, with $\hat{\rho} \geq 0$, $\mathrm{Tr}\,\hat{\rho} = 1$ and $\left[\hat{\rho}\,,\,\hat{U}_t\right] = 0$.

$$\omega(\hat{X}) := \mathrm{Tr}\,\left(\hat{\rho}\hat{X}\right) \quad , \qquad (\hat{X} \in B(\mathbb{H})) \quad . \tag{2}$$

  If a state is *pure* (i.e., cannot be written as a non-trivial convex combination), then $\hat{\rho}$ is a rank-one projection. We will sometimes use the same notation for a density matrix and its state.

- In the more general context of *quantum statistical mechanics*, $\mathcal{A}$ will not necessarily be the whole of $B(\mathbb{H})$, maybe not yet represented on some Hilbert space $\mathbb{H}$. There may be no Hamiltonian $\hat{H} \in \mathcal{A}$ of the system as a whole. Thus the automorphisms σ might not be implemented by unitaries in $\mathcal{A}$ and the states ω over $\mathcal{A}$ will be general, normalised (that is, $\omega(\hat{\mathbb{1}}) = 1$) positive linear functionals $\omega : \mathcal{A} \to \mathbb{C}$, not necessarily representable in the form (2) (see Bratteli and Robinson [11, 12]).

Example. As an instance of this state of affairs let us consider a system of infinitely many Fermions. $\mathcal{A}$ is the *CAR algebra* of the Canonical Anticommutation Relations $\left[\hat{a}^\dagger(f)\,,\,\hat{a}(g)\right]_+ = \langle g\,,\,f\rangle$, arising from the closure with respect to the norm $\|\hat{a}^\sharp(f)\| = \|f\|$ of polynomials in the creation resp. annihilation operators $\hat{a}^\dagger(f)$ resp. $\hat{a}(f)$ of one–particle states $f \in \mathbb{H}$.

The Fock vacuum $|\Omega\rangle$ gives rise to a state $\omega(\hat{X}) = \langle\Omega, \hat{X}\Omega\rangle$ which belongs to a class of states, the so–called *quasi–free states*, that are specified by assigning two–point functions:

$$\omega_A\left(\hat{a}^\dagger(f)\hat{a}(g)\right) := \langle g, \hat{A}f\rangle \quad , \tag{3}$$

where $\hat{A}$ is a one–particle operator on $\mathbb{H}$ and $0 \leq \hat{A} \leq \hat{1\!\!1}$. The higher moments are then given by

$$\omega_A(\hat{a}^\dagger(f_n)\ldots\hat{a}^\dagger(f_1)\hat{a}(g_1)\ldots\hat{a}(g_m)) := \delta_{mn}\det\left(\omega_A(\hat{a}^\dagger(f_i)\hat{a}(g_j))\right). \tag{4}$$

In this class we find the *KMS–states* for inverse temperature β among which the *Fock state* (zero temperature) corresponds to $\hat{A}=0$, while the *tracial state* (infinite temperature) to $\hat{A}=\frac{\hat{1\!\!1}}{2}$. For general β we have

$$\hat{A} := \frac{\exp(-\beta\hat{H})}{\hat{1\!\!1}+\exp(-\beta\hat{H})},$$

$\hat{H}$ denoting the one-particle Hamiltonian.

Establishing an interaction among fermions capable of leading to an automorphism σ_t of the algebra is rather a difficult task, cf. [33, 34]. Much easier to handle are the so–called *quasi–free evolutions* that map $\hat{a}^\sharp$ into themselves. For instance, if $\hat{U}:\mathbb{H}\mapsto\mathbb{H}$ is a one–particle unitary evolution, then $\sigma:\hat{a}^\sharp(f)\mapsto\hat{a}^\sharp(\hat{U}f)$ defines an automorphism of $\mathcal{A}$.

Given $\mathcal{A}$, an automorphism σ and a σ–invariant state ω, we can recover a Hilbert space representation via the so–called *GNS construction* [11, 12]. We are ensured of the existence of a state–dependent Hilbert space $\mathbb{H}_\omega$, a state–dependent representation $\pi_\omega(\mathcal{A})$ of $\mathcal{A}$ as a subalgebra of $B(\mathbb{H}_\omega)$ and a state–dependent unitary implementation $\hat{U}_\omega$ of the automorphism σ. Moreover the state ω corresponds to an invariant vector state $|\Omega\rangle\in\mathbb{H}_\omega$:

$$\pi_\omega\left(\sigma(\hat{a}^\sharp(f))\right) = \hat{U}^*_\omega\pi_\omega\left(\hat{a}^\sharp(f)\right)\hat{U}_\omega\,, \quad \omega\left(\hat{X}\right) = \langle\Omega, \pi_\omega(\hat{X})\Omega\rangle \quad . \tag{5}$$

Finally, the strong–operator closure of $\pi_\omega(\mathcal{A})$ as a C*–algebra of operators on $\mathbb{H}_\omega$ is a von Neumann algebra, denoted by $\pi_\omega(\mathcal{A})''$ that coincides with the bicommutant (commutant of the commutant) of $\pi_\omega(\mathcal{A})\subset B(\mathbb{H}_\omega)$.

As to the CAR algebra $\mathcal{A}$ we last notice that it has the structure of a UHF C*–algebra, namely there exists an increasing sequence of finite–dimensional subalgebras $\mathbf{A}_n$ (isomorphic to $2^n\times 2^n$ matrix algebras) and $\mathcal{A}$ is the norm closure of (the inductive limit) $\bigcup_n \mathbf{A}_n$ [12, Par. 5.2.2]. Once represented via the GNS construction based on some state ω, $\pi_\omega(\mathcal{A})''$ is the strong–operator closure of the corresponding $\bigcup_n \pi_\omega(\mathbf{A}_n)$ (i.e., a hyperfinite von Neumann algebra).

3 CNT Entropy

In this section we introduce and apply the notion of CNT entropy [13] (*quantum dynamical entropy*) of a triple $(\mathcal{A}, \sigma, \omega)$, where $(\mathcal{A}, \sigma)$ is a C*-dynamical system with σ–invariant state ω.

3.1 Entropy of Subalgebras

Since the CNT entropy generalizes the KS entropy, we follow the classical case as far as possible. The key problem consists in finding a suitable definition for the entropy of subalgebras.

The starting point in the definition of the KS entropy of a map $S : \mathcal{X} \to \mathcal{X}$ on phase space $\mathcal{X}$ with probability measure μ is to partition phase space into disjoint measurable atoms $P_i \subset \mathcal{X}$ ($\mathcal{X} = \cup_{i=1}^{d} P_i$, up to μ–measure zero), and to define the *entropy*

$$H_\mu(\mathcal{P}) := \sum_{i=1}^{d} \eta(\mu(P_i))$$

of the partition $\mathcal{P}$, with the positive function on $[0, 1]$,

$$\eta(x) := -x \log x \quad \text{for} \quad 0 < x \leq 1, \qquad \eta(0) := 0.$$

By concavity of η the entropy increases if the partition is refined.

The C*–algebraic version of the entropy of a partition works with the Abelian C*–algebra (actually, von Neumann algebra) $\mathcal{A} := L^\infty(\mathcal{X}, \mu)$, the state $\omega : \mathcal{A} \to \mathbb{C}$, $\omega(f) := \int_{\mathcal{X}} f \, d\mu$ and the characteristic functions $\chi_i \in \mathcal{A}$ of the atoms P_i of the partition $\mathcal{P}$. These span a finite–dimensional (here, d–dimensional) subalgebra $\mathbf{A} \subset \mathcal{A}$, and can be recovered from $\mathbf{A}$ as its unique minimal projections. Then the entropy $H_\mu(\mathcal{P})$ of the partition equals the entropy

$$H_\omega(\mathbf{A}) := \sum_{i=1}^{d} \eta(\omega(\chi_i)) \tag{6}$$

of the associated subalgebra.

In the non-Abelian case of a general C*–algebra $\mathcal{A}$ with subalgebra $\mathbf{A}$ and state ω it is tempting to use the *von Neumann entropy*

$$S(\omega) := -\text{Tr}\,(\hat{\rho} \log \hat{\rho}) \tag{7}$$

of a state ω with density matrix $\hat{\rho}$ to define the entropy of the subalgebra $\mathbf{A} \subset \mathcal{A}$ by $S(\omega\restriction_{\mathbf{A}})$. Indeed, although the state $\omega : \mathcal{A} \to \mathbb{C}$ does not necessarily have a density matrix $\hat{\rho}$ (with $\omega(\hat{X}) = \mathrm{Tr}\,(\hat{\rho}\hat{X})$), the state $\omega\restriction_{\mathbf{A}} : \mathbf{A} \to \mathbb{C}$ has one, since $\dim(\mathbf{A}) < \infty$ (and hence $\mathbf{A}$ can be included in a full matrix algebra). Moreover, $S\left(\omega\restriction_{\mathbf{A}}\right) = H_\omega(\mathbf{A})$ for $\mathbf{A}$ Abelian, so that we have a generalization of the classical definition.

However, unlike $H_\omega(\mathbf{A})$, the von Neumann entropy of a subalgebra of $\mathbf{A}$ need not be smaller than the von Neumann entropy $S\left(\omega\restriction_{\mathbf{A}}\right)$ of $\mathbf{A}$.

Example. We consider a spin $\frac{1}{2}$ particle with algebra $\mathbf{A} = \mathcal{A} = B(\mathbb{C}^2)$. Thus the density matrices have the form $\hat{\rho}_{\vec{b}} := \frac{1}{2}(\hat{1\!\!1} + \vec{b}\cdot\vec{\sigma})$, with $\vec{b}$ in the unit ball $B \subset \mathbb{R}^3$ and the vector $\vec{\sigma} = (\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3) := \left(\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right), \left(\begin{smallmatrix}0&i\\-i&0\end{smallmatrix}\right), \left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)\right)$ of Pauli matrices. The pure states constitute the sphere ∂B and have zero von Neumann entropy, whereas for mixed states

$$S\left(\vec{b}\right) := S\left(\hat{\rho}_{\vec{b}}\restriction_{\mathbf{A}}\right) = \eta(\tfrac{1}{2}(1+|\vec{b}|)) + \eta(\tfrac{1}{2}(1-|\vec{b}|)) > 0.$$

The Abelian subalgebra $\mathbf{B} \subset \mathcal{A}$ generated by $\hat{\sigma}_3$ is used to measure the polarization in the 3–direction. Now $\hat{\rho}_{\vec{b}}\restriction_{\mathbf{B}} = \hat{\rho}_{\vec{b}_{||}}$ with $\vec{b}_{||} := (0, 0, b_3)$ so that

$$S\left(\hat{\rho}_{\vec{b}}\restriction_{\mathbf{B}}\right) = \eta(\tfrac{1}{2}(1+b_3)) + \eta(\tfrac{1}{2}(1-b_3)) \geq S\left(\vec{b}\right) = S\left(\hat{\rho}_{\vec{b}}\restriction_{\mathbf{A}}\right). \tag{8}$$

The two von Neumann entropies are only equal if $\vec{b}_{||} = \vec{b}$, since only then the measurement of the 3–component does not produce additional uncertainty.

In particular, $S\left(\hat{\rho}_{\vec{b}}\restriction_{\mathbf{B}}\right) = \ln(2)$ if $\vec{b}_{||} = 0$, since then both polarizations have probability $\frac{1}{2}$, even if $\hat{\rho}_{\vec{b}}$ is pure.

As the example clearly shows, the von Neumann entropy of a subalgebra does *not* measure the information gained by a suitable experiment using the observables of that subalgebra. Rather, it measures our uncertainty about the outcome of that experiment. Whereas these quantities coincide classically, in quantum mechanics we generally disturb the state by the experiment.

So we have to subtract from the von Neumann entropy $S\left(\omega\restriction_{\mathbf{A}}\right)$ a term which describes the information loss through the experiment and thus leads to a zero entropy of the algebra if ω is pure. This can be done by decomposing $\omega = \sum_{i\in I}\mu_i\hat{\omega}_i$ in a convex combination ($\mu_i > 0$, $\sum_i \mu_i = 1$) of normalized states $\hat{\omega}_i$ and subtracting the weighted sum $\sum_{i\in I}\mu_i S\left(\hat{\omega}_i\restriction_{\mathbf{A}}\right)$ from $S\left(\hat{\omega}\restriction_{\mathbf{A}}\right)$.

Using the *relative entropy*

$$S\left(\hat{\rho}_1\,,\,\hat{\rho}_2\right) := \mathrm{Tr}\,\hat{\rho}_2\left(\log\hat{\rho}_2 - \log\hat{\rho}_1\right) \quad , \tag{9}$$

of $\hat{\rho}_1$ with respect to $\hat{\rho}_2$ [37], we thus consider the positive bounded functional

$$
\begin{aligned}
0 \leq H_{\omega\,,\{\mu_i\hat{\omega}_i\}}(\mathbf{A}) &:= \sum_{i\in I}\mu_i S\left(\omega\restriction_{\mathbf{A}}\,,\,\hat{\omega}_i\restriction_{\mathbf{A}}\right) && (10)\\
&= S\left(\omega\restriction\mathbf{A}\right) - \sum_{i\in I}\mu_i S\left(\hat{\omega}_i\restriction\mathbf{A}\right) && (11)\\
&\leq S\left(\omega\restriction\mathbf{A}\right) \leq \log(\mathrm{rank}(\omega\restriction_{\mathbf{A}})) \quad .
\end{aligned}
$$

on the set of finite dimensional subalgebras $\mathbf{A}$ (where $\mathrm{rank}(\omega\restriction_{\mathbf{A}})$ denotes the rank of the corresponding density matrix). $H_{\omega\,,\{\mu_i\hat{\omega}_i\}}(\mathbf{A})$ is also monotonically increasing with the subalgebra $\mathbf{A}$, since the relative entropy has this property:

$$
S\left(\hat{\rho}_1\restriction_{\mathbf{A}}\,,\,\hat{\rho}_2\restriction_{\mathbf{A}}\right) \leq S\left(\hat{\rho}_1\restriction_{\mathbf{B}}\,,\,\hat{\rho}_2\restriction_{\mathbf{B}}\right) \qquad \text{if} \quad \mathbf{A}\subseteq\mathbf{B} \quad . \tag{12}
$$

Again the restricted states have density matrices so that the definition makes sense.

Positivity, boundedness and monotonicity (with respect to the subalgebra) appear to be necessary properties of any measure of the *amount of information* contained in a given finite–dimensional subalgebra *with respect to a given state.*

The following non–commutative generalization of (6) was proposed in [13] (and already before that, see the references in [13]):

Definition 3.1 (Entropy of a Subalgebra) *Given a C^* or a von Neumann algebra $\mathcal{A}$ and a state ω on it, we will call entropy of a finite–dimensional subalgebra $\mathbf{A}\subseteq\mathcal{A}$ with respect to ω, the following functional*

$$
H_\omega\left(\mathbf{A}\right) := \sup_{\omega=\sum_{i\in I}\mu_i\hat{\omega}_i} H_{\omega\,,\{\mu_i\hat{\omega}_i\}}(\mathbf{A}) \quad , \tag{13}
$$

where the supremum is computed over all decompositions $\omega = \sum_{i\in I}\mu_i\hat{\omega}_i$ of ω as linear convex combinations of states $\hat{\omega}_i$ on $\mathcal{A}$.

Even if in the above definition only decompositions $\omega = \sum_{i\in I}\mu_i\hat{\omega}_i$ into *pure* states $\hat{\omega}_i$ were taken into consideration, unlike in the Abelian case these decompositions would be in general non-unique (e.g., on $B(\mathbb{C}^2)$ we may decompose the tracial state $\rho_{\vec{0}} = \frac{1}{2}\hat{\mathbb{1}}$ into $\rho_{\vec{0}} = \frac{1}{2}(\rho_{\vec{b}} + \rho_{-\vec{b}})$ for arbitrary $\vec{b}\in\partial B$). So it is in any case necessary to perform the supremum over decompositions.

Notation. In the above definition and in the sequel we refer to *states* as to positive normalised linear functionals over algebras that might or might not be represented as density matrices acting on some Hilbert space. Furthermore, we will also use not normalized states when decomposing a given state ω: In this case we will omit the hat, so that $\hat{\omega}_i$ means $\hat{\omega}_i(\hat{\mathbb{1}}) = 1$, whereas $\omega_i(\hat{\mathbb{1}}) = \mu_i < 1$

and $\omega = \sum_{i\in I} \mu_i \hat{\omega}_i = \sum_{i\in I} \omega_i$.

Def. 3.1 is indeed a generalization of (6), since in the Abelian case we may take the decomposition $\omega = \sum_{i=1}^{d} \omega_i$ with $\omega_i(f) := \int_{\mathcal{X}} f(x)\chi_i(x)d\mu(x)$. Then the restricted states $\hat{\omega}_i \restriction_{\mathbf{A}}$ are pure so that $H_\omega(\mathbf{A}) = S(\hat{\omega}\restriction\mathbf{A}) = \sum_{i=1}^{d} \eta(\omega(\chi_i))$.

Example. In the above case of the spin $\frac{1}{2}$ particle with state $\hat{\rho}_{\vec{b}}$ it was shown by Benatti and Grava [8] that the optimal decomposition leading to $H_\omega(\mathbf{B})$ consists in writing $\hat{\rho}_{\vec{b}}$ as a convex combination of $\hat{\rho}_{\vec{b}^+}$ and $\hat{\rho}_{\vec{b}^-}$, with the vectors $\vec{b}^{\pm} := \vec{b}_\perp \pm \sqrt{1 - |\vec{b}_\perp|^2}(0,0,1) \in \partial B$ (and $\vec{b}_\perp := \vec{b} - \vec{b}_{||}$). Using formula (8),

$$S\left(\hat{\rho}_{\vec{b}^{\pm}}\restriction\mathbf{B}\right) = \eta\left(\tfrac{1}{2}\left(1 + \sqrt{1 - |\vec{b}_\perp|^2}\right)\right) + \eta\left(\tfrac{1}{2}\left(1 - \sqrt{1 - |\vec{b}_\perp|^2}\right)\right)$$

and $H_\omega(\mathbf{B}) = S\left(\hat{\rho}_{\vec{b}}\restriction\mathbf{B}\right) - S\left(\hat{\rho}_{\vec{b}^+}\restriction\mathbf{B}\right)$. Thus the entropy of $\mathbf{B}$ only coincides with the von Neumann entropy $S\left(\hat{\rho}_{\vec{b}}\restriction\mathbf{B}\right)$ if $\vec{b}_\perp = 0$, that is, if $\hat{\sigma}_3$ and $\hat{\rho}_{\vec{b}}$ commute. Figure 1 shows a contour plot of $H_\omega(\mathbf{B})$.

In the Abelian case of classical C*-dynamical systems the entropy (6) of *one* subalgebra can be directly used to define the KS dynamical entropy. However, Def. 3.1 is not sufficient for the introduction of the quantum dynamical entropy. Instead, one must first give a definition of the entropy of n subalgebras.

- In the *classical* case the measure-preserving map $S : \mathcal{X} \to \mathcal{X}$ on some phase space $\mathcal{X}$ induces via $\sigma(f) := f \circ S^{-1}$ an automorphism σ on the algebra $\mathcal{A} = L^\infty(\mathcal{X}, \mu)$ of phase space functions. Then the algebra $\mathbf{A} \subset \mathcal{A}$ of a finite partition $\mathcal{P}$ is mapped into the algebras $\sigma^k(\mathbf{A}) \subset \mathcal{A}$ of the partitions $\sigma^k(\mathcal{P})$, which due to the S-invariance of μ all have the same entropy $H_\mu\left(\sigma^k(\mathbf{A})\right) = H_\mu(\mathbf{A})$.

  The algebras $\sigma^l(\mathbf{A}), \ldots, \sigma^r(\mathbf{A})$ (with $l \le r \in \mathbb{Z}$) generate a subalgebra $\mathbf{A}_l^r := \bigvee_{l\le k\le r} \sigma^k(\mathbf{A}) \subset \mathcal{A}$ which is still finite-dimensional. Its entropy is *subadditive* and bounded, that is

  $$H_\mu\left(\mathbf{A}_0^{T-1}\right) \le H_\mu\left(\mathbf{A}_0^{t-1}\right) + H_\mu\left(\mathbf{A}_0^{T-t-1}\right) \le T H_\mu(\mathbf{A}).$$

  Thus, the *average information* $h_\mu(S\,,\,\mathbf{A}) := \lim_{T\to\infty} \frac{1}{T} H_\mu\left(\mathbf{A}_0^{T-1}\right)$ exists. The *Kolmogorov-Sinai entropy* is then defined as the maximal information per unit time coming from finite–dimensional partitions:

  $$h_\mu(S) := \sup_{\mathbf{A}} h_\mu(S\,,\,\mathbf{A}).$$

- In the *non–commutative* case, the idea of replacing the refinement of two finite partitions by the subalgebra $\mathbf{A} \vee \sigma(\mathbf{A})$ generated by a finite dimensional subalgebra $\mathbf{A} \subseteq \mathcal{A}$ and its image $\sigma(\mathbf{A})$ under the evolution (still finite–dimensional) does not in general lead to meaningful results, since $\mathbf{A} \vee \sigma(\mathbf{A})$ might be infinite–dimensional and $H_\omega(\mathbf{A} \vee \sigma(\mathbf{A}))$ undefined. See [46] for a nice example.

  The idea [13] (see also references there) is to replace the classical refinement of the algebras by (multiindexed) decompositions of the state ω. Then one adds the entropies of the algebras, and subtracts from that sum a quantity describing the correlation of the decomposition.

  That is, when dealing with n finite–dimensional subalgebras $\mathbf{A}_1, \ldots, \mathbf{A}_n$, we consider the decompositions of the state which are of the form

$$\omega = \sum_{(i)\in\mathcal{I}} \mu_{(i)} \hat{\omega}_{(i)},$$

  with the multi-index $(i) = (i_1, \ldots, i_n) \in \mathcal{I} := I_1 \times \cdots \times I_n$. Such a decomposition gives rise to the n subordinate decompositions (or partial sums)

$$\omega = \sum_{i_k\in I_k} \mu^k_{i_k} \hat{\omega}^k_{i_k} \qquad (k = 1, \ldots, n) \tag{14}$$

  with

$$\mu^k_{i_k} \hat{\omega}^k_{i_k} := \sum_{(j)\in\mathcal{I}\,,\, j_k = i_k} \mu_{(j)} \hat{\omega}_{(j)} \quad \text{and} \quad \hat{\omega}^k_{i_k}(\hat{\mathbb{1}}) = 1 \quad . \tag{15}$$

  If we denote by $\mathcal{P}$ the natural partition of the index set $\mathcal{I}$ into the atoms $(i) \in \mathcal{I}$ and by $\mathcal{P}^k$ the partition into subsets of the form $P^k_i := \{(j) \in \mathcal{I} \mid j_k = i_k\}$, then $\sum_{k=1}^n \left(H_\mu(\mathcal{P}^k)\right) - H_\mu(\mathcal{P})$ measures the deviation of the probability measure μ on $\mathcal{I}$ from the product measure $\mu^1 \times \ldots \times \mu^n$. Namely by telescoping we obtain

$$\sum_{k=1}^n \left(H_\mu(\mathcal{P}^k)\right) - H_\mu(\mathcal{P}) \;\; = \;\; \sum_{k=2}^n \left(H_\mu(\mathcal{P}^k) - H_\mu(\mathcal{P}^k | \vee_{l=1}^{k-1} \mathcal{P}^l)\right)$$

  with the *conditional entropy* $H_\mu(A|B) := H_\mu(A \vee B) - H_\mu(B) \leq H_\mu(A)$. The terms $H_\mu(\mathcal{P}^k) - H_\mu(\mathcal{P}^k | \bigvee_{l=1}^{k-1} \mathcal{P}^l) \geq 0$ measure how much information about $\mathcal{P}^k$ is gained by measuring the 'previous' partitions $\mathcal{P}^l$, $l < k$. These quantities have to be subtracted from the entropies $H_{\omega,\{\mu^k_{i_k}\omega^k_{i_k}\}}(\mathbf{A}_k) = \sum_{i_k\in I_k}\mu^k_{i_k} S\left(\omega\restriction_{\mathbf{A}_k}, \hat\omega^k_{i_k}\restriction_{\mathbf{A}_k}\right)$ of the single subalgebras $\mathbf{A}_k$. We are thus lead to consider the functional which extends (10) to the case of n subalgebras [13] (see also references there):

$$\begin{aligned} H_{\omega,\{\mu_{(i)}\hat\omega_{(i)}\}}(\mathbf{A}_1,\ldots,\mathbf{A}_n) &:= \sum_{k=1}^n H_{\omega,\{\mu^k_{i_k}\hat\omega^k_{i_k}\}}(\mathbf{A}_k) \\ &+ H_\mu(\mathcal{P}) - \sum_{k=1}^n H_\mu(\mathcal{P}^k) \quad . \end{aligned} \tag{16}$$

Then, the quantum version of the classical entropy $H_\mu(\mathcal{P})$ is:

Definition 3.2 (n–Subalgebra Entropy) *Given the finite–dimensional subalgebras $\mathbf{A}_1,\ldots,\mathbf{A}_n \subset \mathcal{A}$, their entropy $H_\omega(\mathbf{A}_1,\ldots,\mathbf{A}_n)$ with respect to the state ω, is given by taking the supremum of (14) over all multiindexed decompositions $\omega = \sum_{(i)}\mu_{(i)}\hat\omega_{(i)}$:*

$$H_\omega(\mathbf{A}_1,\ldots,\mathbf{A}_n) := \sup_{\omega=\sum_{(i)}\mu_{(i)}\hat\omega_{(i)}} H_{\omega,\{\mu_{(i)}\hat\omega_{(i)}\}}(\mathbf{A}_1,\ldots,\mathbf{A}_n) \quad . \tag{17}$$

Below we list some properties of these n–subalgebra functionals.

1. The *monotonicity* property (12) of the relative entropy carries over to the entropy of n subalgebras, i.e. for $\mathbf{A}_i \subseteq \mathbf{B}_i \subseteq \mathcal{A}$

$$H_\omega(\mathbf{A}_1,\ldots,\mathbf{A}_n) \le H_\omega(\mathbf{B}_1,\ldots,\mathbf{B}_n) \quad . \tag{18}$$

2. If the state ω is σ–invariant, then

$$H_\omega\left(\sigma^j(\mathbf{A}),\ldots,\sigma^{j+n-1}(\mathbf{A})\right) = H_\omega\left(\mathbf{A},\ldots,\sigma^{n-1}(\mathbf{A})\right) \quad . \tag{19}$$

3. The inequality $H_\mu(A|B) \le H_\mu(A)$ for the classical conditional entropy ensures that the second line in (16) is negative so that we deduce *subadditivity* and, using (11), *boundedness*, while *positivity* is almost obvious:

$$\begin{aligned} 0 \le H_\omega(\mathbf{A}_1,\ldots,\mathbf{A}_n) &\le \sum_{k=1}^n H_\omega(\mathbf{A}_k) \\ &\le \sum_{k=1}^n S(\omega\restriction\mathbf{A}_k) \le \sum_{k=1}^n \log(\mathrm{rank}(\omega\restriction_{\mathbf{A}_k})). \end{aligned} \tag{20}$$

4. *Permuting* or *repeating* subalgebras does not alter the n–subalgebra functionals [13]:

$$H_\omega\left(\mathbf{A}_{\pi(1)},\ldots,\mathbf{A}_{\pi(n)}\right) = H_\omega\left(\mathbf{A}_1,\ldots,\mathbf{A}_n,\mathbf{A}_n\right) = H_\omega\left(\mathbf{A}_1,\ldots,\mathbf{A}_n\right). \quad (21)$$

5. The n–subalgebra entropy (17) is indeed a *generalization* of the classical (Abelian) entropy $H_\omega(\mathbf{A})$, $\mathbf{A} := \mathbf{A}_1 \vee \ldots \vee \mathbf{A}_n$, of subalgebras $\mathbf{A}_1,\ldots,\mathbf{A}_n \subseteq \mathcal{A} := L^\infty(\mathcal{X},\mu)$.

   The $\mathbf{A}_k$ are generated by minimal projections $\chi^k_{i_k}$ with indices $i_k \in I_k := \{1,\ldots,\dim(\mathbf{A}_k)\}$ which are characteristic functions on the phase space $\mathcal{X}$. These give rise to decompositions $\hat{\omega} = \sum_{i_k\in I_k}\omega^k_{i_k}$ with $\omega^k_{i_k}(f) := \int_{\mathcal{X}} f(x)\chi^k_{i_k}(x)d\mu(x)$.

   As in the above case of a single algebra, the restricted states $\hat{\omega}^k_{i_k}\restriction_{\mathbf{A}_k}$ are pure so that $H_{\omega\,,\{\mu^k_{i_k}\hat{\omega}^k_{i_k}\}}(\mathbf{A}_k) = S\left(\omega\restriction\mathbf{A}_k\right) = H_\mu(\mathcal{P}^k)$. Thus we deduce from (16) that for this decomposition

$$H_{\omega\,,\{\mu_{(i)}\hat{\omega}_{(i)}\}}(\mathbf{A}_1,\ldots,\mathbf{A}_n) = H_\mu(\mathcal{P}) = H_\omega(\mathbf{A}).$$

   That the above decomposition leads to the supremum in (17) is a consequence of the inequality

$$H_\omega\left(\mathbf{A}_1,\ldots,\mathbf{A}_n\right) \leq H_\omega\left(\mathbf{A}\right).$$

   This inequality, following from $H_\omega\left(\mathbf{A}_1,\ldots,\mathbf{A}_n\right) \leq H_\omega\left(\mathbf{A},\ldots,\mathbf{A}\right) = H_\omega\left(\mathbf{A}\right)$, is not very useful in quantum mechanics, where $\mathbf{A}$ may be of infinite dimension. But in our Abelian case $\mathbf{A}$ is finite–dimensional so that we have seen that the n–subalgebra entropy (17) is also $\leq H_\omega(\mathbf{A})$.

6. A non–commutative situation similar to the classical one is when the reference state ω is *tracial* in the sense that $\omega(\hat{X}\hat{Y}) = \omega(\hat{Y}\hat{X})$ for all $\hat{X},\hat{Y}$ in $\mathcal{A}$. Suppose that the n finite–dimensional subalgebras $\mathbf{A}_j$, $1 \leq j \leq n$, commute with each other. Let $\mathbf{P}_j$ be maximally Abelian subalgebras of the corresponding $\mathbf{A}_j$, with minimal projections $\{\hat{P}^j_{i_j}\}_{i_j=1}^{d_j}$.

   Because ω is tracial, we may decompose it into $\omega = \sum_{(i)}\mu_{(i)}\hat{\omega}_{(i)}$ with the multi–index $(i) = (i_1,\ldots,i_n)$, where

$$\hat{\omega}_{(i)}(\hat{X}) := \frac{\omega\left(\prod_{k=1}^n \hat{P}^k_{i_k}\hat{X}\right)}{\omega\left(\prod_{k=1}^n \hat{P}^k_{i_k}\right)}\,, \quad \mu_{(i)} = \omega\left(\prod_{k=1}^n \hat{P}^k_{i_k}\right)\quad , \quad (22)$$

and we obtain $\omega = \sum_{i_j} \mu^j_{i_j} \hat{\omega}^j_{i_j}$, where $\mu^j_{i_j} = \omega\left(\hat{P}^j_{i_j}\right)$ and $\hat{\omega}^j_{i_j}(\hat{X}) = \dfrac{\omega\left(\hat{P}^j_{i_j}\hat{X}\right)}{\omega\left(\hat{P}^j_{i_j}\right)}$.

Therefore, as in property 5. above,

$$H_{\omega,\{\mu^j_{i_j}\hat{\omega}^j_{i_j}\}}(\mathbf{P}_j) = S(\omega\restriction\mathbf{P}_j) = \sum_{i_j} \eta(\mu^j_{i_j})$$

and, consequently, $H_\omega(\mathbf{P}_1, \ldots, \mathbf{P}_n) = S(\omega\restriction\mathbf{P})$, where $\mathbf{P} = \mathbf{P}_1 \vee \ldots \vee \mathbf{P}_n$ is the finite–dimensional Abelian algebra with minimal projections $\prod_{k=1}^{n} \hat{P}_{i_k}$, which is maximally Abelian in $\mathbf{A} = \mathbf{A}_1 \vee \cdots \vee \mathbf{A}_n$. Then, $H_\omega(\mathbf{A}_1, \ldots, \mathbf{A}_n) \geq S(\omega\restriction\mathbf{P})$ follows from (18).

On the other hand, in full generality,

$$S(\omega\restriction\mathbf{A}) = \min\{S(\omega\restriction\mathbf{P}) \mid \mathbf{P} \subseteq \mathbf{A} \text{ maximallyAbelian}\}.$$

Thus it follows, again e.g. from (18), (20), (21), that $H_\omega(\mathbf{A}_1, \ldots, \mathbf{A}_n) \leq H_\omega(\mathbf{A}) \leq S(\omega\restriction\mathbf{A}) \leq S(\omega\restriction\mathbf{P})$, whence

$$H_\omega(\mathbf{A}_1, \ldots, \mathbf{A}_n) = S(\omega\restriction\mathbf{P}).$$

7. In the above examples we have seen how to optimally decompose a state with respect to the n–subalgebra entropy functionals in the Abelian case and when the reference state is tracial.

   In general quantal situations when neither the algebra $\mathcal{A}$ is commutative, nor the state ω tracial, the way one gets all possible *decompositions of* ω is by considering the von Neumann algebra $\mathcal{M} := \pi_\omega(\mathcal{A})''$ arising from the GNS construction based on ω, touched upon at the end of the introductory Section 2.

   The commutant $\mathcal{M}'$ of $\mathcal{M}$ over $\mathbb{H}_\omega$ contains all sets of positive operators $\hat{X}'_i \in \mathcal{M}'$ such that $\sum_{i\in I} \hat{X}'_i = \hat{1\!\!1}$ are in one–to–one correspondence with decompositions of $\omega = \sum_{i\in I} \mu_i \hat{\omega}_i$ (using the ω–representing vector $|\Omega\rangle \in \mathbb{H}_\omega$ from Section 2):

$$\hat{\omega}_i\left(\hat{Y}\right) = \frac{\langle\Omega, \hat{X}_i'\pi_\omega\left(\hat{Y}\right)\Omega\rangle}{\langle\Omega, \pi_\omega\left(\hat{X}\right)\Omega\rangle}\,, \qquad (\hat{Y}\in\mathcal{A}) \quad . \tag{23}$$

8. The above point is best exemplified by referring to the C* algebra $\mathbf{A} = B(\mathbb{C}^2)$ and to a state on it described by an invertible density matrix $\hat{\rho}$. The GNS construction based on $\hat{\rho}$ has $\mathbf{A}$ represented as $\mathbf{A}\otimes\hat{1\!\!1}$ on the Hilbert space $\mathbb{C}^4$. Its commutant is $\hat{1\!\!1}\otimes\mathbf{A}$ and the GNS cyclic vector is $|\sqrt{\hat{\rho}}\rangle = \sum_{i=1}^{2}\sqrt{\rho_i}|e_i\rangle\otimes|e_i\rangle$, with $|e_i\rangle$ the eigenvectors of $\hat{\rho}$. Thus, formula (23) concretely reads
$$\hat{\omega}_i\left(\hat{Y}\right) = \mathrm{Tr}\left(\frac{\sqrt{\hat{\rho}}\hat{X}_i\sqrt{\hat{\rho}}}{\mathrm{Tr}\,\hat{\rho}\hat{X}_i}\hat{Y}\right)\,,$$
where the $\hat{X}_i$ are positive operators of $\mathbf{A}$ such that $\sum_{i\in I}\hat{X}_i = \hat{1\!\!1}$.

3.2 Non–commutative Dynamical Entropy

Because of (19) and (20), as for the Kolmogorov–Sinai entropy, the limit

$$h_\omega(\sigma\,,\,\mathbf{A}) := \lim_{T\to\infty}\frac{1}{T}H_\omega\left(\mathbf{A},\ldots,\sigma^{T-1}(\mathbf{A})\right) \tag{24}$$

exists.

It is interpreted as the information gained per time unit by repeatedly performing suitable experiments with observables in the subalgebra $\mathbf{A}\subseteq\mathcal{A}$. The *Quantum Dynamical Entropy* of A. Connes, H. Narnhofer and W. Thirring is then defined as the maximal average information contributed by finite–dimensional subalgebras [13] (see also references there):

$$h_\omega(\sigma) := \sup_{\mathbf{A}\subseteq\mathcal{A}} h_\omega(\sigma\,,\,\mathbf{A}) \quad . \tag{25}$$

Some properties and comments.

i. By the above property 5. of the n–subalgebra entropy, the CNT entropy $h_\omega(\sigma)$ is a *generalization* of the Kolmogorov–Sinai entropy.
ii. Generally, the entropy for a fixed subalgebra $\mathbf{A}$ is sublinear with respect to taking positive powers of the automorphism σ:

$$h_\omega(\sigma^n,\mathbf{A}) \leq n\cdot h_\omega(\sigma,\mathbf{A}) \qquad n\in\mathbb{N} \quad . \tag{26}$$

This follows from the properties of the n–subalgebra entropy [13], partly listed after Definition 3.2.

iii. Like classically, we can benefit from a *Kolmogorov–Sinai* type *theorem* [13] which states that, if $\{\mathbf{A}_j\}$ is an increasing sequence, $\mathbf{A}_j \subseteq \mathbf{A}_{j+1}$, of finite–dimensional subalgebras that generate $\mathcal{A}$ as a C*–algebra or as a von Neumann algebra and the state ω is compatible with the corresponding topologies, then

$$h_\omega(\sigma) = \lim_{j\to\infty} h_\omega(\sigma\,,\,\mathbf{A}_j) \quad . \tag{27}$$

In this case, also the converse of the inequality (26) above can be proved [13] for the full CNT entropy: $h_\omega(\sigma^n) = n \cdot h_\omega(\sigma)$ then scales linearly with the power n of σ, as for the classical KS entropy. – Even more generally, a Kolmogorov–Sinai type theorem can be proved [13] for the class of so-called *nuclear* C*–algebras $\mathcal{A}$, see also the brief remark after Def. 4.5 in Sect. 4 below. This is achieved in [13] by extending the entropy functional (24) above from a finite–dimensional subalgebra $\mathbf{A} \subset \mathcal{A}$ (then equivalently viewed as the corresponding canonical inclusion $*$–homomorphism of $\mathbf{A}$ into $\mathcal{A}$) to general *completely positive, unital* (i.e., unity–preserving) maps from abstractly given finite–dimensional C*–algebras into $\mathcal{A}$. For our applications, the definition (24) of entropy for proper subalgebras of $\mathcal{A}$ will be sufficient, whereas we will have to use the concept of positive unital maps of finite rank into $\mathcal{A}$ for the non–commutative generalization of the classical *topological* entropy [23] to be introduced in Sect. T below.

Remark 3.3 *If $\mathcal{A}$ is a C*–algebra, the generating sequence $\{\mathbf{A}_j\}$ must yield $\mathcal{A}$ as a uniform limit $\overline{\bigcup_j \mathbf{A}_j}^{un}$. The state ω, as a positive linear functional over $\mathcal{A}$, is automatically compatible with the uniform topology.*

The case of a von Neumann algebra $\mathcal{A}$ is different. We can think of it as an algebra of operators acting on some Hilbert space $\mathbb{H}$. An increasing sequence of subalgebras $\{\mathbf{A}_j\}$ is generating for it, if the union $\bigcup_j \mathbf{A}_j$ is dense in $\mathcal{A}$ in the strong–operator sense. As the strong–operator topology is coarser than the uniform one, not all positive linear functionals (states) are continuous with respect to it. Those states that enjoy such a propery are called **normal**. *When $\mathcal{A}$ is generated by $\{\mathbf{A}_j\}$ as a von Neumann algebra, it is for normal ω that the Kolmogorov–Sinai like theorem is proved [13].*

iv. As already the Kolmogorov–Sinai entropy is *conjugacy–invariant* [50], here also two isomorphic quantum dynamical systems have the same CNT–entropy. More concretely, let $(\mathcal{A}_1, \sigma_1, \omega_1)$, $(\mathcal{A}_2, \sigma_2, \omega_2)$ be two quantum dynamical systems and $i_{12} : \mathcal{A}_1 \to \mathcal{A}_2$ an isomorphism between the two algebras such that 1) $\omega_2 = \omega_1 \circ i_{12}^{-1}$ and 2) $\sigma_2 = i_{12} \circ \sigma_1 \circ i_{12}^{-1}$. Then

$$h_{\omega_1}(\sigma_1) = h_{\omega_2}(\sigma_2) \quad . \tag{28}$$

3.3 Classical Dynamical Systems

As already in Sect. 3.1 (Property 5 of the final list of properties there), we now consider a discrete classical dynamical system $(\mathcal{X}, S, \mu)$ with phase space $\mathcal{X}$, probability measure μ and a measure-preserving invertible map $S : \mathcal{X} \to \mathcal{X}$. We associate to it the C*–dynamical system $(\mathcal{A}_{cl}, \sigma_{cl}, \omega_{cl})$ with $\mathcal{A}_{cl} = L^\infty(\mathcal{X}, \mu)$, $\sigma_{cl}(f) = f \circ S^{-1}$ for $f \in \mathcal{A}_{cl}$ and $\omega_{cl}(f) = \int_{\mathcal{X}} f d\mu$, and we noticed in 3.2 above that the CNT entropy $h_{\omega_{cl}}(\sigma_{cl})$ coincides with the Kolmogorov-Sinai entropy $h_\mu(S)$.

Now we will follow a von Neumann (Hilbert space) approach instead of the above C*–algebraic approach. The Hilbert space $\mathbb{H}_\mu := L^2(\mathcal{X}, \mu)$ of square integrable phase space functions is then unitarily mapped onto itself by

$$\hat{U} : \mathbb{H}_\mu \mapsto \mathbb{H}_\mu \qquad \left(\hat{U}\psi\right)(x) = \psi(S^{-1}x)\,, \qquad (\psi \in \mathbb{H}_\mu) \quad , \tag{29}$$

since S leaves μ invariant. The algebra $\mathcal{A}_{cl}$ is a maximally Abelian subalgebra of the von Neumann algebra $B(\mathbb{H}_\mu)$ of bounded operators, and the functions $f \in \mathcal{A}_{cl}$ act by multiplication on $\mathbb{H}_\mu$.

The identity function on $\mathcal{X}$, identified with the vector $|\hat{\mathbb{1}}_\mu\rangle \in \mathbb{H}_\mu$, defines the pure state

$$\omega : B(\mathbb{H}_\mu) \to \mathbb{C}, \qquad \omega(\hat{X}) := \langle \hat{\mathbb{1}}_\mu, \hat{X}\hat{\mathbb{1}}_\mu \rangle \tag{30}$$

on $B(\mathbb{H}_\mu)$ whose restriction

$$\omega \restriction_{\mathcal{A}_{cl}} = \omega_{cl}.$$

If we now consider the automorphism

$$\sigma : B(\mathbb{H}_\mu) \to B(\mathbb{H}_\mu), \qquad \sigma(\hat{X}) := \hat{U}^*\hat{X}\hat{U}$$

induced by $\hat{U}$, then σ restricts to the automorphism

$$\sigma \restriction_{\mathcal{A}_{cl}} = \sigma_{cl}.$$

So the CNT entropy of the restricted state ω_{cl} is larger than the CNT entropy of the pure state ω:

$$h_\mu(S) = h_{\omega_{cl}}(\sigma_{cl}) \geq h_\omega(\sigma) = 0,$$

In particular the former CNT entropy is strictly positive if the motion is chaotic, since it coincides with the KS entropy (and since we call a system *chaotic* if its KS entropy is > 0).

There is no contradiction in the fact that $h_{\omega_{cl}}(\sigma_{cl}) > 0$, while $h_\omega(\sigma) = 0$.

In fact, if $\mathcal{N} \subseteq \mathcal{M}$, then the commutant of $\mathcal{N}$ contains that of $\mathcal{M}$. Therefore, according to (23), if ω is a state on $\mathcal{M}$, the restriction $\omega \lceil \mathcal{N}$ has more possibilities of being decomposed. The case of a pure state is extremal in the sense that, in the GNS construction, the commutant of $\mathcal{M}$ is trivial, whereas the commutant of a proper subalgebra of $\mathcal{M}$ is not trivial.

In our case the restriction ω_{cl} of the pure state ω to $\mathcal{A}_{cl}$ is in general not pure. As in Sect. 3.1 we only need to find a partition $\mathcal{P}$ of the phase space $\mathcal{X}$ into atoms P_i of measure $\mu_i := \mu(P_i) \in (0,1)$. The corresponding decomposition $\omega_{cl} = \sum_{i=1}^n \mu_i \hat{\omega}_i$ of the state with $\hat{\omega}_i(f) := \int_{P_i} f d\mu/\mu(P_i)$ is non-trivial which then shows that ω_{cl} is not pure.

Suppose now that the classical dynamical system $(\mathcal{X}, S, \mu)$ corresponds to a so–called $\mathbb{K}$-system. Then $h_{\omega_{cl}}(\sigma_{cl}) > 0$, since by definition the Kolmogorov–Sinai entropy $h_\mu(S\,,\,\mathcal{P})$ of a $\mathbb{K}$-system is strictly positive for all non–trivial finite–dimensional measurable partitions $\mathcal{P}$ of $\mathcal{X}$ [15].

On the other hand in the above situation, there are no other normal, σ–invariant states. In fact, if the classical dynamical system is a $\mathbb{K}$–system, the spectrum of $\hat{U}$ has only 1 as an eigenvalue and its multiplicity is 1, with $|\hat{1\!\!1}_\mu\rangle$ as unique eigenvector.

Thus, in spite of the high randomness of the classical motion, the non–commutative dynamical system naturally arising from the Koopman formulation loses sight of that randomness when measured (on the whole of $B(\mathbb{H})$) from the point of view of normal, invariant states.

While we cannot renounce σ–invariance, we might want to work with invariant states that are not strong–operator continuous, that is not matching the von Neumann structure of $B(\mathbb{H})$, but only its C*–structure: see at the end of Remark 3.3 of Sect. 3.2, why this does not work for computing the CNT entropy in this situation.

3.4 Systems with Purely Discrete Spectrum

1) A typical application of the CNT–entropy construction is to the *quantum spin chain* $\mathcal{A} := \bigotimes_{n\in\mathbb{Z}} \mathbf{M}_d(\mathbb{C})$, with the same full $d\times d$ matrix algebra $\mathbf{M}_d(\mathbb{C})$ at each integer site. $\mathcal{A}$ is understood as a quasi–local C* algebra (inductive uniform limit) with the generating system of increasing, finite–dimensional, subalgebras $\mathbf{A}_{[-n,n]} := \bigotimes_{-n\leq k\leq n} \mathbf{M}_d(\mathbb{C})$.

Equipping $\mathcal{A}$ with the shift $\sigma(\hat{A})_i := \hat{A}_{i+1}$ and the tracial state $\omega(\hat{A}) := \frac{1}{d^{2n+1}}\mathrm{Tr}\,\hat{A}$, $\hat{A} \in \mathbf{A}_{[-n,n]}$, the CNT entropy of the dynamical system $(\mathcal{A},\sigma,\omega)$ equals the entropy density [13]

$$s(\omega) := \lim_{n\to\infty} \frac{1}{2n+1} S\left(\omega\restriction\mathbf{A}_{[-n,n]}\right) = \log d \quad . \tag{31}$$

Since $S\left(\omega\restriction\mathbf{A}_{[-n,n]}\right) = (2n+1)\log d$, $h_\omega(\sigma) \leq \log d$ is easily proved. Indeed,

$$\begin{aligned} h_\omega(\sigma) &= \lim_{n\to\infty} h_\omega\left(\sigma\,,\,\mathbf{A}_{[-n,n]}\right) \quad \text{from (27)} \\ &= \lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{k}H_\omega\left(\mathbf{A}_{[-n,n]},\ldots,\mathbf{A}_{[-n+k-1,k+n-1]}\right) \\ &\leq \lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{k}H_\omega\left(\mathbf{A}_{[-n,k+n-1]}\right) \quad \text{from (18)} \\ &\leq \lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{k}S\left(\omega\restriction\mathbf{A}_{[-n,n+k-1]}\right) \quad \text{from (9)} \quad . \end{aligned} \tag{32}$$

The inequality $h_\omega(\sigma) \geq s(\omega)$ comes from choosing the subalgebra $\mathbf{A}_0$ at the 0-th site and invoking property 6. of the n–subalgebra entropy (see Sect. 3.1):

$$\begin{aligned} h_\omega(\sigma) \geq h_\omega(\sigma\,,\,\mathbf{A}_0) &= \lim_{k\to\infty}\frac{1}{k}H_\omega(\mathbf{A}_0,\mathbf{A}_1,\ldots,\mathbf{A}_{k-1}) \\ &= \lim_{k\to\infty}\frac{1}{k}S\left(\omega\restriction\mathbf{A}_{[0,k-1]}\right) = \log d \quad . \end{aligned} \tag{33}$$

Inequality (32) is independent from the tracial properties of the translation invariant state ω, whereas the characteristic absence of correlations is crucial in getting the equality [13].

2) More physically, let $\mathcal{A}$ be the CAR (CCR) algebra of Fermions (Bosons) over the single particle Hilbert space $L^2(\mathbb{R}^\nu, \mathrm{d}^\nu x)$ and

$$\theta^n(\hat{a}^\dagger(f)) := \hat{a}^\dagger(\hat{U}(n)f) \quad \text{with} \quad (\hat{U}(n)f)(x) := f(x-n)\,, n\in\mathbb{Z}^\nu \tag{34}$$

the ν–dimensional *space translation group*. Finally, let $\hat{A}$ be a positive one–particle operator, $\leq \hat{\mathbb{1}}$ for Fermions, such that

$$\omega_A\left(\hat{a}^\dagger(f)\hat{a}(g)\right) := \langle g, \hat{A}f\rangle = \int_{\mathbb{R}^\nu}\int_{\mathbb{R}^\nu} \bar{g}(x)K_A(x-y)f(y)\mathrm{d}^\nu x\,\mathrm{d}^\nu y \qquad (35)$$

defines a translation invariant quasi–free state, and the Fourier transform $\hat{K}_A(k) := \int_{\mathbb{R}^\nu} \mathrm{e}^{-i\,k\cdot x}K_A(x)\mathrm{d}^\nu x$ enjoys sufficiently rapid decreasing properties [38].

Then, the CNT entropy of the full–translation group is again proved to coincide with the entropy density (upper signs for Fermions, lower ones for Bosons) [39]:

$$h_{\omega_A}(\theta) = \frac{1}{(2\pi)^\nu}\int \left[\eta(\hat{K}_A(k)) \pm \eta(1 \mp \hat{K}_A(k))\right]\mathrm{d}^\nu k \quad . \qquad (36)$$

3) In [35] the case of the CAR algebra $\mathcal{A}$ over $L^2(\mathbb{R}, \mathrm{d}x)$ is studied, with the quasi–free time evolution

$$\sigma_\epsilon\left(\hat{a}^\dagger(f)\right) = \hat{a}^\dagger(\hat{U}_\epsilon f)\,, \quad (\hat{U}_\epsilon f)(p) = \mathrm{e}^{-i\,\epsilon(p)}f(p) \quad , \qquad (37)$$

and the σ_ϵ–invariant quasi–free state

$$\omega_\epsilon\left(\hat{a}^\dagger(f)\hat{a}(g)\right) = \int \mathrm{d}p\,\bar{g}(p)f(p)\underbrace{\frac{1}{1+\mathrm{e}^{\epsilon(p)}}}_{\rho(p)} \quad . \qquad (38)$$

Under suitable conditions on the one–particle energy $\epsilon(p)$, the CNT entropy is computed to be

$$h_{\omega_\epsilon}(\sigma_\epsilon) = \frac{1}{2\pi}\int \left|\frac{\mathrm{d}\epsilon(p)}{\mathrm{d}p}\right| \left[\eta(\rho(p)) + \eta(1-\rho(p))\right]\mathrm{d}p \quad . \qquad (39)$$

4) Finally, Störmer and Voiculescu prove in [45] that, given the quasi–free state ω_A in (3), if $\hat{A}$ has pure point spectrum and commutes with the one–particle evolution $\hat{U}$, then only the absolutely continuous component of the spectrum of $\hat{U}$ contributes to the CNT entropy which equals

$$h_{\omega_A}(\sigma_U) = \frac{1}{2\pi}\int_0^{2\pi} m(\theta)\,\left[\eta(A(\theta)) + \eta(1-A(\theta))\right]\mathrm{d}\theta \quad , \qquad (40)$$

where $A(\theta)$ is the diagonalization of $\hat{A}$ according to the spectral representation of $\hat{U}$ and $m(\theta)$ is its spectral multiplicity.

The fact that the singular components (both discrete and continuous) of the spectrum of $\hat{U}$ have zero CNT entropy is obtained by different arguments in [44].

5) It is none the less useful to examine the result from a less abstract point of view than in [45, 44].

Indeed, most of the quantum systems under investigation as instances of chaotic behaviour have finite degrees of freedom, while the CNT entropy seems to be nontrivial only for systems containing infinitely many particles. It is thus interesting to understand what role is played by the invariant state, respectively the evolution in fixing the value of the CNT entropy.

The case when the algebra $\mathcal{A}$ is *finite–dimensional*, say a matrix algebra of bounded operators over a finite–dimensional Hilbert space $\mathbb{H}$, is clear. The CNT entropy of any automorphism with respect to any invariant state ω is zero, as all n–subalgebra entropy functionals are bounded by the entropy $H_\omega(\mathcal{A}) \leq S(\omega\restriction\mathcal{A}) \leq \log\dim(\mathbb{H})$.

Let us now examine a typical quantum mechanical situation where $\mathbb{H}$ is *not* finite–dimensional, $\mathcal{A} = B(\mathbb{H})$ and the evolution is given as in equation (1) with $\hat{U}_t = \mathrm{e}^{-i\hat{H}t}$ and assume that there is an invariant normal state ρ as in (2), with $\left[\hat{\rho}\,,\,\hat{U}\right] = 0$. Then,

Proposition 3.4 *Given the time evolution* $B(\mathbb{H}) \ni \hat{X} \mapsto \sigma(\hat{X}) = \mathrm{e}^{i\hat{H}}\hat{X}\mathrm{e}^{-i\hat{H}}$*, and any invariant normal state* ρ *on* $B(\mathbb{H})$*, then* $h_\rho(\sigma) = 0$*.*

Proof. By assumption ρ is represented by the trace with respect to a density matrix $\hat{\rho}$ such that $\left[\hat{\rho}\,,\,\hat{H}\right] = 0$. Let $\left\{\hat{P}_j\right\}_{j\in\mathbb{N}}$ be any resolution of the identity by one–dimensional, pairwise orthogonal eigenprojectors of $\hat{\rho}$, $\hat{\rho}\hat{P}_j = \rho_j\hat{P}_j$, the eigenvalues ρ_j being repeated according to their multiplicities and enumerated in decreasing order (if there are zero eigenvalues, also possibly with infinite multiplicity, we order them alternatingly with the decreasing non–zero eigenvalues in the sequence ρ_j).

Let $\hat{P}_{n]} := \bigoplus_{j=0}^n \hat{P}_j$, $\hat{Q}_{n]} := \hat{1\!\!1} - \hat{P}_{n]}$. Then, consider $B_{n]} := \hat{P}_{n]}B(\mathbb{H})\hat{P}_{n]} \oplus \mathbb{C}\cdot\hat{Q}_{n]}$. These are finite–dimensional subalgebras of $B(\mathbb{H})$ with the same identity, whose elements are finite–rank operators (of rank at most $(n{+}1)$). Moreover, the sequence is increasing and the strong–operator closure of $\bigcup_{n\in\mathbb{N}} B_{n]}$ is the whole of $B(\mathbb{H})$. Furthermore, due to the assumption that $\left[\hat{\rho}\,,\,\hat{U}\right] = 0$, the subalgebras $B_{n]}$ are σ–invariant: $\sigma\left(B_{n]}\right) \subseteq B_{n]}$. Therefore, we can argue as in (32):

$$
\begin{aligned}
h_\rho(\sigma) &= \lim_{n\to+\infty} h_\rho\left(\sigma\,,\,B_{n]}\right) \\
&= \lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{k}H_\rho\left(B_{n]},\sigma\left(B_{n]}\right),\ldots\right) \\
&\leq \lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{k}H_\rho\left(B_{n]},B_{n]},\ldots\right)
\end{aligned}
$$

$$\leq \lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{k}H_\rho\left(B_{n]}\right) \leq \lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{k}S\left(\rho\restriction B_{n]}\right) = 0 \quad . \quad \square$$

Remark 3.5 *Notice that the normal states over the von Neumann algebra $B(\mathbb{H})$ coincide with the density matrices and, according to Remark 3.3, the above result holds for them and not necessarily for other states that are only continuous in the norm–topology of $B(\mathbb{H})$: with respect to the latter, the closure of $\bigcup_{n\in\mathbb{N}} B_{n]}$ would give the compact operators over $\mathbb{H}$ (with the identity operator adjoined) and not all the bounded ones.*

3.5 Quantum Mechanical Randomness

In this section we would like to deepen the question addressed in section 3.3, there concerning the Koopman formulation of classical mechanics. Namely, we will consider cases where a classically chaotic behaviour can be directly transfered to the quantum level, and we will investigate whether there is a way to put this quantum chaoticity into evidence by entropic means.

However, if we decide to signal the presence of quantum chaos by means of the positivity of the CNT–entropy, then according to Proposition 3.4 of the preceding section, at least all systems of finitely many degrees of freedom, even with significantly 'erratic' quantum evolution in finite time–intervals, will not match anyway the time average in the entropy definition, and will thus not be chaotic according to the chosen criterium.

3.5.1 Finite Degrees of Freedom

Sometimes one hears the wrong argument that quantum mechanics, by the mere linearity of the Schrödinger equation, should be incompatible with chaos. As Berry noticed in [9], that reasoning would equally apply to classical mechanics in the Koopman formulation (29).

As a counterexample, we discuss in this subsection a Schrödinger equation with random properties.

In a general setting we start with a vector field $\vec{V}$ on a manifold $\mathcal{X}$ which is divergence-free for some phase space volume μ. This vector field then induces the ordinary differential equation

$$\dot{x} = \vec{V}(x) \tag{41}$$

on $\mathcal{X}$ whose flow transforms a phase space density ρ on $\mathcal{X}$ according to

$$\frac{\partial}{\partial t}\rho_t = d\rho_t(\vec{V}). \tag{42}$$

On the Hilbert space $L^2(\mathcal{X},\mu)$ this Liouville equation has the form

$$i\hbar\frac{\partial}{\partial t}\rho_t = \hat{\mathcal{H}}\rho_t \tag{43}$$

of a Schrödinger equation, with the 'Hamiltonian' operator $\hat{\mathcal{H}} := \sum_{a=1}^{\dim(\mathcal{X})}\vec{V}_a\hat{\pi}_a$ and 'momenta' $\hat{\pi}_a := -i\hbar\frac{\partial}{\partial x^a}$. These momenta have the usual commutator $[\hat{x}^a\,,\,\hat{\pi}_b] = i\hbar\delta^a_b$ with the coordinates $\hat{x}^a$, and $\hat{\mathcal{H}}$ is formally hermitean since the vector field $\vec{V}$ has no divergence.

Clearly, the solutions of (43) will follow classical trajectories and, in case the latter behave chaotically, the support of the former will develop characteristic features like whorls and tendrils, no $\hbar$ smoothing effect being at work.

One class of such systems is given by Hamiltonian vector fields $\vec{V} := J\bigtriangledown H$ on a phase space $\mathcal{X} := \mathbb{R}^n_q \times \mathbb{R}^n_p$ with Hamilton function $H : \mathcal{X} \to \mathbb{R}$ and $J := \left(\begin{smallmatrix} 0 & \hat{1\!\!1} \\ -\hat{1\!\!1} & 0\end{smallmatrix}\right)$. Then, however, the Hamiltonian operator $\hat{\mathcal{H}}$ acts on $L^2(\mathcal{X},\mu)$, that is, on the phase space functions instead of the configuration space functions, so that we definitely do *not* consider a quantization of the classical dynamical system.

If we want to consider the quantization of a classical motion, we should thus start with a vector field on *configuration space.*

Indeed, in spite of its abstractness, the above construction indicates the possibility that quantum Hamiltonians, linear in the momentum operators, be used to transfer erratic classical behaviours to the quantum case.

This is exactly what done in a paper [40] by Pasmanter, where, given an incompressible velocity field $\mathbf{u}(\mathbf{x})$, $\operatorname{div}\mathbf{u}(\mathbf{x}) = 0$, he constructs the Schrödinger–type equation:

$$i\hbar\frac{\partial\psi_t}{\partial t} = \left(\mathbf{u}(\mathbf{x})\cdot\hat{\mathbf{p}} + \hat{\sigma}_3E_0 + \hat{\sigma}_2\kappa\right)\psi_t\,, \quad \text{where} \tag{44}$$

$$\hat{\mathbf{p}} = -i\hbar\vec{\bigtriangledown}\,, \quad \hat{\sigma}_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}\,, \quad \hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad . \tag{45}$$

The incompressibility of $\mathbf{u}(\mathbf{x})$ ensures the hermiticity of the Hamiltonian in (44).

The model describes a two–particle system (ψ^1,ψ^2) whose components are advected by the velocity field $\mathbf{u}(\mathbf{x})$ and spontaneously converted one into the other at a rate $\kappa/\hbar$. From the linearity of the Hamiltonian it follows that the total density $\rho_t(\mathbf{x}) := |\psi^1_t(\mathbf{x})|^2 + |\psi^2_t(\mathbf{x})|^2$ satisfies the advection equation:

$$\frac{\partial}{\partial t}\rho_t(\mathbf{x}) = -\mathrm{div}(\mathbf{u}(\mathbf{x})\,\rho_t(\mathbf{x})) \quad . \tag{46}$$

The interest of the above model lies in the fact that there are choices of the incompressible velocity field giving rise to chaotic patterns in the dynamics of planar and tridimensional fluids. Again, these features would be transmitted to the solutions of (44). Moreover, from possible eigenfunctions of (46) with real eigenvalues ω_n, $-\bigtriangledown\cdot[\mathbf{u}(\mathbf{x})\psi_n(\mathbf{x})] = \omega_n\psi_n(\mathbf{x})$, one obtains eigenvalues Ω_n and eigenfunctions Ψ_n of (44) [40].

The latter possibility renders the non–commutative situation somewhat richer than the one arising from the Koopman approach of subsection 3.3. In fact, convex linear combinations of eigenprojectors would provide non–trivial invariant states. However, their normality would permit to follow exactly the argument of Proposition 3.4 and to show that the CNT–entropy for the above dynamical system is zero. As before, the persistence (less abstract in such a case) of classically erratic behaviour affecting the supports of the solutions of the quantum dynamics (44) is not reflected by the strict positivity of the corresponding CNT–entropy with respect to normal invariant states.

3.5.2 Infinite Degrees of Freedom

Typically, one goes from a one-particle system to infinitely many degrees of freedom through second quantization. As a consequence, there is abundance of non-normal states that remain invariant under a given evolution and thus allow us to avoid the consequences of Proposition 3.4.

Moreover, the possibility that information can get lost is greatly enhanced by a mechanism that we describe by considering a one-particle system evolving according to a discrete group of unitaries $\hat{U}(n)$ on a Hilbert space $\mathbb{H}$. Further, we assume that $\hat{U}$ has *homogeneous Lebesgue spectrum*. This means that there exists an increasing sequence $\mathbb{H}_k \subseteq \mathbb{H}_{k+1} \subseteq \mathbb{H}$, $k \in \mathbb{Z}$, of Hilbert spaces such that 1) $\hat{U}\mathbb{H}_k = \mathbb{H}_{k+1}$, 2) $\bigcap_k \mathbb{H}_k = \emptyset$, while 3) the closure of the linear span $\bigcup_k \mathbb{H}_k$ is either $\mathbb{H}$ or the orthogonal subspace to the unique $\hat{U}$–invariant state $|\Omega\rangle$, if the latter exists.

It turns out that, by considering the orthogonal complements $\mathbb{K}_k \subset \mathbb{H}_k$ of $\mathbb{H}_{k-1}$, we can choose a basis $|e_{0,j}\rangle$, $1 \leq j \leq J$, in $\mathbb{K}_0$ such that the vectors $|e_{k,j}\rangle := \hat{U}(k)|e_{0,j}\rangle$ form a basis in $\mathbb{K}_k$,

$$\langle e_{k_1,j_1}\,,\, e_{k_2,j_2}\rangle = \delta_{k_1,k_2}\delta_{j_1,j_2} \quad , \tag{47}$$

and $\{|e_{k,j}\rangle\}$ is a basis in $\mathbb{H}$ (or in $|\Omega\rangle^\perp$), J being the multiplicity of the spectrum.

The spectrum of $\hat{U}$ on the orthogonal subspace $|\Omega\rangle^\perp$ is absolutely continuous; thus, according to Proposition 3.4, the absence at all of normal invariant states or of nonpure normal invariant states means that either we cannot use a Kolmogorov–Sinai type approximation as in (27) or that the result is trivially zero as in section 3.3.

Nevertheless, for future purposes (see around equation (74) in Sect. 4), we elaborate on that argument. That is, we keep for a moment the one–particle description and thus consider the C*–algebra $B(\mathbb{H})$ over the Hilbert space $\mathbb{H}$. For sake of simplicity we suppose $|\Omega\rangle$ not to exist (otherwise our considerations will be valid with reference to the Hilbert space $|\Omega\rangle^\perp$) and that the multiplicity $J<\infty$. Thus, let $\hat{E}_{k,j}$ be the one–dimensional, pairwise orthogonal projections corresponding to the basis vectors $|e_{k,j}\rangle$ and construct

$$\hat{E}_{[-n,n]} := \bigoplus_{-n\leq k\leq n} \bigoplus_{1\leq j_k\leq J} \hat{E}_{k,j_k}\,, \qquad \hat{Q}_{[-n,n]} := \hat{1\!\!1} - \hat{E}_{[-n,n]} \quad . \tag{48}$$

In this way, the strong–operator limit of the double sequence of finite rank orthogonal projections $\hat{E}_{[-n,n]}$ is the identity operator on $\mathbb{H}$ and the sequence of finite–dimensional subalgebras

$$B_{[-n,n]} := \hat{E}_{[-n,n]} B(\mathbb{H}) \hat{E}_{[-n,n]} \oplus \mathbb{C}\cdot\hat{Q}_{[-n,n]} \tag{49}$$

is such that the strong–operator closure of $\bigcup_{n\in\mathbb{N}} B_{[-n,n]} = B(\mathbb{H})$.

The subalgebras $B_{[-n,n]}$, as linear spaces, have dimension $(2n+1)J+1$. Moreover, $\hat{U}|e_{i,j}\rangle = |e_{i+1,j}\rangle$, whence $\sigma^l\left(B_{[-n,n]}\right) = B_{[-n+l,n+l]}$. It follows that the finite–dimensional subalgebras $B_{[-n+l,n+l]}$, for $0\leq l\leq k-1$, can be embedded into $B_{[-n,n+k-1]}$ which has dimension $(2n+k)J+1$ that increase linearly with k. Thus, even if we could find a normal invariant state, the proof of Proposition 3.4 would give zero CNT entropy, for such an increase would not be enough to match the asymptotic average $\lim_n \frac{1}{n}$ in (24).

Let us now consider the *CAR algebra* $\mathcal{A}$ over $\mathbb{H}$ with the quasi–free evolution $\sigma\left(\hat{a}^\dagger(f)\right) = \hat{a}^\dagger\left(\hat{U}f\right)$ as in (34), (37) and the unitary $\hat{U}$ considered above. The situation radically changes. Because of (47), the creation and annihilation operators $\hat{a}^\natural_{k,j} := \hat{a}^\natural(e_{k,j})$ associated with the basis vectors $|e_{k,j}\rangle$ fulfil $\hat{a}^\dagger_{k_1,j_1}\hat{a}_{k_2,j_2} + \hat{a}_{k_2,j_2}\hat{a}^\dagger_{k_1,j_1} = \delta_{k_1,k_2}\delta_{j_1,j_2}$. Therefore, by introducing (see [12, Par. 5.2.2])

$$\begin{aligned} \hat{e}^{0,j}_{11} &:= \hat{a}_{0,j}\hat{a}^\dagger_{0,j}\,, \qquad \hat{e}^{0,j}_{12} := \hat{a}_{0,j}\hat{V}^0_{j-1} \\ \hat{e}^{0,j}_{21} &:= \hat{V}^0_{j-1}\hat{a}^\dagger_{0,j}\,, \quad \hat{e}^{0,j}_{22} := \hat{a}^\dagger_{0,j}\hat{a}_{0,j} \quad , \end{aligned} \tag{50}$$

where

$$\hat{V}_j^0 := \prod_{i=1}^{j} \left(\hat{1\!\!1} - \hat{a}_{0,i}^\dagger \hat{a}_{0,i} \right) \quad \text{and} \quad \hat{V}_0^0 := \hat{1\!\!1} \quad ,$$

we have a complete set of 2×2 matrix units, one for each $1 \leq j \leq J$ with which to establish an isomorphism between the subalgebra $\mathbf{A}_0 \subseteq \mathcal{A}$ generated by the $\hat{a}_{0,j}^\natural$, $1 \leq j \leq J$ and $\hat{1\!\!1} - \sum_{1 \leq j \leq J} \hat{a}_{0,j}^\dagger \hat{a}_{0,j}$, and the full $2^J \times 2^J$ matrix algebra $\mathbf{M}_{2^J}(\mathbb{C})$.

The same argument holds for the subalgebras $\sigma^l(\mathbf{A}_0)$, $1 \leq l \leq k-1$, generated by $\sigma^l\left(\hat{a}_{0,j}^\natural\right) = \hat{a}_{l,j}^\natural$. Let us denote by $\mathbf{M}_l$, $l = 0, \ldots, k-1$ the corresponding images under the isomorphism. Because of (47), the matrix algebras $\mathbf{M}_l$ pairwise commute. Therefore, $\bigvee_{0 \leq l \leq k-1} \sigma^l(\mathbf{A}_0)$ is isomorphic to the full matrix algebra $\mathbf{M}_{2^{kJ}}(\mathbb{C})$ whose dimension increases now exponentially with k, unlike the linear increase on the one–particle level. Therefore, the possibility remains that the asymptotic average might be matched and that there can be states such that the CNT entropy of the quasi-free automorphism σ is not zero. For instance, let us take the tracial state τ on $\mathcal{A}$. Thus we can apply the result (40) which gives $h_\tau(\sigma) = J \log 2$, the multiplicity of the spectrum being constant and equal to J by assumption.

4 Non–commutative Topological Entropy

What emerges from the previous sections is that states of ordinary quantum mechanical systems either are too regular to keep track of irregular dynamics or they are too irregular and good approximation theorems cannot be used. Therefore, one might hope to get hold of quantum randomness by avoiding reference to invariant states and by considering the C*–algebraic properties of the evolution only.

In classical ergodic theory this corresponds to passing from the measure-theoretic point of view to the topological one, the latter being based on the analysis of classical dynamical systems on topological spaces $\mathcal{X}$ (that we shall assume to be compact and Hausdorff resp. even metrizable) equipped with continuous (usually even invertible continuous) maps $S : \mathcal{X} \to \mathcal{X}$ representing the evolution. Such couples may be viewed in algebraic terms by considering the algebra $C(\mathcal{X})$ of continuous functions $x \mapsto f(x)$ over $\mathcal{X}$ evolving under the automorphism $\sigma : C(\mathcal{X}) \to C(\mathcal{X})$, $(\sigma f)(x) = f(S^{-1}x)$. $C(\mathcal{X})$ is a C*–algebra with respect to the sup–norm.

Central in the classical theory of the topological entropy (cf. [50]) is the notion of *open cover* of $\mathcal{X}$ by a set $\mathcal{U}$ of open subsets U_i, $i \in I_{\mathcal{U}}$. Since by our compactness assumption we can always reduce to finite open subcovers, we will consider the class $\mathcal{O}(\mathcal{X})$ of $\mathcal{U}$ with $\mathrm{card}\, I_{\mathcal{U}} < \infty$.

Obviously, $\mathcal{U} \in \mathcal{O}(\mathcal{X})$ may contain many more open subsets U_i than needed to cover $\mathcal{X}$. Let then denote

$$N(\mathcal{U}) := \min\{\mathrm{card}\,\mathcal{U}' \mid \mathcal{U}' \subset \mathcal{U}\,, \mathcal{U}' \in \mathcal{O}(\mathcal{X})\} \quad \text{and} \tag{51}$$

$$H(\mathcal{U}) := \log N(\mathcal{U}) \quad . \tag{52}$$

The latter will define the entropy of $\mathcal{U} \in \mathcal{O}(\mathcal{X})$.

Supposing that S is a homeomorphism, the image $S(\mathcal{U}) := \{S(U_i)\}_{i\in I}$ of a finite open cover is still in $\mathcal{O}(\mathcal{X})$ and we can define the joining of $\mathcal{U}$ and $S(\mathcal{U})$ as the finite open cover $\mathcal{U} \vee S(\mathcal{U})$ whose elements are all the intersections $U_i \cap S(U_j)$. Clearly,

$$N(S(\mathcal{U})) = N(\mathcal{U}) \quad \text{since } S \text{ is assumed invertible}\,, \tag{53}$$

$$N(\mathcal{U} \vee S(\mathcal{U})) \le N(\mathcal{U})^2 \Rightarrow H(\mathcal{U} \vee S(\mathcal{U})) \le 2H(\mathcal{U}) \quad \text{and} \tag{54}$$

$$h(S\,, \mathcal{U}) := \lim_{n\to\infty} \frac{1}{n} H\left(\bigvee_{j=0}^{n-1} S^j(\mathcal{U})\right) \quad \text{exists.} \tag{55}$$

In analogy with the Kolmogorov–Sinai entropy, the maximal state–independent average information coming from the open covers of $\mathcal{X}$, namely

$$h(S) := \sup_{\mathcal{U}\in\mathcal{O}(\mathcal{X})} h(S\,, \mathcal{U}) \quad , \tag{56}$$

is defined as the *topological entropy* of $(\mathcal{X}, S)$, cf. [50].

Let $\mathcal{V}\,, \mathcal{U} \in \mathcal{O}(\mathcal{X})$. If for all $V \in \mathcal{V}$ there is $U \in \mathcal{U}$ with $V \subset U$, we will say that $\mathcal{V}$ is a refinement of $\mathcal{U}$. Then, $H(\mathcal{U}) \le H(\mathcal{V})$.

Moreover, if a sequence of $\mathcal{U}_n \in \mathcal{O}(\mathcal{X})$ is refining and 'cofinal', in the sense that: each open cover is a refinement of the previous one, and that for all $\mathcal{V} \in \mathcal{O}(\mathcal{X})$ there is $n \in \mathbb{N}$ such that $\mathcal{U}_n$ is a refinement of $\mathcal{V}$, then we have a *Kolmogorov–Sinai type theorem* which states that

$$h(S) = \lim_{n\to\infty} h(S\,, \mathcal{U}_n) \quad . \tag{57}$$

The topological entropy of $(\mathcal{X}, S)$ is related by a so–called *variational principle* to the Kolmogorov–Sinai entropy $h_\mu(S)$ of $(\mathcal{X}, S, \mu)$ where μ is any S–invariant

Borel measure on $\mathcal{X}$. Let $M(\mathcal{X}, S)$ denote the convex, compact set of such measures. Then:

$$h(S) = \sup_{\mu \in M(\mathcal{X},S)} h_\mu(S) \quad . \tag{58}$$

We will now concentrate on *quantum dynamical systems* $(\mathcal{A}, \sigma)$ without referring to any invariant state, thus to the intrinsic properties of the dynamics, and as before we will deal with unital C*–algebras $\mathcal{A}$ and with their automorphisms $\sigma : \mathcal{A} \to \mathcal{A}$. Following [23, 24], in the non–commutative case $(\mathcal{A}, \sigma)$ we start by replacing open covers $\mathcal{U} \in \mathcal{O}(\mathcal{X})$, introducing the so–called (positive) operator covers.

Definitions 4.1

1. *An* **operator cover** *for $\mathcal{A}$ is any finite subset $\alpha = \left\{\hat{A}_i\right\}_{i\in I}$ of $\mathcal{A}$ such that the sum $\sum_{i\in I} \hat{A}_i^* \hat{A}_i$ is an invertible operator, namely strictly > 0. If this is the case, we will write $\alpha \in \mathcal{O}(\mathcal{A})$.*

2. *A* **positive operator cover** *for $\mathcal{A}$ is any finite set of operators $0 \leq \hat{A}_i \leq \hat{1\!\!1}$ such that $\sum_{i\in I} \hat{A}_i > 0$. We will denote their class by $\mathcal{O}^+(\mathcal{A})$.*

3. *Let $\alpha, \beta \in \mathcal{O}(\mathcal{A})$. The* **ordered join** *of α, β is the operator cover*

$$\alpha \vec{\vee} \beta := \left\{\hat{B}_i \cdot \hat{A}_j \mid \hat{B}_i \in \beta\, , \, \hat{A}_j \in \alpha\right\} \quad . \tag{59}$$

4. *We will denote by $\overline{N}(\alpha)$ the minimum number of elements of $\alpha \in \mathcal{O}(\mathcal{A})$ such that they still constitute an operator cover:*

$$\overline{N}(\alpha) := \min\left\{\mathrm{card}\,\alpha' \mid \alpha' \subseteq \alpha\, , \, \alpha' \in \mathcal{O}(\mathcal{A})\right\} \quad . \tag{60}$$

Notice:

1. The non–commutative join generalizes the classical join of two open covers by specifying which operator cover has its elements coming first (this is superfluous in the commutative case). If $\sum_i \hat{A}_i^* \hat{A}_i > 0$, $\sum_j \hat{B}_j^* \hat{B}_j > 0$, both $\sum_{i,j} \hat{B}_j^* \hat{A}_i^* \hat{A}_i \hat{B}_j$ and $\sum_{i,j} \hat{A}_i^* \hat{B}_j^* \hat{B}_j \hat{A}_i$ are invertible.

   While $\alpha \vec{\vee} \beta \in \mathcal{O}(\mathcal{A})$ if $\alpha, \beta \in \mathcal{O}(\mathcal{A})$, the ordered join of $\alpha, \beta \in \mathcal{O}^+(\mathcal{A}) \subset \mathcal{O}(\mathcal{A})$ need not be in $\mathcal{O}^+(\mathcal{A})$.

2. $\overline{N}(\alpha) \leq \overline{N}\left(\alpha \vec{\vee} \beta\right)$, but $\overline{N}(\beta)$ might be bigger.

3. $\overline{N}\left(\alpha \vec{\vee} \alpha \vec{\vee} \cdots \vec{\vee} \alpha\right) = \overline{N}(\alpha)$ for all $\alpha \in \mathcal{O}^{+}(\mathcal{A})$, but this is not necessarily true for operator covers $\alpha \in \mathcal{O}(\mathcal{A}) \setminus \mathcal{O}^{+}(\mathcal{A})$.

4. However, like in the commutative situation the following inequality holds:
$$\overline{N}\left(\alpha \vec{\vee} \beta\right) \leq \overline{N}(\alpha) \cdot \overline{N}(\beta) \quad . \tag{61}$$

5. Furthermore, denoting by $\sigma(\alpha)$, for an automorphism σ of $\mathcal{A}$, the (positive) operator cover with elements $\sigma(\hat{A}_i)$, $\hat{A}_i \in \alpha$, then
$$\overline{N}(\sigma(\alpha)) = \overline{N}(\alpha) \quad . \tag{62}$$

6. If $\mathbf{B}$ is a *finite*–dimensional C*–algebra isomorphic to $\bigoplus_{k=1}^{n} \mathbf{M}_{d_k}(\mathbb{C})$ and $d = \sum_{k=1}^{n} d_k$, then $\overline{N}(\alpha) \leq d$ for all $\alpha \in \mathcal{O}(\mathbf{B})$. Given any partition of the identity into orthogonal one–dimensional projections of the matrix algebra, the isomorphic image in $\mathbf{B}$ is a positive cover $\alpha^* \in \mathcal{O}(\mathbf{B})$ for which
$$\max\left\{\overline{N}(\alpha) \mid \alpha \in \mathcal{O}(\mathbf{B})\right\} = \overline{N}(\alpha^*) = d \quad . \tag{63}$$

Since C*–algebras need not contain proper finite–dimensional subalgebras, like $C(\mathcal{X})$, and we want them, together with their (positive) operator covers, to replace the classical open covers, we will do, in general, by relying upon *positive* (i.e., positivity–preserving) *unital maps* $\gamma : \mathbf{B} \mapsto \mathcal{A}$, $\gamma(\hat{1}_{\mathbf{B}}) = \hat{1}$, $\hat{1}_{\mathbf{B}} \in \mathbf{B}$ a finite–dimensional C*–algebra.

We will also need to identify as *equivalently covering* ($\gamma_1 \simeq \gamma_2$) two positive unital maps $\gamma_k : \mathbf{B}_k \to \mathcal{A}$, $k = 1, 2$, such that $\gamma_1 = \gamma_2 \circ \theta_{12}$, where $\theta_{12} : \mathbf{B}_1 \to \mathbf{B}_2$ is any *–isomorphism. Notice that positive unital maps $\gamma : \mathbf{B} \to \mathcal{A}$ map $\beta \in \mathcal{O}^{+}(\mathbf{B})$ into $\gamma(\beta) \in \mathcal{O}^{+}(\mathcal{A})$.

Definition 4.2 *Given positive unital maps $\gamma_k : \mathbf{B}_k \to \mathcal{A}$ from finite–dimensional C* algebras $\mathbf{B}_k$ into $\mathcal{A}$, $k = 1, \ldots, n$, their* **entropy** *is defined by*
$$\overline{H}(\gamma_1, \ldots, \gamma_n) := \max_{\alpha_j \in \mathcal{O}^{+}(\mathbf{B}_j),\, j=1,\ldots,n} \left\{\log \overline{N}\left(\gamma_1(\alpha_1) \vec{\vee} \cdots \vec{\vee} \gamma_n(\alpha_n)\right)\right\}, \tag{64}$$
with the restriction that, if $\gamma_k \simeq \gamma_l$ for $k < l$, then the trivial cover $\alpha_l = \left\{\hat{1} \in \mathbf{B}_l\right\}$ is to be used for the later map with index $l > k$.

Some comments and properties:

1. The restriction on the evaluation of the maximum in (64) is necessary in view of the third observation after (60). In fact, we want the entropy not to be sensitive of repeated unital maps in different places.

2. For a single $\gamma : \mathbf{B} \to \mathcal{A}$, from (63) it follows that $\overline{H}\,(\gamma) \leq \log D(\mathbf{B})$, where $D(\mathbf{B})$ is what is d in (63). If $\mathbf{B}$ is a finite–dimensional subalgebra of $\mathcal{A}$, we will denote by $\overline{H}\,(\mathbf{B}) := \log D(\mathbf{B})$ the entropy of the inclusion map (which is hence independent of the inclusion into $\mathbf{A}$).

3. For positive unital maps $\theta_k : \mathbf{B}_k \to \mathbf{A}_k$ and $\gamma_k : \mathbf{A}_k \to \mathcal{A}$, $k = 1, \ldots, n$ on finite dimensional algebras $\mathbf{A}_k, \mathbf{B}_k$, such that if $\gamma_i \simeq \gamma_i$ also $\gamma_i \circ \theta_i \simeq \gamma_j \circ \theta_j$, we have:

$$\overline{H}\,(\gamma_1 \circ \theta_1, \ldots, \gamma_n \circ \theta_n) \leq \overline{H}\,(\gamma_1, \ldots, \gamma_n) \quad . \tag{65}$$

4. If $\sigma : \mathcal{A} \mapsto \mathcal{A}$ is an automorphism, then from (62) we deduce

$$\overline{H}\,(\sigma \circ \gamma_1, \ldots, \sigma \circ \gamma_n) = \overline{H}\,(\gamma_1, \ldots, \gamma_n) \quad . \tag{66}$$

5. It follows from the definition and (61) :

$$\begin{aligned} \overline{H}\,(\gamma_{i_1}, \ldots, \gamma_{i_l}) \leq \overline{H}\,(\gamma_1, \ldots \gamma_n) \quad \leq \quad & \overline{H}\,(\gamma_1, \ldots, \gamma_k) \\ & + \overline{H}\,(\gamma_{k+1}, \ldots, \gamma_n) \quad , \end{aligned} \tag{67}$$

where $1 \leq i_1 \leq \ldots \leq i_l \leq n$, $l < n$ and none of the maps equivalently covering.

6. Additivity rather than mere subadditivity for all the single arguments $\gamma_1, \ldots, \gamma_n$ in property 5 above should follow from some algebraic independence of these n arguments. For such a result, we need some preliminary definitions for the general case of positive unital maps into $\mathcal{A}$:

Definitions 4.3

1. *A positive unital map $\gamma : \mathbf{B} \to \mathcal{A}$ from a finite-dimensional algebra into $\mathcal{A}$ is called* **faithfully covering***, if there exists $\alpha' \in \mathcal{O}^+(\mathbf{B})$ such that $\overline{H}\,(\gamma) = \log \overline{N}\,(\gamma(\alpha')) = \log card\, \alpha'$.*

2. *Given n positive unital maps $\gamma_k : \mathcal{B}_k \to \mathcal{A}$, $k = 1, \ldots, n$, they are called* **independently covering**, *if for all sets of $0 \leq B_k \in \mathbf{B}_k$, $k = 1, \ldots, n$, such that $\gamma_k(B_k)$ are not invertible, there exists a single state ω on $\mathcal{A}$ such that $\omega \circ \gamma_k(B_k) = 0$, $k = 1, \ldots, n$.*

3. *Two positive unital maps $\gamma_k : \mathbf{B}_k \to \mathcal{A}$, $k = 1, 2$, are called* **commuting** *if $\gamma_1(B_1)\gamma_2(B_2) = \gamma_2(B_2)\gamma_1(B_1)$ for all $B_k \in \mathbf{B}_k$, $k = 1, 2$.*

The above definitions generalize the case when one is dealing with pairwise commuting, algebraically independent, finite–dimensional subalgebras $\mathbf{B}_k \subseteq \mathcal{A}$ whose natural inclusion $*$–homomorphisms are thus commuting, faithfully and independently covering [23].

Further, if the positive unital maps $\gamma_k : \mathbf{B}_k \to \mathcal{A}$, $k = 1, \ldots, n$, are pairwise commuting, each one faithfully and all together independently covering, then [23]

$$\overline{H}\left(\gamma_1, \ldots, \gamma_n\right) = \sum_{k=1}^{n} \overline{H}\left(\gamma_k\right) \quad . \tag{68}$$

Using properties 5. and 4., we define as for the Kolmogorov–Sinai entropy in the classical case and for the CNT–entropy in the non–commutative one (Sect. 3.2 above):

Definition 4.4 *For a positive unital map $\gamma : \mathbf{B} \to \mathcal{A}$ from a finite–dimensional C^*–algebra $\mathbf{B}$ and for an automorphism $\sigma : \mathcal{A} \to \mathcal{A}$, the* **entropy of σ with respect to γ** *is defined by:*

$$\hbar\left(\sigma\,,\,\gamma\right) := \lim_{n\to\infty} \frac{1}{n} \overline{H}\left(\gamma, \sigma\circ\gamma, \ldots, \sigma^{n-1}\circ\gamma\right) \quad . \tag{69}$$

Among the other properties of $\hbar\left(\sigma\,,\,\gamma\right)$ we quote [23, 24]:

$$\hbar\left(\sigma\,,\,\gamma\right) \;\leq\; \overline{H}\left(\gamma\right) \tag{70}$$

$$\hbar\left(\theta\circ\sigma\circ\theta^{-1}\,,\,\theta\circ\gamma\right) \;=\; \hbar\left(\sigma\,,\,\gamma\right), \quad \theta : \mathcal{A} \to \theta(\mathcal{A}) \text{ a } *\text{-isomorphism.} \tag{71}$$

In analogy with the measure–theoretic Kolmogorov–Sinai entropy, with the classical topological entropy and with the CNT–entropy, a straightforward definition of *non–commutative topological entropy* would be:

$$\hbar\left(\sigma\right) := \sup_{\gamma} \hbar\left(\sigma\,,\,\gamma\right) \quad , \tag{72}$$

where $\gamma : \mathbf{A} \to \mathcal{A}$ is any linear, positive, unital map from a finite–dimensional C*–algebra $\mathbf{A}$ into $\mathcal{A}$.

However, a major difference between the above definition and that of the CNT–entropy lies in that (72) is not supported by a Kolmogorov–Sinai like theorem as (27), or (57) for the classical topological entropy.

Indeed, there is no control over the continuity of the entropy functionals (64) with respect to the appropriate (norm–) topology on the space of γ: there are instances of γ_1, γ_2 from $\mathbf{B}$ into $\mathcal{A}$, arbitrarily close to each other, with different entropy functionals [23, 24].

A more workable definition which explicitly depends on the existence of a finite approximation of the C*–algebra $\mathcal{A}$ by means of an increasing sequence of finite–dimensional C*–algebras included or positively mapped into it, is contained in the following:

Definitions 4.5

1. *Suppose that a sequence* $\mathbf{B}_n$ *of finite–dimensional C*–algebras is given together with positive unital maps* $\tau_n : \mathbf{B}_n \to \mathcal{A}$*. The sequence* $\tau := \{\tau_n\}_{n\in\mathbb{N}}$ *will be called 'cover increasing' if* $\tau_n\left(\mathcal{O}^+(\mathbf{B}_n)\right) \subseteq \tau_{n+1}\left(\mathcal{O}^+(\mathbf{B}_{n+1})\right)$.

2. *In this case, the* τ–**topological entropy of an automorphism** $\sigma : \mathcal{A} \to \mathcal{A}$ *is defined by [23]:*

$$\hbar_\tau(\sigma) = \lim_{n\to\infty} \hbar(\sigma\,,\,\tau_n) \quad , \tag{73}$$

where the increasing limit exists due to assumption 1., see the definitions 4.2 and following ones.

This is typically the case when $\mathcal{A}$ is the C*–inductive limit of an increasing sequence of finite–dimensional subalgebras $\mathbf{A}_n$, $\mathcal{A} = \overline{\bigcup_n \mathbf{A}_n}$, in which case we choose as τ_n the corresponding inclusions. – More in general, the structure of $\mathcal{A}$ might be that of a *nuclear C*–algebra*, that is there exists an increasing sequence $\{\mathbf{A}_n\}_{n\in\mathbb{N}}$ of finite–dimensional C*–algebras and completely positive maps $\sigma_n : \mathcal{A} \mapsto \mathbf{A}_n$, $\tau_n : \mathbf{A}_n \mapsto \mathcal{A}$ such that $\|\tau_n \circ \sigma_n(\hat{X}) - \hat{X}\| \to 0$ for all $\hat{X} \in \mathcal{A}$ when $n \to \infty$. This is not sufficient, however, to ensure that $\hbar(\sigma) = \lim_n \hbar(\sigma\,,\,\tau_n)$; see [23] for an alternative definition instead of 4.4 for this case.

The above theory does not distinguish between Abelian and nonabelian algebras. Therefore we might ask whether, when $\mathcal{A}$ is the Abelian C*–algebra $C(\mathcal{X})$ of continuous functions over a compact *metric* space $\mathcal{X}$, (72) resp. (73) coincides with (56). At least one inequality between (72) and (56) is indeed easy to show:

Namely let $\mathcal{U} = \{U_i\}_{i\in I} \in \mathcal{O}(\mathcal{X})$ be given. Correspondingly, we have a partition of the identity by positive functions $f_i \in \mathcal{A} = C(\mathcal{X})\,,\ i \in I$ supported by the open sets $U_i \in \mathcal{U}$. Clearly, $\alpha_{\mathcal{U}} = \{f_i\}_{i\in I} \in \mathcal{O}(\mathcal{A})$ and $N(\mathcal{U}) = \overline{N}(\alpha_{\mathcal{U}})$. Given the automorphism $\sigma : \mathcal{A} \to \mathcal{A}$, defined by $\sigma f(x) = f(S^{-1}x)$, according to (51), Definitions 4.1 and owing to commutativity of the operator algebra $\mathcal{A}$, it is also true that $N\left(\bigvee_{j=0}^{n} S^j(\mathcal{U})\right) = \overline{N}\left(\overrightarrow{\bigvee}_{j=0}^{n}\sigma^j(\alpha_U)\right)$. Therefore, $h(S\,,\mathcal{U}) = \hbar(\sigma\,,\alpha_{\mathcal{U}})$. Comparing definitions (56) and (72), we thus deduce $h(S) \leq \hbar(\sigma)$. See [23], in particular Remark (2.12),(5) resp. Lemma (2.10) there, for the more complicated converse inequality.

Remark 4.6 *In the above example one could start off with an abstract Abelian algebra $\mathcal{A}$ and represent it via the Gelfand transform as an algebra of continuous functions over the space of its characters (see [11, Par. 2.3.5]) which plays the role of $\mathcal{X}$. However, the fact that $\mathcal{A}$ is assumed to contain an identity forces $\mathcal{X}$ to be compact as a topological space. Indeed, the quantum topological entropy defined by (72) mimicks the construction of the classical topological entropy (56) that is based on compact topological spaces.*

However, if $\mathcal{X}$ is endowed with a metric, then a metric dependent definition of topological entropy was given by Bowen (see Def. 5.3 and [50]). On compact metrizable spaces, equivalent metrics give the same Bowen's entropy which in turn equals the expression (56).

For a noncompact metrizable space $\mathcal{X}$ it is Bowen's construction that must be used and to different, not uniformly equivalent, metrics there can correspond different topological entropies. One then wonders whether an algebraic version of Bowen's entropy can be envisaged, to be possibly extended to non-unital C–algebras.*

We come now to some concrete *examples* that aim at comparing the use of the quantum topological entropy introduced here versus the CNT quantum dynamical entropy.

From (63) and inequality (70) it trivially follows that the topological entropy of whatever evolution over *finite dimensional C^*–algebras* vanishes exactly as does the CNT entropy.

Let now $\mathbb{H}$ be an *infinite dimensional* Hilbert space and let $U : \mathbb{H} \to \mathbb{H}$ be the unitary evolution considered in section 3.5.2. We have seen that, despite the presence of homogeneous Lebesgue spectrum (of multiplicity J), the CNT entropy of the corresponding automorphism vanishes with respect to normal states and is out of control for more general states because of lack of continuity.

With the topological entropy the situation is more or less equivalent in the following sense. By using the finite rank subalgebras $B_{[-n,n]}$ in (49) as a sequence τ generating the C*–algebra $\tilde{B}(\mathbb{H}) :== C^*(B_\infty(\mathbb{H}) \oplus \mathbb{C}\cdot\hat{1\!\!1})$ of compact operators plus the identity, we get $\hbar_\tau(\sigma) = 0$ (see (73)) for the automorphism σ on $B(\mathbb{H})$ defined by U. In fact, $\sigma^l(B_{[-n,n]})$, $l = 0, \ldots, k-1$, are all included in $B_{[-n,n+k-1]}$. Therefore, considering the inclusions $\gamma_n^l : \sigma^l(B_{[-n,n]}) \to B_{[-n,n+l-1]}$ and $\gamma_n : B_{[-n,n+l-1]} \to \tilde{B}(\mathbb{H})$, from (65) and (63) we get

$$\overline{H}\left(\gamma_n \circ \gamma_n^1, \ldots, \gamma_n \circ \gamma_n^k\right) \leq \overline{H}\left(\gamma_n\right) = \log(J(2n+k)) \quad . \tag{74}$$

Thus, $\hbar(\sigma\,,\,\tau_n) = 0$ for all inclusions $\tau_n : B_{[-n,n]} \to \tilde{B}(\mathbb{H})$. However, we do not know whether the result extends to the whole of $B(\mathbb{H})$ which is the strong-operator closure of the sequence τ.

Again, as in the case of the CNT entropy we can pass to the infinitely many degrees of freedom by *second quantization*. We shall work not with the CAR algebra $\mathcal{A}$ itself, but with an isomorphic dynamical system and use (71). In fact, the isomorphism constructed in Sect. 3.5.2 by means of the system of matrix unit extends to an isomorphism between the CAR algebra $\mathcal{A}$ and the C*–closure $\mathcal{C} = \bigotimes_{-\infty}^{+\infty}\mathbf{M}_l$ of the increasing sequence τ of finite tensor products $\bigotimes_{l=-k}^{k}\mathbf{M}_l$, that is the spin-chain algebra with a $J \times J$ matrix algebra at each site. Clearly, the automorphism σ on $\mathcal{A}$ becomes isomorphic to the bilateral shift $\tilde{\sigma} : \mathbf{M}_l \mapsto \mathbf{M}_{l+1}$ as automorphism on $\mathcal{C}$. Now it is easy to show, applying (65), that [23]

$$\hbar_\tau\left(\tilde{\sigma}\right) = \hbar\left(\tilde{\sigma}, \mathbf{M}_0\right) = \overline{H}\left(\mathbf{M}_0\right) = J\log 2 \quad , \tag{75}$$

where by $\hbar\left(\tilde{\sigma}, \mathbf{M}_0\right)$ we denote the entropy defined in Def. 4.4 for the inclusion map of $\mathbf{M}_0$ into $\mathcal{C}$..
Notice:

It is very doubtful if the equality between this result and that obtained at the end of Sect. 3.5.2 reflects the presence of a general quantum variational principle linking the quantum topological entropy constructed in this section and the CNT entropy (which would then generalize the classical relation 58); but here this is revealing the peculiar properties of the tracial state from an entropic point of view, too.

Despite the previous result, it is not necessary to go to infinitely many degrees of freedom in order to get nontrivial results. Indeed, unlike the CNT–entropy, the cases dealt with in subsections 3.3 and 3.5.1 show that the non–commutative topological entropy is capable of keeping track of 'erratic' behaviour in these cases.

Given the Koopman suspension of a classical dynamical system with strictly positive topological entropy, the next, simple Lemma follows:

Lemma 4.7 *Let $(\mathcal{X}, S, \mu)$ be a classical dynamical system (with $\mathcal{X}$ compact, metric and μ an invariant Borel probability measure) with a positive topological entropy, $h\,(S) > 0$. Let $(\mathcal{M}_{cl} = L^\infty(\mathcal{X}, \mu), \sigma_{cl}, \omega_{cl})$ be the algebraic classical dynamical system emerging from the Koopman approach as in Sect. 3.3, and $(B(\mathbb{H}_\mu), \sigma, \omega_\mu)$ be the non–commutative 'Hilbert space' dynamical system naturally arising from the previous one. Then, the the full, non–commutative topological entropy of the latter, defined as in (72), is also positive, $\hbar\,(\sigma) > 0$.*

Proof. By assumption, there exists an open cover $\mathcal{U} = \{U_i\} \in \mathcal{O}\,(\mathcal{X})$ such that $h\,(S\,,\mathcal{U}) > 0$. The characteristic functions $\hat{X}_i := \chi_{U_i}$, as multiplication operators, belong to the von Neumann subalgebra $\mathcal{M}_{cl} = L^\infty_\mu(\mathcal{X}) \subset B(\mathbb{H}_\mu)$ and constitute a positive operator cover $\alpha_U \in \mathcal{O}\,(\mathcal{M}_{cl})$, $\sum_i \hat{X}_i = \hat{1\!\!1}$. As $\sigma(\hat{X}_i) = \chi_{S(U_i)}$, we can repeat the argument used above for the Abelian case $\mathcal{A} = C(\mathcal{X})$ after 4.5, to show that $\hbar\,(\sigma) \geq h\,(S,\mathcal{U})$. □

As to the more physical model (44), let a proper *advecting velocity field* $\mathbf{u}$ on $\mathbb{R}^3$ be chosen that develops at least one (bounded) chaotic region $\mathcal{X} \subset \mathbb{R}^3\,, \mathbb{R}^3\,(\ni \mathbf{x})$ mapped into itself by the dynamics $\dot{S}_t(\mathbf{x}) = \mathbf{u}(S_t(\mathbf{x}))$. Given the C*–algebra $B\,(\mathbb{H})$ and the evolution

$$\sigma(\hat{X}) = \mathrm{e}^{i\,\hat{H}}\hat{X}\mathrm{e}^{-i\,\hat{H}}\,, \quad \hat{H} = \mathbf{u}(\mathbf{x})\cdot\hat{\mathbf{p}} + \beta E_0 + \alpha\kappa \quad , \tag{76}$$

the multiplication operators by functions supported within this region provide the necessary tool to get $\hbar\,(\sigma) > 0$.

In fact, due to our assumptions we can concentrate on the invariant chaotic region only, where an open cover $\mathcal{U}(\mathcal{X}) = \{U_i\}$ can be found such that the classical $h\left(S_1\restriction_{\mathcal{X}}\right) > 0$. It is clear that, for the set of multiplication operators $\hat{X}_i := \chi_{U_i}$ by the corresponding characteristic functions, we can repeat the argument of Lemma 4.7.

5 Motion in a Crystal

In this section we illustrate the various relations between classical and quantum chaos by the example of an electron in a n–dimensional crystal. The dynamical properties of this electron will be compared with the ones of a free particle.

In the one-electron approximation of solid state physics the effect of the nuclei and the other electrons is taken into account in the form of a potential V.

We assume the potential to be $\mathcal{L}$-periodic with a *lattice*

$$\mathcal{L} := \left\{ \sum_{j=1}^{n} z_j \ell_j \mid z_1, \ldots, z_n \in \mathbb{Z} \right\}$$

spanned by a basis $\ell_1, \ldots, \ell_n \in \mathbb{R}^n_q$ of configuration space $\mathbb{R}^n_q$.

The *fundamental domain*

$$\mathcal{D} := \left\{ \sum_{j=1}^{n} x_j \ell_j \mid 0 \le x_1, \ldots, x_n < 1 \right\}$$

is then naturally isomorphic as a set to the n–dim. configuration space torus $\mathbb{T} := \mathbb{R}^n_q / \mathcal{L}$, and V can be considered to be a function $V : \mathbb{T} \to \mathbb{R}$.

In the quantum mechanical context the dynamics exists for more singular potentials than in the classical case.

However, we will discuss one example in both cases, namely the one of motion in a planar crystal with attracting Coulombic forces. There in the fundamental domain $m \ge 1$ nuclei are situated at the positions $s_1, \ldots, s_m \in \mathcal{D}$ which attract the electron with the *charges* $Z_1, \ldots, Z_m > 0$. That is, we assume the potential of the form $V(q) \sim -Z_i/|q - s_i|$ for q near s_i. Now by the periodicity of the crystal the potential is singular at the points of

$$\mathcal{S} := \{ q \in \mathbb{R}^2 \mid q = s_i + \ell, \ell \in \mathcal{L} \}$$

and thus only defined in the punctured configuration plane $\tilde{M} := \mathbb{R}^2 \setminus \mathcal{S}$. Sometimes we identify the plane $\mathbb{R}^2$ with $\mathbb{C}$.

We assume that V has the following form

Definition 5.1 *A potential $V \in C^\infty(\tilde{M}, \mathbb{R})$ which is $\mathcal{L}$-periodic*

$$V(q+\ell) = V(q), \quad (q \in \tilde{M},\, \ell \in \mathcal{L})$$

is called **Coulombic** *if for $\varepsilon > 0$ small the functions $f_1, \ldots, f_m$,*

$$f_i(Q) := \begin{cases} V(s_i + Q^2) \cdot Q\bar{Q} & , 0 < |Q| < \varepsilon \\ -Z_i & , Q = 0 \end{cases}$$

are C^∞ (where $Q \in \mathbb{C}$ is a so-called regularizing complex coordinate, related to the complex coordinate q in the plane by the Levi-Civita transformation $Q^2 = q - s_i$).

Obviously we have a finite $V_{\max} := \sup_{q \in \tilde{M}} V(q)$. We assume without loss of generality that $V_{\max} \le 0$.

Example (Periodic Yukawa potentials).
We choose 'masses' $\mu_1, \ldots, \mu_m > 0$ and set

$$V(q) := \sum_{\ell \in \mathcal{L}} \sum_{i=1}^{m} -Z_i \frac{\exp(-\mu_i \cdot |q - s_i - \ell|)}{|q - s_i - \ell|}, \qquad (q \in \tilde{M}).$$

Due to the positivity of the μ_i this sum is absolutely converging together with its derivatives and thus leads to a smooth, $\mathcal{L}$-periodic V. The f_i have the form

$$f_i(Q) = -Z_i \cdot \exp(-\mu_i \cdot Q\bar{Q}) + g_i(Q) \cdot Q\bar{Q}$$

with g_i smooth and are thus smooth, too.

The reason for the somewhat odd-looking definition is that we want to regularize the Coulomb singularities by using the so-called Levi-Civita transformation.

5.1 The Classical Motion (One Particle)

Now we consider the topological and metric entropy of a classical particle of energy E in the periodic potential V.

If $V : \mathbb{R}^n \to \mathbb{R}$ is *smooth* (C^2 being sufficient), then the Hamiltonian flow $\Phi^t : P \to P$ on the phase space $P := T^*\mathbb{R}^n \cong \mathbb{R}^n_p \times \mathbb{R}^n_q$ generated by the Hamiltonian function $H : P \to \mathbb{R}$, $H(p,q) := \frac{1}{2}p^2 + V(q)$ exists for all times t. Moreover for $E > V_{\max}$ the *energy shell*

$$\Sigma_E := \{x \in P \mid H(x) = E\}$$

is a smooth $2n-1$-dimensional submanifold, and we denote the restricted flow $\Phi^t\restriction_{\Sigma_E}$ by Φ^t_E.

In the case of a *Coulombic* potential the classical motion is generated by the Hamiltonian function

$$\tilde{H}(p,q) := \tfrac{1}{2}p^2 + V(q), \quad ((p,q) \in T^*\tilde{M}).$$

Due to collisions with the singularities in $\mathcal{S}$ the Hamiltonian flow on the cotangent bundle $T^*\tilde{M}$ of the punctured plane $\tilde{M}$ does not exist for all times.

However, as described in Lemma 5.2 below, the flow can be smoothly regularized.

Lemma 5.2 *There exists a unique smooth extension (P,ω,H) of the Hamiltonian system $(T^*\tilde{M}, dq_1 \wedge dp_1 + dq_2 \wedge dp_2, \tilde{H})$, where the phase space P is a smooth four-dimensional manifold with*

$$P := T^*\tilde{M} \cup \bigcup_{\mathcal{S}} \mathbb{R} \times S^1 \tag{77}$$

as a set, ω is a smooth symplectic two-form on P with

$$\omega|_{T^*\tilde{M}} = dq_1 \wedge dp_1 + dq_2 \wedge dp_2,$$

and $H : P \to \mathbb{R}$ is a smooth Hamiltonian function with $H|_{T^*\tilde{M}} = \tilde{H}$.

The smooth Hamiltonian flow

$$\Phi^t : P \to P, \qquad (t \in \mathbb{R}) \tag{78}$$

generated by H is complete.

For all energies E which are regular values of V, the energy shell

$$\Sigma_E := \{x \in P \mid H(x) = E\} \tag{79}$$

is a smooth, three-dimensional manifold, and we write $\Phi^t_E := \Phi^t|_{\Sigma_E}$.

Proof. The construction works locally near the singularities $s \in \mathcal{S}$. We shortly explain the method by considering the simplest case. For more details see Prop. 2.3 of [26], where a scattering potential is considered.

One may linearize the *Kepler flow* with Hamiltonian function

$$\tilde{H}_K(p,q) := \tfrac{1}{2}p^2 - Z/|q|$$

in a suitable neighbourhood of $\mathbb{R}^2_p \times \{0\}$ in the phase space $T^*(\mathbb{R}^2_q \setminus \{0\})$, using the canonical coordinates $\tilde{H}_K$, $\tilde{T}$, $\tilde{L}$ and $\tilde{\varphi}$, where $\tilde{L}(p,q) := p \wedge q$ is the angular momentum, $\tilde{T}(p,q)$ is the time needed to come from the phase space point (p,q) to the pericenter of the Keplerian conic section and $\tilde{\varphi}(p,q)$ is the angle between the direction of that pericenter and, say, the 1-direction. Except $\tilde{T}$ these phase space functions are constant along the Kepler flow, and the collision points correspond to $\tilde{T}=0$, $\tilde{L}=0$. The remaining coordinates $(\tilde{H}_K, \tilde{\varphi})$ take values in a cylinder $\mathbb{R}\times S^1$.

Similarly, because the singularities of V are of the Kepler form, one may thus complete the phase space $T^*\tilde{M}$ by gluing one cylinder for each singularity in $\mathcal{S}$. $\square$

So after this regularization the Hamiltonian flow exists for all time, and we are in a similar situation as in the case of a smooth periodic potential.

However, in both cases the energy shells extend to spatial infinity and are thus non–compact. Therefore the Liouville measure μ_E on Σ_E is not normalizable and we cannot define a *metric entropy* of the flow Φ_E^t w.r.t. that measure.

But it is natural to use the invariance of H under the symplectic diffeomorphisms

$$\Psi^\ell : P \to P, \quad \Psi^\ell(p,q) := (p, q+\ell), \qquad (\ell \in \mathcal{L}) \tag{80}$$

of the phase space P generated by the lattice translations. So H descends to a function $\hat{H}$ on the phase space $\hat{P} := P/\mathcal{L} \cong T^*\mathbb{T}$ over the configuration torus $\mathbb{T}$, and generates a flow $\hat{\Phi}_E^t : \hat{\Sigma}_E \to \hat{\Sigma}_E$, $t\in\mathbb{R}$ on its energy shells $\hat{\Sigma}_E := \{x \in \hat{P} \mid \hat{H}(x) = E\}$. For regular values E of $\hat{H}$ (and thus in particular for $E > V_{\max}$) the Liouville measure $\hat{\mu}_E$ on $\hat{\Sigma}_E$ can be normalized. Then we will consider the metric entropy of $\hat{\Phi}_E^t$ w.r.t. the probability measure $\hat{\mu}_E$.

In the Coulombic case the flow is defined as Φ_E^t in Lemma 5.2.

The *topological entropy* of our flow Φ_E^t on the non–compact energy shell Σ_E can be defined directly. Namely we use the definition by Bowen of topological entropy which also applies to non-compact phase spaces X. This definition is not (and cannot be) purely topological, and one needs a metric d on X.

The topological entropy will then be invariant under uniformly continuous changes of the metric d. Therefore, for compact metrisable spaces X the topological entropy will only depend on the topology generated by the metric.

Definition 5.3 (Bowen) *Let (X,d) be a metric space and $T: X\to X$ a uniformly continuous map. Then for $m\in\mathbb{N}$, $\varepsilon>0$, a subset $F\subset X$ is said to* (m,ε)-span *a compact $K\subset X$ if*

$$\forall x \in K\, \exists y \in F : d_m(x,y) \le \varepsilon,$$

with the metric $d_m(x,y) := \max_{0\le i\le m-1} d(T^i x, T^i y)$*.*

Let $r_m(\varepsilon, T, K)$ *be the smallest cardinality of an* (m,ε)*-spanning set* F *of* K*,*

$$h_r(\varepsilon, T, K) := \limsup_{m\to\infty} \frac{1}{m} \ln(r_m(\varepsilon, T, K)),$$

and $h_{\text{top}}(T,K) := \lim_{\varepsilon\to 0} h_r(\varepsilon, T, K)$*.*

Then the **topological entropy of** T *is*

$$h_{\text{top}}(T) := \sup \left\{ h_{\text{top}}(T,K) \mid K \subset X \text{ } \textit{compact} \right\}.$$

Note that $h_r(\varepsilon, T, K)$ is monotonically increasing in ε, so that its limit $h_{\text{top}}(T,K)$ exists (it can be ∞).

In estimating the topological entropy, the relation

$$h_{\text{top}}(T^m, K) = m \cdot h_{\text{top}}(T,K), \qquad (m \in \mathbb{N}) \tag{81}$$

for the iterated map is useful.

The topological entropy of a *flow* $\Phi^t : X \to X$ is defined to be $h_{\text{top}}(\Phi^1)$.

In our case it is natural to use a metric d_E on Σ_E which is compatible with the topology on that energy shell and invariant under the lattice translations Ψ^ℓ, $\ell \in \mathcal{L}$.

Lemma 5.4 *The topological entropy for energy* E *of the flow on the configuration space* $\mathbb{R}^n_q$ *coincides with the one of the flow on the configuration torus* $\mathbb{T}$*:*

$$h_{\text{top}}(\Phi^1_E) = h_{\text{top}}(\hat{\Phi}^1_E) \tag{82}$$

Proof. Clearly $h_{\text{top}}(\hat{\Phi}^1_E) \le h_{\text{top}}(\Phi^1_E)$.

In fact, considering the projection

$$\Pi_{\Sigma_E, \hat{\Sigma}_E} : \Sigma_E \to \hat{\Sigma}_E \ ,$$

it follows that $d(\Pi_{\Sigma_E, \hat{\Sigma}_E}(x), \Pi_{\Sigma_E, \hat{\Sigma}_E}(y)) \le d(x,y)$. This implies

$$r_m(\epsilon, \hat{\Phi}^1_E, \Pi_{\Sigma_E, \hat{\Sigma}_E}(K)) \le r_m(\epsilon, \Phi^1_E, K)$$

for all $\epsilon > 0$ and compact $K \subset \mathbb{R}^n_q$. Therefore,

$$\sup_{K\subset\mathbb{R}^n_q} h_{\rm top}(\hat{\Phi}^1_E, \Pi_{\Sigma_E,\hat{\Sigma}_E}(K)) \le h_{\rm top}(\Phi^1_E)$$

and the inequality follows, for every compact $K \subset \hat{\Sigma}_E$ is the image of a compact in Σ_E under the projection $\Pi_{\Sigma_E,\hat{\Sigma}_E}$.

On the other hand, any (m, ε)-spanning set F of a compact $K \subset \Sigma_E$ is contained in the compact ε-neighbourhood

$$K_\varepsilon := \{x \in \Sigma_E \mid \exists y \in K : d(x, y) \le \varepsilon\},$$

of K, and the maximal multiplicity

$$M_{\max} := \sup_{x\in K_\varepsilon} \left|\left\{\Pi^{-1}_{\Sigma_E,\hat{\Sigma}_E}(\Pi_{\Sigma_E,\hat{\Sigma}_E}(x)) \cap K_\varepsilon\right\}\right|$$

of the projection $\Pi_{\Sigma_E,\hat{\Sigma}_E}$ is finite on K_ε.

Now if F is a (m, ε)-spanning set of $\Pi_{\Sigma_E,\hat{\Sigma}_E}(K)$, then it is contained in $\Pi_{\Sigma_E,\hat{\Sigma}_E}(K_\varepsilon)$, and $\left|\Pi^{-1}_{\Sigma_E,\hat{\Sigma}_E}(F) \cap K_\varepsilon\right| \le M_{\max} \cdot |F|$ which implies $h_{\rm top}(\Phi^1_E) \le h_{\rm top}(\hat{\Phi}^1_E)$ and thus (82). □

Proposition 5.5 *If the periodic potential V is twice continuously differentiable, the topological entropy for the flow is bounded above:*

$$h_{\rm top}(\Phi^1) \le 2n \cdot \max_q \|D^2V(q)\|^{\frac{1}{2}}. \tag{83}$$

On the other hand for $n \ge 3$ dimensions there exist smooth periodic potentials for which the topological entropy is bounded below above a threshold energy $E_{\rm th}$

$$h_{\rm top}(\Phi^1_E) \ge C > 0 \qquad (E > E_{\rm th}). \tag{84}$$

Proof. Phase space P is a Riemannian manifold w.r.t. the canonical Riemannian metric $\sum_{i=1}^n dp_i \otimes dp_i + dq_i \otimes dq_i$.

If the potential is constant, the flow is integrable and (83) is trivially true. Otherwise $b := \max_q \|D^2V(q)\|^{\frac{1}{2}} > 0$.

By Thm. 7.15 of [50] we have on the $2n$-dim. manifold P the bound

$$h_{\rm top}(\Phi^t) \le 2n \cdot \ln\left(\max_{x\in P}\|U^t(x)\|\right),$$

where $\|U^t(x)\|$ is the operator norm of the linearization $U^t(x) := D\Phi^t(x)$ of the flow at x.

But $U^t(x)$ is the solution of the initial value problem

$$\frac{d}{dt}U^t(x) = \begin{pmatrix} 0 & -D^2V(q(t,x)) \\ \hat{1\!\!1} & 0 \end{pmatrix} U^t(x), \qquad U^0(x) = \hat{1\!\!1}.$$

We set $W^t(x) := BU^t(x)$ with $B := \begin{pmatrix} \hat{1\!\!1} & 0 \\ 0 & b \cdot \hat{1\!\!1} \end{pmatrix}$. Thus $W^t(x)$ solves

$$\frac{d}{dt}W^t(x) = \begin{pmatrix} 0 & -D^2V(q(t,x))/b \\ b \cdot \hat{1\!\!1} & 0 \end{pmatrix} W^t(x), \qquad W^0(x) = B$$

or

$$W^t(x) = B + \int_0^t \begin{pmatrix} 0 & -D^2V(q(s,x))/b \\ b \cdot \hat{1\!\!1} & 0 \end{pmatrix} W^s(x) ds.$$

Thus Gronwall's inequality says $\|W^t(x)\| \le \|B\| \exp(bt)$ so that $\|U^t(x)\| \le \|B^{-1}\| \|B\| \exp(bt)$.

Using the formula $h_{\mathrm{top}}(\Phi^1) = h_{\mathrm{top}}(\Phi^t)/|t|$ in the $t \to \infty$ limit, we prove (83).

Concerning the lower bound, we use the fact that there exist two–dimensional smooth $\mathcal{L}'$–periodic potentials V' with positive entropy $h := h_{\mathrm{top}}(\Phi^1_{E_{\mathrm{th}}}) > 0$ for some energy E_{th}. Examples can be found in the paper [16] by Donnay and Liverani (we even expect it to be a generic property). Let $V : \mathbb{R}^n \to \mathbb{R}$ be the potential $V(q) := V'(q_1, q_2)$ and let $\mathcal{L} := \mathcal{L}' \times \mathbb{Z}^{n-2} \subset \mathbb{R}^n = \mathbb{R}^2 \times \mathbb{R}^{n-2}$ be a n–dim. lattice based on the lattice $\mathcal{L}'$ of V'. Then $F^1 : P^1 \to \mathbb{R}$, $F^1(p,q) = \frac{1}{2}(p_1^2 + p_2^2) + V(q)$ is a constant of the motion generated by $\hat{H}$. For $E > E_{\mathrm{th}}$ the submanifold

$$X := \{x \in \hat{\Sigma}_E \mid F^1(x) = E_{\mathrm{th}}\}$$

is thus flow–invariant, and the flow on this product manifold is the product flow of the flow in V' and a free flow. But the topological entropy of a product flow is the sum of the entropies of the factors (Thm. 7.10 of [50]) so that the flow on X has entropy equal to h. But $h_{\mathrm{top}}(\Phi^1_E) \ge h_{\mathrm{top}}(\Phi^1_E|_X)$ which proves (84). $\square$

However, the *metric* entropy of smooth periodic potentials decays in the high energy limit:

Proposition 5.6 *For $3n$ times continuously differentiable periodic potentials on $\mathbb{R}^n$ the metric entropy $h_{\mu_E}(\hat{\Phi}^1_E)$ w.r.t. Liouville measure μ_E is of order $\mathcal{O}(\sqrt{1/E})$.*

Proof. In [4] it is shown, using KAM theory, that the μ_E–measure of the complement of the invariant tori in $\hat{\Sigma}_E$ is $\mathcal{O}(\sqrt{1/E})$. Since on the KAM tori the motion is conditionally periodic, only that complement contributes in the Shannon–McMillan–Breiman formula

$$h_{\mu_E}(\hat{\Phi}_E^1) = \int_{\hat{\Sigma}_E} h_{\mu_E}(\hat{\Phi}_E^1, x) d\mu_E(x),$$

(see, e.g. Mañé [32], Chapter IV). But by (83) and the variational principle $h_{\mu_E}(\hat{\Phi}_E^1, x)$ is bounded above by a constant independent of E. □

Remark 5.7 *If the potential is* separable*, i.e. if the lattice $\mathcal{L}$ is rectangular (say, oriented in the coordinate directions) and V of the form $V(q) = \sum_{j=1}^n V_j(q_j)$, then the motion is integrable and has zero topological entropy. In particular the topological entropy vanishes for $n = 1$ dim.*

However, there does not seem to exist another example of a smooth periodic potential leading to integrable motion.

For these potentials the motion is ballistic *in the sense that for almost all initial points $x_0 \in \Sigma_E$ on an energy shell with $E > V_{\max}$ the* asymptotic velocity

$$\bar{v}(x) := \lim_{t \to \infty} \frac{q(t, x_0)}{t}$$

is non-zero.

In the simplest case of classical free motion

$$\Phi^t(p, q) = (p, q + tp) \tag{85}$$

with Hamiltonian function $H(p, q) := \frac{1}{2}p^2$, one has $|\bar{v}(x)| = \sqrt{2E}$.

Of course a ballistic form of the motion does not contradict positive entropy of the flow, See [4].

We now calculate the topological entropy for the Coulombic potentials in the high energy limit.

Although Lemma 5.2 solves the problem of collision orbits and regularizes the motion without changing it otherwise, we will now introduce a second regularization which is more useful to calculate quantities like the topological entropy, whereas it leads to a completely different phase space and a new time parametrization.

It is well-known that in general the solution curves for a Hamiltonian function of the form 'kinetic + potential' and energy E coincide with the geodesics of the *Jacobi metric* which is the Euclidean metric in configuration space, multiplied at point q with the conformal factor $(1 - V(q)/E)$, the only difference consisting in a modified time parametrization.

In our case, the Jacobi metric becomes singular near the positions $\mathcal{S}$ of the nuclei. Nevertheless one may consider for the Kepler flow the regularizing complex coordinate $Q^2 = q$, that is, the *Levi-Civita transformation*. It turns out that in this coordinate the Jacobi metric, originally defined only for $Q \neq 0$, can be smoothly extended to a non-singular Riemannian metric on the whole complex Q plane. Note that the Q plane is a two-fold branched covering of the original q plane, with a branch point at the position $q = 0$ of the singularity.

In [27] this local construction was globalized using the toral Riemann surfaces $\mathbb{T} = M/\mathcal{L}$ with projection $\Pi_{M,\mathbb{T}} : M \to \mathbb{T}$, its four-fold covering torus $\mathbb{T}^2 := M/(2\mathcal{L})$ (with projections $\Pi_{M,\mathbb{T}^2} : M \to \mathbb{T}^2$, $\Pi_{\mathbb{T}^2,\mathbb{T}} : \mathbb{T}^2 \to \mathbb{T}$) and the compact Riemann surface

$$M_4 := \left\{ (q,Q) \in \mathbb{T}^2 \times \mathbb{P} \,\middle|\, Q^2 = \frac{\prod_{i=1}^m \sigma(q - s_i + \ell_1)\sigma(q - s_i + \ell_1 + \ell_2)}{\prod_{i=1}^m \sigma(q - s_i)\sigma(q - s_i + \ell_2)} \right\}, \quad (86)$$

$$\sigma(z) := z \prod_{w \in 2\mathcal{L}\setminus\{0\}} (1 - z/w) \exp\left(z/w + \tfrac{1}{2}(z/w)^2\right)$$

being the Weierstrass σ-function and $\mathbb{P} := \mathbb{C} \cup \infty$ the Riemann sphere. The map $\Pi_{M_4,\mathbb{T}^2} : M_4 \to \mathbb{T}^2$, $(q,Q) \mapsto q$ is a two-fold branched covering with branch points at the singularities, all branch numbers equalling one.

Thus by the Riemann-Hurwitz relation the genus $\mathcal{G}(M_4)$ of M_4 equals $\mathcal{G}(M_4) = 2m + 1$ (m being the number of singularities in the fundamental domain). Since thus the genus is ≥ 3, by Gauss-Bonnet the integrated Gaussian curvature $\int_{M_4} K_E dM_4 = -4\pi \cdot (\mathcal{G}(M_4) - 1)$ of the lifted Jacobi metric $g_{4,E}$ on M_4 becomes negative. Due to the branched covering construction the metric $g_{4,E}$, originally not defined at the branch points, is be *smoothly* extended to these points by taking limits. So the geodesic flow $\phi^t_{4,E}$ on the unit tangent bundle $T_1 M_4$ of the surface is smooth and defined for all times.

In terms of the potential V the Gaussian curvature K_E equals

$$K_E(q) = \frac{(1 - V(q)/E)\Delta V(q)/E + (\nabla V(q)/E)^2}{2(1 - V(q)/E)^3} = -\frac{\Delta \ln(E - V(q))}{2(E - V(q))} \quad (87)$$

with Δ and ∇ denoting the Euclidean Laplacian and gradient, respectively.

For many potentials V the Gaussian curvature becomes strictly negative ($K_E(x) < 0$ for all $x \in M_4$) if E is large enough. Clearly this can only happen if $\Delta V < 0$ in (87), and the negativity is then preserved if one enlarges the energy E.

In our example of Yukawa potentials Nobbe [36] estimated analytically an upper bound for the threshold energy E_{th} above which $K_E < 0$ of $E_{\text{th}} < 5.17$, if one has a square unit lattice $\mathcal{L}$ and $m = 1$ singularity with $\mu = 1$ in the fundamental domain. The actual E_{th} is probably even much smaller.

Furthermore, as shown in [27], the negative curvature property is preserved by convex combinations of our Coulombic potentials. So it is a quite common property. As is well-known, it leads to a geodesic flow on the unit tangent bundle $T_1 M_4$ which is a transitive Anosov flow and is mixing w.r.t. the Liouville measure.

Moreover the autocorrelation of this flow decays rapidly enough that for many phase space functions a central limit theorem holds true. This made it possible to show in [27] that for probability measures ν_E of initial conditions $x_0 \in \Sigma_E$ which are absolutely continuous w.r.t. Liouville measure μ_E on the energy shell Σ_E (and with $\int q^2 d\nu_E < \infty$) the motion in the crystal is *diffusive*, i.e.

$$D(E) := \lim_{t\to\infty} \frac{\int_{\Sigma_E} q^2(t, x_0) d\nu_E(x_0)}{t} > 0 \tag{88}$$

if $E > E_{\mathrm{th}}$. In fact the diffusion constant D only depends on the energy E and not on the probability measure ν_E of initial conditions.

Nevertheless, there are many ν_E *not* absolutely continuous w.r.t. μ_E which do *not* lead to diffusive motion. For example, this is the case if ν_E is supported on a periodic orbit.

Such a diffusive behaviour does not follow from good ergodic properties alone. Like our system, the Sinai billard is Bernoulli, but the corresponding motion in the plane (Lorenz gas) is diffusive only if the so-called finite horizon condition is met, that is, if all trajectories hit the scattering centers.

In [36] Nobbe gave analytical and numerical evidence for a divergence of the diffusion constant as $D(E) \sim c \cdot E^{3/2}$.

Theorem 5.8 *If there exists a threshold energy E_{th} for which $\Delta(E_{\mathrm{th}} - V) < 0$, then on $(E_{\mathrm{th}}, \infty)$ the topological entropy $h_{\mathrm{top}}(\hat{\Phi}_E^1)$ is a smooth positive monotone increasing function of E asymptotic to*

$$h_{\mathrm{top}}(\Phi_E^1) \sim h_{\mathrm{top}}^{\infty} \cdot \sqrt{2E} \qquad (E \to \infty),$$

and the constant $h_{\mathrm{top}}^{\infty} > 0$ depends only on the set $\mathcal{S}$ of singularities.

Remark 5.9 *Below E_{th} the topological entropy is not expected to be a smooth function of the energy but to exhibit a singular continuous (devil's staircase) dependence on E. The reason for this kind of behaviour is a transition from regular (small E) to chaotic ($E > E_{\mathrm{th}}$) dynamics, see e.g. Troll [48].*

Proof. By the formula (87) for Gaussian curvature the condition $\Delta(E_{\mathrm{th}}-V)<0$ implies that For $E \geq E_{\mathrm{th}}$ that curvature is strictly negative. As shown in [27], then the flow $\hat{\Phi}^t_E$ on the compact manifold $\hat{\Sigma}_E$ is Bernoulli for each energy $E > E_{\mathrm{th}}$. Thus $h_{\mathrm{top}}(\Phi^1_E) > 0$ (see [50]).

Moreover it was shown in [27] that this flow is Anosov.

Since $E_{\mathrm{th}} > V_{\max}$, all the Σ_E for $E > E_{\mathrm{th}}$ are diffeomorphic (the diffeomorphisms leaving the configuration space point q invariant and rescaling momentum p). Thus Φ^t_E can be considered as a family of flows on a *fixed* manifold smoothly depending on E. But by Thm. 2 of Katok et al. [25] for smooth families of Anosov flows the topological entropy varies smoothly, too (this is a deep result since their invariant (un)stable foliations are very non–smooth in general).

We will now estimate $h_{\mathrm{top}}(\hat{\Phi}^1_E)$ by comparing it with the topological entropy $h_{\mathrm{top}}(\Phi^1_{4,E})$ of the *geodesic* flow $\Phi^t_{4,E}$ on unit tangent bundle T_1M_4 of the branched covering surface M_4.

The limit

$$\lim_{E\to\infty} h_{\mathrm{top}}(\Phi^1_{4,E}) \tag{89}$$

exists, since $h_{\mathrm{top}}(\Phi^1_{4,E})$ *is increasing in E.*

This can be seen by noticing that the topological entropy of the geodesic flow equals the asymptotic exponential growth rate in L of the number of closed geodesics whose length is $\leq L$. Now the geodesic flow $\Phi^t_{4,E}$, being Anosov, is structurally stable so that for two given energies $E, E' > E_{\mathrm{th}}$ there exists a homeomorphism

$$H_{E',E} : T_1M_4 \to T_1M_4$$

which maps oriented orbits on oriented orbits. In particular the closed orbits of the two flows are conjugated. If $E \geq E'$, then the length $l_{E'}(\gamma_{E'})$ of each closed orbit $\gamma_{E'}$ of $\Phi^t_{4,E'}$ is larger than the length $l_E(\gamma_E)$ of the closed orbit $\gamma_E := H_{E',E}(\gamma'_E)$ of $\Phi^t_{4,E}$. This follows since

- the length $l_E(\gamma_{E'})$ w.r.t. the Jacobi metric $g_{4,E}$ is smaller than the length $l_{E'}(\gamma'_E)$ w.r.t. $g_{4,E'}$, since the conformal factor $(1-V/E)$ decreases in E (we assumed $V_{\max} \leq 0$),
- the closed geodesics are unique in their conjugacy class, due to the negativity of the Gaussian curvature K_E,
- and we can thus find the closed geodesic γ_E by shortening the closed loop $\gamma_{E'}$ in the metric $g_{4,E}$.

The decrease in length of the closed orbits then leads to an increase of the topological entropy, proving our claim.

We will now show that (89) is finite. This is not immediately clear since as $E \to \infty$, the Gaussian curvature K_E concentrates near the singularities, so that the geodesic flow becomes singular there.

On the other hand, using the relation

$$h_{\mathrm{top}}(\Phi^1_{4,E}) = \lim_{L\to\infty} \frac{1}{L} \ln(N_E(L)),$$

$N_E(L)$ being the number of closed geodesics of length not exceeding L, we are done if we can show the existence of a $c \geq 1$ with

$$l_E(\gamma_E) \geq l_{E'}(\gamma_{E'})/c \tag{90}$$

with $\gamma_E := H_{E',E}(\gamma'_E)$ for all closed geodesics $\gamma_{E'}$ and all energies $E \geq E'$. Then $N_E(L) \leq N_{E'}(c \cdot L)$ so that $h_{\mathrm{top}}(\Phi^1_{4,E}) \leq c \cdot h_{\mathrm{top}}(\Phi^1_{4,E'})$.

To estimate the length of the geodesics, we consider ε-neighbourhoods of the singularities with Euclidean radius $\varepsilon = 1/E$ (see also [26], Chap. 5).

Since the singularities of V are Coulombic, outside these neighbourhoods the conformal factor of the Jacobi metric is uniformly bounded by

$$1 \leq 1 - V(q)/E \leq C(E')$$

for all energies $E \geq E'$.

For E' large the $1/E$-neighbourhoods, $E \geq E'$, are not intersecting each other, and by the above remark there exists a E-independent minimal length $L_{\min}$ of a geodesic segment which connects two different disks.

The boundaries of these disks are geodesically convex. Because of the negative Gaussian curvature each geodesic entering a disk has a maximal length of $\pi \cdot \sqrt{C(E')}/E$ inside that disk (it must be shorter than half the circumference).

Moreover, after leaving a disk D, it cannot reenter the same disk after a geodesic segment which is homotopic to one of the circle segments of ∂D between the points $x_1, x_2 \in \partial D$ of leave and re-entrance. This is a consequence of the Gauss-Bonnet theorem, the negativity of K_E and the geodesic convexity of ∂D.

Thus the length $l_E(\gamma_E)$ of a closed geodesic γ_E which has k encounters with a disk is

$$l_E(\gamma_E) \geq k \cdot L_{\min}.$$

On the other hand the length $l_{E'}(\gamma_{E'})$ of the homotopic closed geodesic $\gamma_{E'}$ is

$$l_{E'}(\gamma_{E'}) \leq k\sqrt{C(E')} \cdot (L_{\min} + \pi/E'),$$

since this is an upper bound for the length $l_{E'}(\gamma)$ of the loop γ which coincides outside the disks with $\gamma_{E'}$ but whose points of entrance and leave of the disks D are connected along the shorter circle segment of ∂D. Thus

$$l_E(\gamma_E) \geq l_{E'}(\gamma_{E'})/c$$

with $c := \sqrt{C(E')} \cdot (1 + \pi/(E' L_{\min}))$, showing (90).

So the topological entropy of the geodesic flow $\Phi^t_{4,E}$ has a high energy limit h^∞_{top}. In that limit the length of the geodesic segments between consecutive encounters of disks is given by the Euclidean distance between the two corresponding points in the set $\mathcal{S}$ of singularities. So h^∞_{top} depends only on the geometry of $\mathcal{S}$.

We now relate $h_{\text{top}}(\hat{\Phi}^1_E)$ to that limit.

The proportion of the total time spent by the orbits of that flow inside disks of radius $1/\sqrt{E}$ goes to zero as $E \to \infty$, since the speed inside that disk is larger than the speed outside, multiplied by a suitable E-independent constant C, $0 < C \leq 1$.

The period $T(\tilde{\gamma}_E)$ of a closed orbit $\tilde{\gamma}_E$ of $\hat{\Phi}^t_E$ covered n times by a closed geodesic flow line γ_E of $\hat{\Phi}^t_E$ is related to the length $l_E(\gamma_E)$ by the reparametrization formula

$$T(\tilde{\gamma}_E) = n \cdot l_E(\gamma_E) \cdot \frac{1}{\sqrt{2E}} \cdot \frac{1}{T(\gamma_E)} \int_0^{T(\gamma_E)} (1 - V(q(t))/E)^{-1} dt \qquad (91)$$

which takes the speed $\sqrt{2(E - V(q))}$ and the geodesic length element $\sqrt{1 - V(q)/E}$ into account.

The disks shrink to zero, and for the region outside the disks the integrand goes to one as $E \to \infty$, Thus (91) is asymptotic to $n \cdot l_E(\gamma_E)/\sqrt{2E}$.

Since the covering of $\hat{\Sigma}_E$ by $\Sigma_{4,E}$ has finite multiplicity (namely 8, a factor of two coming from the double branched covering of $\Pi_{M_4,\mathbb{T}^2} : M_4 \to \mathbb{T}^2$ in (86) and a factor of four coming from $\Pi_{\mathbb{T}^2,\mathbb{T}} : \mathbb{T}^2 \to \mathbb{T}$), n is bounded and we obtain the statement of the theorem. □

Remark 5.10 *The measure theoretic entropy $h_{\hat{\mu}_E}(\hat{\Phi}^1)$ is continuously differentiable in the energy $E > E_{\text{th}}$. This can be derived from a result by Knieper and Weiss [31] for geodesic flows of negative curvature.*

5.2 The Quantum Motion (One Particle)

Now we describe the quantum motion and its semiclassical limit as Planck's constant $\hbar \searrow 0$.

So we analyze the Hamiltonian operator

$$\hat{H}_\hbar := -\tfrac{1}{2}\hbar^2\Delta + V \tag{92}$$

on $L^2(\mathbb{R}^n)$, with an $\mathcal{L}$ periodic potential V.

In $n \geq 2$ dimensions $H_\hbar$ is self-adjoint, and the spectrum of $H_\hbar$ is known to be purely absolutely continuous and bounded below, if $V \in L^{n-1+\varepsilon}_{\mathrm{loc}}$.

This condition is also met by the Coulomb potentials, although they are so singular in two dimensions that $H_\hbar$ is only defined as a quadratic form, see [28].

Using the dual basis $\ell_1^*, \ldots, \ell_n^* \in \mathbb{R}^{n,*}$,

$$(\ell_i^*, \ell_j) = 2\pi\delta_{i,j} \tag{93}$$

spanning the dual lattice $\mathcal{L}^*$ in momentum space, we define the dual torus $\mathbb{T}^* := \mathbb{R}^{n,*}/\mathcal{L}^*$ (a fundamental domain of $\mathbb{T}^*$ adapted to the symmetries of V is called the *Brillouin zone*).

Denoting by $\mathrm{d}k := d^n k = dk_1 \cdots dk_n$ the elementary volume in cartesian coordinates and by $|\mathbb{T}^*| = \det(\ell_1^*, \ldots, \ell_n^*)$ the volume of the Brillouin zone, the unitary transformation

$$\hat{U} : L^2(\mathbb{R}^n) \to \mathcal{H} := \int_{\mathbb{T}^*}^{\oplus} L^2(\mathbb{T}) \frac{\mathrm{d}k}{|\mathbb{T}^*|}, \tag{94}$$

which on wave functions $f \in \mathcal{S}(\mathbb{R}^n)$ of rapid decrease is given by

$$(\hat{U}f)_k(q) = \sum_{\ell \in \mathcal{L}} \exp\left(-ik \cdot (q+\ell)\right) f\left(q+\ell\right),$$

defines the *Bloch decomposition.*

The Hamiltonian is transformed into a direct integral

$$\hat{U}\hat{H}_\hbar\hat{U}^{-1} = \int_{\mathbb{T}^*}^{\oplus} \hat{H}_\hbar(k) \frac{\mathrm{d}k}{|\mathbb{T}^*|}$$

of Hamiltonians $\hat{H}_\hbar(k) = \frac{1}{2}\hbar^2(-i\nabla + k)^2 + V$ on $L^2(\mathbb{T})$. The operators $\hat{H}_\hbar(k)$ have compact resolvent and spectrum $\{E_{\hbar,l}(k)\}_{l=1}^{\infty}$.

Now by this decomposition we have ballistic motion in the plane (see Asch and Knauf [4]):

$$\lim_{t\to\infty} \frac{(\psi, q^2(t)\psi)}{t^2} =: C > 0 \tag{95}$$

for ψ in the form domain of $\hat{H}_\hbar$ with $(\nabla\psi, \nabla\psi) + (q\psi, q\psi) < \infty$.

This is qualitatively different from the classical diffusive behaviour (88).

On the other hand the constant C for the squared speed of the ballistic motion is given by

$$C = \sum_{l=1}^{\infty} \int_{\mathbb{T}^*} \left|\hbar^{-1}\nabla E_{\hbar,l}(k)\right|^2 d\mu_\psi(l,k),$$

μ_ψ being the spectral measure of the wave function ψ. The gradient $\nabla E_{\hbar,l}$ of the band function appearing in the above expression is physically interpreted as the group velocity.

In [28] it was shown for Coulombic periodic potentials that

Proposition 5.11 *Above E_{th} in each compact energy interval $[E_1, E_2]$ and for each $\varepsilon > 0$ the number of bands with*

$$\left|\hbar^{-1}\nabla E_{\hbar,n}\right| < \varepsilon$$

is of density one as $\hbar \searrow 0$.

This can be interpreted in the sense that due to quantum chaotic effects the typical wave function is ballistic but very slow in the semiclassical limit.

For the quantum *free particle* with Hamiltonian $\hat{H}_\hbar := -\frac{\hbar^2}{2}\Delta$ the ballistic constant C equals $2(\psi, \hat{H}_\hbar\psi)$, independent of the value of Planck's constant $\hbar$.

In both the free and the potential case, the CNT entropy is undefined, as there is no normal state on $B(L^2(\mathbb{R}^2))$ invariant under the time evolution $\hat{U}_t := \exp(-i\hat{H}_\hbar t/\hbar)$.

On the other hand, by Proposition 3.4, the CNT entropy for the operators $\hat{H}_\hbar(k)$, which generate the motion on the configuration torus $\mathbb{R}^n/\mathcal{L}$, equals zero, given any density matrix describing the time-invariant state.

5.3 The Classical Electron Gas

We consider now the ergodic properties of the system of infinitely many classical non-interacting electrons in the crystal. Of course by our non-interaction assumption the dynamics of the infinite system is determined by the dynamics of a single electron. However, ergodic properties involve dynamics *and* measure.

A third aspect comes in when we discuss entropy, namely the question of the kinds of observation which we are able to make.

Due to the possibility of an arbitrarily large particle number within a given compact region of the one-particle phase space P, the space $\overline{P}$ describing a many-particle system is non-compact for usual choices of the topology, even if P is compact. Whereas Bowen's Definition 5.3 of *topological entropy* needs no compactness of the phase space, some metric on it must be chosen. Since we know no physically natural choice of such a metric on $\overline{P}$, we restrict ourselves to a discussion of *measure-theoretical entropy.*

Although the Liouville measure of a phase space of finitely many particles is infinite, the state of the infinite ensemble will be described by a *probability* measure. That measure describes a Poisson distribution of particles on the one-particle phase space P w.r.t. the invariant measure μ on P which one considers (as an example, μ may be Liouville measure on one energy shell or the measure of a Boltzmann distribution for a given temperature).

Now it turns out that even an *ideal gas*, i.e. an ensemble of free particles, is a Bernoulli system w.r.t. time evolution and has infinite total entropy. The reason for these optimal stochastic properties is the fact that the particles move away to infinity and are thus not observed any longer. These questions are analyzed in the articles [18] and [1] by Aizenman, Goldstein and Lebowitz.

As a consequence of Ornstein's theorem (see Walters [50], Thm. 4.28) all infinite entropy Bernoulli system are isomorphic. So from the measure-theoretic point of view the ideal gas cannot be discerned from, say, the classical electron gas in a Coulombic periodic potential whose particle energies are above the energy threshold E_{th}. On the other hand, unlike for the ideal gas, in our example of Coulombic potentials there exists a local mechanism leading to positive entropy for the motion of one particle. One would like to have a measure-theoretical notion which reflects that distinction between the two dynamical systems.

A clue to that problem is the observation by Goldstein in [17] that systems of statistical mechanics typically have a larger symmetry group than finite particle systems, since in addition to time evolution they are invariant under a group of space translations. This enabled Goldstein to define what he called *space-time entropy* (entropy density) and other related notions.

So the general setting starts with an Abelian group G acting on the measure space (P, Σ, μ) of a single particle by automorphisms $\Phi^g : P \to P$, $g \in G$. The measure space is assumed to be totally σ-finite and non-atomic. If μ is a probability measure (P, Σ, μ, Φ) is called a *generalized dynamical system.* Such systems are discussed by Conze in [14].

We first describe the Poisson construction, the classical analog of second quantization.

Definition 5.12 *The* **Poisson system** $(\overline{P}, \overline{\Sigma}, \overline{\mu}, \overline{\Phi})$ built over (P, Σ, μ, Φ) *has phase space* $\overline{P}$ *which is the set of countable subsets of* P*. The* σ*-algebra* $\overline{\Sigma}$ *of* $\overline{P}$ *is the smallest* σ*–algebra on* $\overline{P}$ *w.r.t. which for all* $A \in \Sigma$ *the 'particle number' functions*

$$N_A : \overline{P} \to \mathbb{N} \cup \{\infty\}, \qquad N_A(\overline{x}) := |A \cap \overline{x}|,$$

are measurable. Its probability measure $\overline{\mu}$ *is fixed by setting*

$$\overline{\mu}\left(\left\{\overline{x} \in \overline{P} \mid N_A(\overline{x}) = m\right\}\right) := \exp(-\mu(A)) \cdot \frac{\mu(A)^m}{m!}.$$

For $g \in G$ *the automorphism* $\overline{\Phi}^g : \overline{P} \to \overline{P}$ *is given by*

$$\overline{\Phi}^g(\overline{x}) := \{\Phi^g(x) \mid x \in \overline{x}\}.$$

In the case of $\mathcal{L}$-periodic potentials V we take

- the one-particle *phase space* $P := \mathbb{T}^*\mathbb{R}^n_q$ if V is smooth. In the Coulombic case P will be the four-dimensional manifold defined in (77).
- In both cases the one-particle σ*-algebra* Σ consists of the Borel subsets of the phase space P.
- *Measures:* Starting from the phase space volume form $\mu := \frac{1}{n!}\omega \wedge \ldots \wedge \omega$ on P, we will consider the Liouville measures μ_E induced by μ which have support on the energy shells $\Sigma_E \subset P$.

  Moreover, we will use the Boltzmann measures ν_β which are given by

  $$d\nu_\beta := \exp(-\beta \cdot H) d\mu$$

  for inverse temperatures $\beta > 0$.

  In the Coulombic case $d\nu_\beta := \theta(H - E_{\rm th}) \exp(-\beta \cdot H) d\mu$, θ being the Heaviside function. The main reason why we give zero measure to the phase space region below the threshold energy $E_{\rm th}$ is that otherwise the Boltzmann measures for $\beta > 0$ would be concentrated at the negative energies where the particles are bounded by the Coulombic singularities.

A partial physical justification for this cutoff is given by the fact that quantum mechanically the Pauli exclusion principle forbids the electrons to be in those low-energy states which are already occupied by electrons bounded to the nuclei of the crystal.

In all cases we may adjust the *particle density* by multiplying the one-particle measure by a constant.

- The *group actions* of interest are the discretized flow Φ^t, $t \in \mathbb{Z}$, on P generated by the Hamiltonian function H, and the Abelian space-time translations

$$\Xi^{t,\ell} : P \to P, \qquad \Xi^{t,\ell} := \Phi^t \circ \Psi^\ell \qquad (t \in \mathbb{R}, \ell \in \mathcal{L})$$

with the lattice translations Ψ^ℓ on P generated by the maps $q \mapsto q + \ell$ on the configuration plane M, see (80).

The notion of the measure-theoretic entropy of a generalized dynamical system is a direct generalization of the case of one iterated map (see [17]):

Definition 5.13 *The* **entropy** $h_\mu(\Phi)$ **of a generalized dynamical system** (P, Σ, μ, Φ) *with the action* $\Phi^g : P \to P$ *of an Abelian group* G *with finitely many generators* $g_1, \ldots, g_n \in G$ *is given by*

$$h_\mu(\Phi) := \sup_X h_\mu(\Phi, X),$$

where the supremum is w.r.t. all finite partitions X *of* P. *Here*

$$h_\mu(\Phi, X) := \lim_{k \to \infty} \frac{H_\mu(\bigvee_{\|g\| \le k} \Phi^g(X))}{|\{g \in G \mid \|g\| \le k\}|}$$

is the μ*-entropy for the partition* X*, and the norm on* G *is* $\|\sum_{i=1}^n k_i g_i\| := \sum_{i=1}^n |k_i|$.

The definition does not depend on the choice of the generators.

We will also discuss the information gain by local measurements in a region $B \subset \mathbb{R}^n_q$ of configuration space. Denoting the phase space over this region by $\mathbf{B} := \{(p,q) \in P \mid q \in B\}$, we thus consider the *dynamical entropy of* B given by

$$h_{\overline{\mu},B}(\overline{\Phi}) := \sup_{A \subset \mathcal{A}(\mathbf{B})} h_{\overline{\mu}}(\overline{\Phi}, A), \tag{96}$$

where the supremum is taken over all finite-dimensional subalgebras A of the algebra $\mathcal{A}(\mathbf{B})$ of classical observables over $\mathbf{B}$. Note that by the inclusion $\mathcal{A}(\mathbf{B_1}) \subset \mathcal{A}(\mathbf{B_2})$ for $B_1 \subset B_2$ this entropy is monotonic:

$$h_{\overline{\mu},B_1}(\overline{\Phi}) \leq h_{\overline{\mu},B_2}(\overline{\Phi}) \qquad (B_1 \subset B_2). \tag{97}$$

For simplicity we state our result for a compact configuration space region $B \subset \mathbb{R}^n_q$ which we assume to be an n-manifold with boundary (or a finite transversal intersection $B = B_1 \cap \ldots \cap B_l$ of such manifolds). However (97) immediately implies statements about unbounded B, in particular $B = \mathbb{R}^n_q$.

Theorem 5.14 *If the $\mathcal{L}$-periodic potential V is smooth ($V \in C^{3n}(\mathbb{R}^n, \mathbb{R})$ suffices), then above some threshold energy $E_{\rm th}$ the classical microcanonical subregion entropy is infinite*

$$h_{\overline{\mu_E},B}(\overline{\Phi}) = \infty \qquad (E > E_{\rm th}). \tag{98}$$

The same holds for the canonical subregion entropy for inverse temperature $\beta > 0$:

$$h_{\overline{\nu_\beta},B}(\overline{\Phi}) = \infty. \tag{99}$$

On the other hand

$$h_{\overline{\mu_E},B}(\overline{\Phi}) < \infty \tag{100}$$

for low energies $E > V_{\rm min}$ for which the components of Σ_E are compact.

The microcanonical space-time entropy equals the density of particles multiplied by the time-entropy per particle:

$$h_{\overline{\mu_E}}(\overline{\Xi}) = \hat{\mu}_E(\hat{P}) \cdot h_{\overline{\mu}_E}(\overline{\Phi}). \tag{101}$$

Similarly the canonical space-time entropy meets

$$h_{\overline{\nu_\beta}}(\overline{\Xi}) = \hat{\nu}_\beta(\hat{P}) \cdot h_{\overline{\nu}_\beta}(\overline{\Phi}) \tag{102}$$

(thus in particular both quantities are finite).

Proof. Let $\bar{v} : P \to \mathbb{R}^n$ be the asymptotic velocity of the classical particle

$$\bar{v}(x_0) := \lim_{T\to\infty} \frac{1}{T} \int_0^T p(t, x_0)dt.$$

By Birkhoff's ergodic theorem (applied to the phase space $\hat{P}$ over the configuration torus $\mathbb{T}$) this quantity exists $\hat{\mu}$-almost everywhere for an invariant measure $\hat{\mu}$, (and we set $\bar{v}(x_0) := 0$ otherwise for definiteness). See [4] for an extensive discussion.

We consider the restriction of this classical observable to the energy shell Σ_E. By KAM theory we know that for energies $E > E_{\rm th}$ above some threshold there exists a set $\hat{B}_E \subset \hat{\Sigma}_E$ of positive Liouville measure

$$k_E := \hat{\mu}_E(\hat{B}_E) > 0$$

composed of invariant tori. On each of these KAM tori the asymptotic velocity $\bar{v}$ is constant. By compactness of the energy shell $\hat{\Sigma}_E$ the deviation of the configuration space trajectory from a straight line in the direction $\bar{v}$ is uniformly bounded by some constant $C_E > 0$:

$$\|q(t,x_0) - q_0 - \bar{v}(x_0)\cdot t\| \le C_E \qquad (x_0 = (p_0,q_0) \in B_E,\, t \in \mathbb{R}).$$

Moreover for initial conditions on these tori the motion is ballistic:

$$v_{\min} := \inf_{x\in B_E} |\bar{v}(x)| > 0.$$

Using the asymptotic velocity as an observable we partition the region $B_E \cap \mathbf{B}$ of B_E which projects to the observation region B into r parts of equal size.

Namely for arbitrary $r \in \mathbb{N}$ we can find a partition $(U_1,\ldots,U_r)$ of the space $\mathbb{R}^n_{\bar{v}}$ of asymptotic velocities such that the preimages $(P_1,\ldots,P_r)$

$$P_j := \{x \in B_E \cap \mathbf{B} \mid \bar{v}(x) \in U_j\}$$

have equal volume

$$\mu_E(P_1) = \ldots = \mu_E(P_r) = \frac{k_E}{r} > 0 \tag{103}$$

(this is actually possible since the image of $\nu_E\restriction_{B_E}$ is non-atomic, every invariant torus having its specific asymptotic velocity). This partition of $B_E \cap \mathbf{B}$ induces an infinite partition $\mathcal{Q}$ of the many–particle phase space $\overline{P}$ whose atoms $Q_{m_1,\ldots,m_r}$, $m_j \in \mathbb{N}_0$, are of the form

$$Q_{m_1,\ldots,m_r} := \left\{\overline{x} \in \overline{P} \mid N_{P_1}(\overline{x}) = m_1, \ldots, N_{P_r}(\overline{x}) = m_r\right\}.$$

Observe the crucial fact that the partition ignores the number of particles which do not belong to the KAM component. For times t larger than

$$T := \left[\frac{\operatorname{diam}(B) + C_E}{v_{\min}}\right] + 1$$

($[x]$ denoting the integral part of x)

$$\Phi^t(B_E \cap \mathbf{B}) \cap \mathbf{B} = \emptyset.$$

Thus the partitions

$$\mathcal{Q}\,,\ \overline{\Psi}(\mathcal{Q})\,,\ldots,\ \overline{\Psi}^l(\mathcal{Q})\,,\ldots \tag{104}$$

are independent for the time T evolution $\overline{\Psi} := \overline{\Phi}^T : \overline{P} \to \overline{P}$. We will show that $h_{\overline{\mu_E},B}(\overline{\Psi}) = \infty$ which then implies $h_{\overline{\mu_E},B}(\overline{\Phi}) = \infty$, since in general $h_\mu(\Phi^1, \xi) \geq h_\mu(\Phi^T, \xi)/T$ for any partition ξ.

By independence of the partitions (104) and by independence and equidistribution of the r events $\{N_{P_1}(\overline{x}) = m_1\}, \ldots, \{N_{P_r}(\overline{x}) = m_r\}$

$$h_{\overline{\mu_E}}(\overline{\Psi}, \mathcal{Q}) = H_{\overline{\mu_E}}(\mathcal{Q}) = r \cdot H_{\overline{\mu_E}}(\tilde{\mathcal{Q}}), \tag{105}$$

the partition $\tilde{\mathcal{Q}}$ consisting of the atoms $\{N_{P_1}(\overline{x}) = m\}$, $m \in \mathbb{N}_0$. By (103) these atoms have measure

$$\overline{\mu_E}\{\overline{x} \in \overline{P} \mid N_{P_1}(\overline{x}) = m\} = \exp(-c)\frac{c^m}{m!}$$

with $c := k_E/r$. Thus (105) diverges as $r \to \infty$.

Note that technically Definition 5.13 uses finite partitions. However, our infinite partitions can be approximated by finite ones (merging the atoms with large particle numbers), so that we obtain a proof of (98).

The corresponding statement (99) for the canonical distribution is obtained along the same lines.

Next we show that the microcanonical subregion entropy (100) is finite for low energies E, such that connected components of the energy shell Σ_E are compact.

By the monotonicity property (97) we can estimate (100) from above by $h_{\overline{\mu_E},B_2}(\overline{\Phi})$, where the compact configuration space region $B_2 \subset \mathbb{R}^n_q$ contains B but additionally contains the projections of full energy shell components. That is, we assume the energy shell region

$$\{(p, q) \in \Sigma_E \mid q \in B_2\}$$

to be flow-invariant. But this implies that the particle numbers $N_{B_2}(\overline{\Phi}^t(\overline{x}))$ are t-invariant, too. Since the microcanonical measure

$$\mu_E(\{(p,q) \in \Sigma_E \mid q \in B_2\}) < \infty,$$

that particle number has finite expectation

$$\int_{\overline{P}} N_{B_2}(\overline{x}) d\overline{\mu_E}(\overline{x}) < \infty \tag{106}$$

The total entropy of distinguishable independent particles equals the entropy per particle, multiplied by the expectation (106). But the dynamical entropy per particle is finite (it was first shown by Kushnirenko that a C^1 transformation on a compact manifold has finite entropy), so that $h_{\overline{\mu_E},B_2}(\overline{\Phi}) < \infty$.

(101) and (102) follow from Thm. 6.8 of [17], since the systems $(\overline{P}, \overline{\Sigma}, \overline{\mu_E}, \overline{\Phi})$ and $(\overline{P}, \overline{\Sigma}, \overline{\nu_\beta}, \overline{\Phi})$ meet the condition of that theorem to be of *periodic-σ-bounded type*. Roughly speaking this means:

1. The one-particle system has a $\mathbb{Z}^n$ lattice symmetry commuting with time evolution.
2. Although the particle speed $|p|$ is unbounded in phase space P, it is bounded in each region $H^{-1}([V_{\min}, E]) \subset P$, which exhausts P as the maximal energy E goes to infinity. □

Now we turn to the case of *Coulombic potentials*. The motion in these potentials is diffusive for high energies and thus qualitatively different from the ballistic case of smooth potentials discussed above.

Proposition 5.15 *For $E > E_{\mathrm{th}}$ and $\beta > 0$ the infinite particle systems*

$$(\overline{P}, \overline{\Sigma}, \overline{\mu_E}, \overline{\Xi}) \quad \textit{resp.}\ (\overline{P}, \overline{\Sigma}, \overline{\nu_\beta}, \overline{\Xi})$$

are space-time $\mathbb{K}$-systems with infinite (time) dynamical entropy

$$h_{\overline{\mu_E}}(\overline{\Phi}) = \infty = h_{\overline{\nu_\beta}}(\overline{\Phi}) \tag{107}$$

and the (micro)canonical space-time entropies are positive:

$$h_{\overline{\mu_E}}(\overline{\Xi}) = \hat{\mu}_E(\hat{P}) \cdot h_{\overline{\mu}_E}(\overline{\Phi}) > 0, \tag{108}$$

$$h_{\overline{\nu_\beta}}(\overline{\Xi}) = \hat{\nu}_\beta(\hat{P}) \cdot h_{\overline{\nu}_\beta}(\overline{\Phi}) > 0. \tag{109}$$

Proof. Although the phase space $\hat{P} = P/\mathcal{L}$ over an elementary configuration torus $\mathbb{T} = \mathbb{R}^2/\mathcal{L}$ is non-compact, the projected measures $\hat{\mu}_E$ and $\hat{\nu}_\beta$ on it are finite for all energies $E \in \mathbb{R}$ resp. inverse temperature $\beta > 0$.

Moreover, although in the Coulombic case the maximal *speed* $|p|$ of a particle is unbounded on the energy shells Σ_E, the *maximal distance* $|q(1) - q(0)|$ traversed by that particle within one time unit is bounded. Namely, outside a ε-neighbourhood $\mathcal{S}_\varepsilon \subset \mathbb{R}^2$ of the singularity set $\mathcal{S}$ the maximal speed $\sup\{|p| \mid (p,q) \in \mathbb{T}^*(\mathbb{R}^2 \setminus \mathcal{S}_\varepsilon), H(p,q) = E\}$ is finite, and for small ε the disks of $\mathcal{S}_\varepsilon$ are disjoint so that trajectories with $|q(1) - q(0)| > 2\varepsilon$ intersect $\mathbb{R}^2 - \mathcal{S}_\varepsilon$.

Thus the system $(\overline{P}, \overline{\Sigma}, \overline{\mu_E}, \overline{\Phi})$ is of *periodic-bounded type* in the language of [17].

Furthermore, although the motion of the particle in the configuration plane $\mathbb{R}^2$ is not a $\mathbb{K}$-flow (since the Liouville measures μ_E are not finite so that ergodic notions do not apply), it is closely related to a family of $\mathbb{K}$-flows. Namely for $r \in \mathbb{N}$ we may consider the sublattice $r\mathcal{L} \subset \mathcal{L}$ and periodize phase space w.r.t. that lattice in the way we did using $\mathcal{L}$.

Then for energies $E > E_{\text{th}}$ the dynamical system $(P^{r\mathcal{L}}, \Sigma^{r\mathcal{L}}, \mu_E^{r\mathcal{L}}, \Phi^{r\mathcal{L}})$ is a Bernoulli system which implies the $\mathbb{K}$-property. So $(\overline{P}, \overline{\Sigma}, \overline{\mu_E}, \overline{\Phi})$ is of *periodic* $\mathbb{K}$-*type* in the sense of [17], and Thm. 6.1 of [17] implies that $(\overline{P}, \overline{\Sigma}, \overline{\mu_E}, \overline{\Xi})$ is a space-time $\mathbb{K}$-system.

On the other hand, the Boltzmann measure ν_β is not supported on a single invariant energy shell, so that the systems $(P^{r\mathcal{L}}, \Sigma^{r\mathcal{L}}, \nu_\beta^{r\mathcal{L}}, \Phi^{r\mathcal{L}})$ cannot even be ergodic. But, given the partition of phase space P into energy shells and the fact that for $E > E_{\text{th}}$ the dynamical systems $(P^{r\mathcal{L}}, \Sigma^{r\mathcal{L}}, \mu_E^{r\mathcal{L}}, \Phi^{r\mathcal{L}})$ are Bernoulli, $(\overline{P}, \overline{\Sigma}, \overline{\nu_\beta}, \overline{\Phi})$ is of *periodic* $\sigma - \mathbb{K}$-*type* (see [17]).

The $\mathbb{K}$ property for the space-time system $(\overline{P}, \overline{\Sigma}, \overline{\nu_\beta}, \overline{\Xi})$ follows immediately from Theorem 6.3 of [17], since $(\overline{P}, \overline{\Sigma}, \overline{\nu_\beta}, \overline{\Phi})$ is of $\sigma - \mathbb{K}$ type.

The formulas (108), (109) for the space-time entropies are consequences of Theorem 6.8 of [17]. Since by the $\mathbb{K}$ property these are strictly positive, the dynamical entropies (107) must be infinite. □

Remark 5.16 *Whereas the* ideal gas *(i.e. the Poisson system built over the free flow (85) with the canonical distribution ν_β) is a $\mathbb{K}$ system w.r.t. to time, it is not a space-time $\mathbb{K}$ system [17]. Although its time entropies are infinite, the entropy densities are zero in that case. So from the measure-theoretical point of view the ideal gas and the classical gas in a periodic array of attracting Coulombic potentials are really different.*

It is also possible that the Coulomb case is qualitatively different from the case of a smooth potential as described in Prop. 5.14 in that the finite region entropy could be finite for large energies.

An argument in favour of that idea is that the motion on long time scales resembles the random walk so that each particle should recur to B with probability one (as we are in dimension two).

Conversely, because of the finite density of particles, the number of particles visiting B for the first time should go to zero as time goes to infinity. So one could argue that in the $T \to \infty$ limit the dynamical one-particle mechanism of entropy production could be dominant over the fresh information about the phase space position of incoming particles.

5.4 The Quantum Electron Gas

As shown in Subsection 5.3, the (time) dynamical entropy of noninteracting classical electrons has a density which may well be positive.

Our conjecture is that the quantum (time) dynamical entropy of electrons within some bounded configuration space region B is not proportional to the *volume* but to the *surface* of B. Thus in $n = 1$ dimension the total quantum dynamical entropy of the gas, being a finite positive quantity, has density zero, whereas for $n > 1$ the entropy of the scaled region $\lambda \cdot B$ scales like λ^{n-1} as $\lambda \to \infty$, see (134).

The general setting will be as follows: we will second–quantize the Schrödinger operator $\hat{H}_\hbar = -\frac{1}{2}\hbar^2\Delta + V$ with the $\mathcal{L}$-periodic potential $V \in L^{n-1+\varepsilon}_{\mathrm{loc}}(\mathbb{R}^n)$ on the Hilbert space $L^2(\mathbb{R}^n)$.

In addition to the spectral properties discussed in Subsection 5.2, Wilcox [52] showed that the Bloch generalized eigenfunctions $\psi_{m,k} \in L^\infty(\mathbb{R}^n)$, $m \in \mathbb{N}$, $k \in \mathbb{T}^*$,

$$\begin{aligned} \hat{H}_\hbar \psi_{m,k} &= E_m(k)\psi_{m,k} && (110) \\ \psi_{m,k}(x+\ell) &= \exp(ik\cdot\ell)\psi_{m,k}(x), \qquad (\ell \in \mathcal{L}) \ , && (111) \end{aligned}$$

can be chosen in such a way that up to zero measure sets in $\mathbb{T}^*$ they are analytic functions of the quasi-momentum vector k, and have L^2–norm one on each elementary cell.

The bands are assumed to be enumerated so that $E_{m+1}(k) \geq E_m(k)$. The functions $u_{m,k} \in L^\infty(\mathbb{R}^n)$,

$$u_{m,k}(x) := \psi_{m,k}(x) \cdot \exp(-ik \cdot x) \tag{112}$$

are $\mathcal{L}$-periodic and thus may be considered as functions in $L^2(\mathbb{T})$.

We shall consider the CAR algebra $\mathcal{A}(\mathbb{R}^n)$ generated by creation and annihilation operators $\hat{a}^\dagger(f)$, $\hat{a}(g)$ of single-particle Fermionic states f, $g \in L^2(\mathbb{R}^n)$ satisfying

$$\hat{a}^\dagger(f)\ \hat{a}(g)\ +\ \hat{a}(g)\ \hat{a}^\dagger(f)\ =\ \langle g\,,\,f\rangle \tag{113}$$

$$\hat{a}^\dagger(f)\ \hat{a}^\dagger(g)\ +\ \hat{a}^\dagger(g)\ \hat{a}^\dagger(f)\ =\ 0 \tag{114}$$

$$\hat{a}(f)\ \hat{a}(g)\ +\ \hat{a}(g)\ \hat{a}(f)\ =\ 0\ . \tag{115}$$

The observables measuring the electrons in a region $\Lambda \subset \mathbb{R}^n$ are elements of the CAR subalgebra of the whole CAR algebra $\mathcal{A}(\mathbb{R}^n)$ based on the Hilbert space $L^2(\Lambda)$ which we denote by $\mathcal{A}(\Lambda)$. In a natural way $\mathcal{A}(\Lambda_1) \subset \mathcal{A}(\Lambda_2)$ if $\Lambda_1 \subset \Lambda_2$.

Though the general aim is the study of the entropic properties of the quasi-free automorphism

$$\alpha_H^t(\hat{a}^\dagger(f))\ =\ \hat{a}^\dagger\left(e^{-i/\hbar \hat{H}_\hbar\ t} f\right)\ , \tag{116}$$

in this paper we shall limit ourselves, as a preliminary step, to the study of the CNT-entropy of the group of translations by multiples of a lattice vector.

For an arbitrary vector $v \in \mathbb{R}^n$ we denote by $\hat{V} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, the unitary map $\hat{V}f(q) := f(q - v)$, and by α_v the Bogoliubov transformation $\alpha_{\hat{V}}$ on $\mathcal{A}(\mathbb{R}^n)$:

$$\alpha_v(\hat{a}(f)) := \hat{a}(\hat{V}f), \qquad (f \in L^2(\mathbb{R}^n))\ .$$

If v is a lattice vector, then α_v leaves the state ω_ρ (introduced below) invariant.

So α_v incorporates the shift of the lattice gas by v. We are inconsistent to use in one case the generator H and in the other case the unitary $\hat{V}$ (or rather, the velocity vector v) as an index. However, the use will be clear from the context.

In sight of our later application to the transformation α_H we are interested in α_v–invariant states on $\mathcal{A}(\mathbb{R}^n)$ *which are also* α_H*–invariant.* Now by Theorem XIII.98 of Reed and Simon we can write a wave function $f \in L^2(\mathbb{R}^n)$ as the superposition

$$f(x) = \sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \tilde{f}(m,k)\psi_{m,k}(x) \frac{\mathrm{d}k}{|\mathbb{T}^*|^{\frac{1}{2}}}. \tag{117}$$

of Bloch functions $\psi_{m,k}$ with coefficients $\tilde{f}(m,k) := \left(u_{m,k}, (\hat{U}f)_k\right)_{L^2(\mathbb{T})}$, $\hat{U}$ being defined in (94).

Thus suitable densities $\rho : \mathbb{N} \times \mathbb{T}^* \to \mathbb{R}^+$ of Bloch functions define quasifree states ω of non–interacting electrons which are fixed by their two–point functions

$$\omega(\hat{a}^\dagger(f)\hat{a}(g)) := \sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \tilde{f}(m,k)\overline{\tilde{g}(m,k)}\rho(m,k)\mathrm{d}k \tag{118}$$

Assumption 5.17 *We assume nondegeneracy of the bands and decay and smoothness of the density ρ:*

$$\rho \in C^{n+1}(\mathbb{N} \times \mathbb{T}^*, (0,1)) \tag{119}$$

and for some $\alpha > 1 + 1/n$

$$\max_{k \in \mathbb{T}^*} \partial_{k_1}^{i_1}, \ldots, \partial_{k_n}^{i_n} \rho^{1/2}(m,k) = \mathcal{O}(m^{-\alpha}) \qquad (i_1 + \ldots + i_n \leq n+1). \tag{120}$$

In particular we may consider the inverse temperature β state ω_{ρ_β},

$$\rho_\beta(m,k) := (1 + \exp(\beta(E_m(k) - \mu)))^{-1}, \tag{121}$$

whose chemical potential $\mu \in \mathbb{R}$ is determined by the prescribed density $D > 0$ of particles in configuration space. Under the nondegeneracy assumption $k \mapsto E_m(k)$ is a real-analytic function, and it even decays exponentially.

The nondegeneracy assumption is imposed in order to avoid technicalities alien to our question. One way to relax it is to consider ρ as a function on the Fermi surface and to formulate the assumptions accordingly.

The Bogoliubov automorphism α_v leaves the state ω invariant, since the latter derives from the one–particle Hamiltonian H which commutes with $\hat{V}$.

It proves convenient to introduce the Wannier functions $\phi_{m,\ell} \in L^2(\mathbb{R}^n)$ defined by

$$\phi_{m,\ell} := \int_{\mathbb{T}^*} e^{-ik\cdot\ell}\psi_{m,k} \frac{\mathrm{d}k}{|\mathbb{T}^*|} , \qquad (m \in \mathbb{N}, \ell \in \mathcal{L}) , \tag{122}$$

(see Ashcroft and Mermin [5]). The index m refers to the band.

Using that

$$\sum_{\ell \in \mathcal{L}} e^{i(k_1 = k_2)\ell} \;=\; |\mathbb{T}^*| \; \delta(k_1 - k_2) , \tag{123}$$

we obtain the inversion formula

$$\psi_{m,k} = \sum_{\ell \in \mathcal{L}} e^{ik\ell} \phi_{m,\ell} \; . \tag{124}$$

Furthermore, from the completeness of the Bloch functions $\psi_{m,k}$ one concludes that the Wannier functions form an orthonormal basis of $L^2(\mathbb{R}^n)$.

By (112) the Wannier functions of the m-th band are translates of each other:

$$\phi_{m,\ell}(q+\ell) = \phi_{m,0}(q) \qquad (q \in \mathbb{R}^n, \ell \in \mathcal{L}).$$

Thus they are somewhat localized in configuration space $\mathbb{R}^n$ near l.

Comparing the defining relation of the Wannier functions with the decomposition (117), one sees that their expectation

$$\omega\left(\hat{a}^\dagger(\phi_{m_1,\ell_1})\hat{a}(\phi_{m_2,\ell_2})\right) = \delta_{m_1,m_2}\tilde{\rho}_{m_1}(\ell_1 - \ell_2), \tag{125}$$

where

$$\tilde{\rho}_m(\ell) := \int_{\mathbb{T}^*} \rho(m,k)\; e^{ik\cdot\ell} \frac{\mathrm{d}k}{|\mathbb{T}^*|} \qquad (m \in \mathbb{N}, \ell \in \mathcal{L}) \tag{126}$$

is proportional to the ℓ-th Fourier coefficient of the density on the m-th band.

As all quasi-free states, ω in (118) has its two-point functions determined by a single-particle operator $0 \leq \hat{A} < \hat{\mathbb{1}}$:

$$\omega(\hat{a}^\dagger(f)\hat{a}(g)) = \langle g\,,\, \hat{A}f\rangle. \tag{127}$$

In our case, by means of the Wannier functions, $\hat{A}$ reads

$$\hat{A} = \sum_{m=1}^{\infty} \sum_{\ell_1,\ell_2 \in \mathcal{L}} \tilde{\rho}_m(\ell_1 - \ell_2) \cdot |\phi_{m,\ell_1}\rangle\langle\phi_{m,\ell_2}| \; . \tag{128}$$

We now consider a bounded configuration space region $B \in \mathbb{R}^n$ and assume that B is a n–dimensional submanifold with boundary (e.g. a ball) or a finite intersection

$$B = B_1 \cap \ldots \cap B_l \tag{129}$$

of such regions B_i whose boundaries ∂B_i are intersecting transversally (like a cube).

Then we introduce (using Def. (24)) a measure of the information loss per time unit within B.

Definition 5.18 *Let $\omega : \mathcal{A} \to \mathbb{C}$ be a state invariant under an automorphism $\alpha : \mathcal{A} \to \mathcal{A}$. Then we call*

$$h_{\omega,B}(\alpha) := \sup_{A \subset \mathcal{A}(B)} h_\omega(\alpha, A) \tag{130}$$

the **volume**–B *(or* **local***)* **quantum dynamical entropy** *of α w.r.t. ω*

Enlarging B by a factor λ and considering the scaling of $h_{\omega,\lambda B}(\alpha_v)$ with λ we have the following

Theorem 5.19 *If $B \subset \mathbb{R}^n$ is a finite, convex volume, then*

$$\lim_{\lambda\to\infty} \frac{1}{\lambda^{n-1}} h_{\omega,\lambda B}(\alpha_v) = \tfrac{1}{2} \int_{\partial B} |v \cdot dn| \cdot s(\omega)\ , \tag{131}$$

where

$$s(\omega) := \sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \frac{\mathrm{d}k}{|\mathbb{T}^*|} \eta_F(\rho(m,k)) \tag{132}$$

with the fermionic function

$$\eta_F : [0,1] \to \mathbb{R} \quad \textit{given by} \quad \eta_F(x) := \eta(x) + \eta(1-x)$$

is the mean entropy of ω.

More generally, for arbitrary (not necessarily convex) regions B of the form (129)

$$\lim_{\lambda\to\infty} \frac{1}{\lambda^{n-1}} h_{\omega,\lambda B}(\alpha_v) = |\mathrm{Pr}_v(B)| \cdot |v| \cdot s(\omega) \tag{133}$$

where $\mathrm{Pr}_v(B)$ denotes the shadow of the volume B with respect to projection in the v direction.

Proof. (131) reduces to (133) if B is convex, since then each line of projection through B (parallel to v) is either tangential to the surface ∂B and thus does not contribute to both expressions (see Remark 5.28 below), or intersects ∂B in exactly two points.

The proof of (133) will be split into an upper bound (Prop. 5.30) and a lower bound (Prop. 5.35). □

Remarks 5.20 *1. We plan to prove in a second paper that the local CNT-entropy for the non-interacting electron gas in a periodic potential, too, scales with the boundary:*

$$\lim_{\lambda\to\infty} \frac{1}{\lambda^{n-1}}\ h_{\omega,\lambda B}(\alpha_H)$$
$$= \tfrac{1}{2}\sum_{m=1}^{\infty}\int_{\mathbb{T}^*}\int_{\partial B}\left|\frac{\nabla_k E_m(k)}{\hbar}\cdot dn\right|\ \eta_F(\rho(m,k))\frac{\mathrm{d}k}{|\mathbb{T}^*|}\ . \quad (134)$$

To see how our theorem on the shift is related to this question, consider the Appendix, where we introduce a family of Hamiltonians $\hat{H}_\hbar^r$ (defined in (196)) which approximate $\hat{H}_\hbar$ in the $r\to\infty$ limit. These Hamiltonians act as shifts on the subbands.

2. *It should be inessential for the result (but simplify the proof) that we increase the size of B without changing its form. What is certainly essential is a van Hove type bound on the expanding region which ensures that ultimately most points are far from the boundary (see Def. 5.24 below).*

   On the other hand we do not believe that a van Hove condition is sufficient. As an example one may consider a region $B := B_1\dot{\cup}B_2 \subset \mathbb{R}^n$ where B_1 is n-dimensional (say, a ball) and B_2 is of dimension $n-1$, (say, a disk). Now $\lambda\mapsto\lambda B$ forms a van Hove sequence, since in that limit the volume of λB_1 dominates the surface of λB_2. However, the r.h.s. of (134) is enlarged by the existence of B_2.

   Although there is no conceptual contradiction (particles can in principle also be detected at B_2), we do believe that due to a large entropy defect that formula becomes wrong for this B.

Our interpretation of (134) is that the contribution of the individual electrons to the local CNT entropy is negligible if λ is large. Then the electrons typically spend a long time within λB. Thus an initial quasiclassical behaviour (ascertained by Egorov's Theorem) with an eventually exponential separation rate is followed by a spreading of the wave packet and a quasifree ballistic behaviour.

Hence for large λ the only remaining entropy contribution comes from incoming particles measured for the first time near the boundary of λB.

We work out this interpretation in the simplest case of a vanishing potential:

Example: The free electron gas.
In the low density limit (and in the semiclassical limit $\hbar\searrow 0$) $\mu\to-\infty$ in (121) so that the Fermi–Dirac distribution converges to the Boltzmann distribution. For example, for the 2-dim. free electron gas with mass m (and two spin states) one has

$$\mu = \ln(\exp(\pi D\hbar^2\beta/m) - 1)/\beta,$$

since the nonrelativistic dispersion relation $E(k) = \frac{(\hbar k)^2}{2m}$ leads to the density $\int \rho_\beta(k) d^2k/(4\pi^2) = D$.

More generally, for the n-dimensional free electron gas one obtains from the equation $\int_0^\infty \exp(-\beta(E-\mu)) d(E) dE = D$ with density of states $d(E) = (2\pi\hbar)^{-n} \cdot |B^n|\, n\, E^{n/2-1}$ that

$$\beta\mu \sim \ln\left(cD(2\pi\hbar)^n(\beta/m)^{n/2}\right)$$

in the low density (resp. $\hbar$) limit (c being a numerical constant depending on the dimension d).

Then in $\rho \searrow 0$ and only the $\rho\ln(\rho)$–term gives a contribution to (134) , which is asymptotic to

$$D\sqrt{\frac{T}{2\pi m}}\,|\partial B| \ln\left(cD^{-1}(2\pi\hbar)^{-n}(T\,m)^{n/2}\right).$$

The interpretation is as follows: $D\sqrt{\frac{T}{2\pi m}}$ is the number of particles per unit surface element and time unit entering (and leaving) the region λB of surface area $\lambda^{n-1}|\partial B|$ so that the total number per time unit equals

$$N := \lambda^{n-1}|\partial B| \cdot D\sqrt{\frac{T}{2\pi m}}.$$

These incoming particles are detected in a mean distance $\sqrt{\frac{T}{2\pi m}}$ from the boundary of λB and thus may be in one of

$$\approx \frac{\sqrt{\frac{T}{2\pi m}}\lambda^{n-1}|\partial B| \cdot (T\,m)^{n/2}}{(2\pi\hbar)^n}$$

phase space cells. The logarithm of that expression gives the contribution of each electron to the quantum dynamical entropy.

But the particles are indistinguishable, so that one has to subtract from the entropy the term $N\ln N$.

Of course the interpretation of formula (134) for general states and non–constant periodic potentials is exactly analogous to the above one for the free electron gas and the Fermi–Dirac distribution.

5.4.1 One–Particle Estimates

We first prove that the state ω is *locally normal*. That is, its restriction $\omega\restriction_\Lambda$ to any finite volume Λ is a state with a density matrix, and this belongs to the local algebra $\mathcal{A}_\Lambda$ with eigenvectors in the Fock space $\mathbb{H}_\Lambda$ generated by $\mathcal{A}_\Lambda$ acting on the Fock vacuum [38]–[39]. In the following we shall basically use restrictions of the global state ω to finite volumes $\Lambda \subset \mathbb{R}^n$. It is thus convenient to introduce at this point some useful notations and comments.

Remarks 5.21 *1. By the restriction of the state ω to a finite volume $\Lambda \subset \mathbb{R}^n$ we shall mean taking expectation (with respect to ω) of observables from the CAR algebra $\mathcal{A}(\Lambda)$ localized within Λ. The assumed quasi-freeness of ω relates it to the restriction*

$$\hat{A}_\Lambda := \chi_\Lambda \ \hat{A} \ \chi_\Lambda \ ,$$

of the single-particle operator $\hat{A}$, where χ_Λ is the characteristic function of the volume Λ.

This means that $\hat{A}_\Lambda$ will be considered to act on the square-summable functions supported within Λ.

2. Since $0 \leq \hat{A} < \hat{\mathbb{1}}$, the single-particle

$$\hat{B} = \frac{\hat{A}}{\hat{\mathbb{1}} - \hat{A}}$$

is positive. We shall consider the finite-volume restrictions

$$\hat{B}_\Lambda := \chi_\Lambda \ \hat{B} \ \chi_\Lambda$$

and also

$$\hat{B}^\Lambda := \frac{\hat{A}_\Lambda}{\hat{\mathbb{1}} - \hat{A}_\Lambda} \ .$$

The latter operator $\hat{B}^\Lambda$ is quite different from the restriction $\hat{B}_\Lambda$. Indeed, we have [39]:

$$\hat{B}^\Lambda = \chi_\Lambda \ \sqrt{\hat{B}} \ \frac{1}{\hat{\mathbb{1}} + \sqrt{\hat{B}} \ \chi_{\mathbb{R}^n \setminus \Lambda} \ \sqrt{\hat{B}}} \sqrt{\hat{B}} \ \chi_\Lambda \ .$$

Lemma 5.22 *Under the above assumptions on ρ the state ω is locally normal, and for bounded regions Λ the operator $\hat{B}_\Lambda$ of Remark 5.21.2 meets the estimate*

$$\mathrm{Tr}\,(\hat{B}_\Lambda) = \mathcal{O}(|\Lambda|). \tag{135}$$

The (unnormalized!) energy expectation

$$\sum_{m\in\mathbb{N}} \int_{\mathbb{T}^*} \rho(m,k) E_m(k) \frac{d^n k}{|\mathbb{T}^*|} \tag{136}$$

is finite.

Proof. Local normality follows from the estimate $\mathrm{Tr}\,(\hat{A}_\Lambda) < \infty$ for for $\hat{A}_\Lambda$ in Remark 5.21.1 (see [12]). But $\hat{B} = \hat{A}/(\hat{1\!\!1} - \hat{A}) \geq \hat{A}$ so that $\hat{B}_\Lambda \geq \hat{A}_\Lambda$ and we need only show (135). By our assumptions on ρ we conclude that

$$\rho_{\max} := \sup_{m\in\mathbb{N}, k\in\mathbb{T}^*} \rho(m,k) < 1.$$

Indeed by (120) a density $\rho(m,k) = 1$ can only occur on finitely many bands m, by (119) $\rho(m,k) < 1$, ρ is continuous and $\mathbb{T}^*$ is compact.

From (118) and (127) we see that the unitary Bloch transformation defined in (94) conjugates $\hat{A}$ with multiplication by ρ.

So in fact $\hat{A} \leq \rho_{\max} \hat{1\!\!1}$ which implies

$$\hat{B} \leq \hat{A}/(1 - \rho_{\max}) \ . \tag{137}$$

Therefore we can equally well show that $\mathrm{Tr}\,(\hat{A}_\Lambda) = \mathcal{O}(|\Lambda|)$ to prove the a priori stronger (135).

After expressing the one-particle operator $\hat{A}$ in terms of the Bloch functions, by means of (122), (123) and (124), we get the kernel

$$\begin{aligned} A(x,y) &= \sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \rho(m,k) \bar{\psi}_{m,k}(x) \psi_{m,k}(y) \frac{\mathrm{d}k}{|\mathbb{T}^*|} \\ &= \sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \rho(m,k) \bar{u}_{m,k}(x) u_{m,k}(y) \exp(ik(y-x)) \frac{\mathrm{d}k}{|\mathbb{T}^*|}, \end{aligned}$$

(the last form being manifestly $\mathcal{L}$-invariant).

By an L^∞-bound on the Wannier functions (see [52]), the Weyl estimate

$$E_m(k) \sim C \cdot m^{n/2} \qquad (m \to \infty)$$

and the decay assumption (120) for ρ that expression converges. So

$$\mathrm{Tr}\,(\hat{A}_\Lambda) = \int_\Lambda A(x,x)d^n x = \mathcal{O}(|\Lambda|) \tag{138}$$

(actually one sees from the L^2-normalization of the Wannier functions $\psi_{m,k}$ on $\mathbb{R}^n/\mathcal{L}$ that

$$\mathrm{Tr}\,(\hat{A}_\Lambda) = |\Lambda| \sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \rho(m,k) \frac{\mathrm{d}k}{|\mathbb{T}^*|} + \mathcal{O}(|(\partial\Lambda)_\varepsilon|),$$

where $(\partial\Lambda)_\varepsilon$ is a thickening of the boundary of Λ). Finiteness of (136) follows from the same argument, since by Assumption (120) $\alpha - 1$ is strictly larger than the exponent $n/2$ in the Weyl estimate. □

Lemma 5.23 *There exists a constant $c > 0$ such that for all bounded regions $\Lambda \subset \mathbb{R}^n$ with finite surface area $|\partial\Lambda|$ (defined as in (168))*

$$\mathrm{Tr}\,\left(\chi_\Lambda(\hat{B}^{1/2} - (\hat{B}^\Lambda)^{1/2})^2 \chi_\Lambda\right) \leq c|\partial\Lambda|,$$

with $\hat{B}^\Lambda$ as in 5.21 2..

Proof. We use the abstract inequality

$$\begin{aligned} &\mathrm{Tr}\,\left(\chi_\Lambda(\hat{B}^{1/2} - (\hat{B}^\Lambda)^{1/2})^2 \chi_\Lambda\right) \leq \\ &\quad \mathrm{Tr}\,\left(\chi_\Lambda \hat{B} \chi_{\mathbb{R}^n \setminus \Lambda} \hat{B} \chi_\Lambda\right) + 2\mathrm{Tr}\,\left(\chi_\Lambda \hat{B}^{1/2} \chi_{\mathbb{R}^n \setminus \Lambda} \hat{B}^{1/2} \chi_\Lambda\right) \end{aligned} \tag{139}$$

from the proof of Lemma 5.2 in [39]. Here we need decay estimates for the kernel of $\hat{B}$. Similar to $\hat{A}$, the kernel of $\hat{B}$ can be written in the form

$$B(x,y) = \sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \rho_B(m,k) \bar{\psi}_{m,k}(x) \psi_{m,k}(y) \frac{\mathrm{d}k}{|\mathbb{T}^*|}\ ,$$

with the density $\rho_B = \rho/(1-\rho)$.

By functional calculus, the representation of the kernel of $B^{1/2}$ is similar, but with density $\rho_B^{1/2}$.

Note that by $0 < \rho < 1$, $\rho_B > 0$, too, so that no smoothness is lost when taking the root $\rho_B^{1/2}$. Moreover the decay rate for $\rho_B^{1/2}$ is the same as for $\rho^{1/2}$:

$$\max_{k \in \mathbb{T}^*} \partial_{k_1}^{i_1}, \ldots, \partial_{k_n}^{i_n} \rho_B^{1/2}(m,k) = \mathcal{O}(m^{-\alpha}) \qquad (i_1 + \ldots + i_n \leq n+1) \tag{140}$$

and double as much for ρ_B.

Our nondegeneracy assumption implies that the phases of the Bloch functions can be chosen in a way that for each $x \in \mathbb{R}^n$ the maps

$$\mathbb{T}^* \to \mathbb{C}, \qquad k \mapsto \psi_{m,k}(x) \qquad (m \in \mathbb{N})$$

are analytic. Thus the Fourier coefficients

$$\mathcal{F}_{x,y,m}(\ell) := \int_{\mathbb{T}^*} \exp(+ik\cdot\ell)\bar{\psi}_{m,k}(x)\psi_{m,k}(y)\frac{\mathrm{d}k}{\sqrt{|\mathbb{T}^*|}} \qquad (\ell \in \mathcal{L})$$

decay faster than any power of $\|\ell\|$.

In fact, by writing the vector $\ell \in T$ in terms of the direct lattice basis vectors ℓ_i as $\ell = \sum_{i=1}^n l^i \ell_i$ and $k \in \mathbb{T}^*$ in terms of the dual lattice basis vectors ℓ_j^* (see (93)) as $k = \sum_{j=1}^n s^j \ell_j^*$ we have, using partial integration and dual lattice periodicity

$$\begin{aligned} l^j\ \mathcal{F}_{x,y,m}(\ell) &= -\frac{i}{2\pi}\int_0^1 \mathrm{d}s^1\cdots\mathrm{d}s^n\ \frac{\partial}{\partial k^j}\left(e^{2\pi\ i\sum_{i=1}^n s^i l^i}\right)\bar{\psi}_{m,k}(x)\psi_{m,k}(y) \\ &= i\int_0^1 \mathrm{d}s^1\cdots\mathrm{d}s^n\ e^{2\pi\ i\sum_{i=1}^n s^i l^i}\ \frac{\partial}{\partial k^j}\left(\bar{\psi}_{m,k}(x)\psi_{m,k}(y)\right)\ . \end{aligned}$$

This equality can be generalized to powers of the components l^i of $\ell \in \mathcal{L}$ and the decay properties result from application of the Riemann-Lebesgue Lemma.

In an analogous manner can be handled the Fourier coefficients of ρ_B

$$\tilde{\rho}_{B,m}(\ell) = \int_{\mathbb{T}^*} \rho_B(m,k)\exp(+ik\cdot\ell)\frac{d^n k}{\sqrt{|\mathbb{T}^*|}}, \tag{141}$$

that, due to the assumed decay properties of ρ, can be proved to obey the decay rate

$$|\tilde{\rho}_{B,m}(\ell)| \le Cm^{-\alpha}\|l\|^{-n-1} \qquad (m \in \mathbb{N}, \ell \in \mathcal{L}).$$

Now we assume w.l.o.g. (using $\mathcal{L}$-translation invariance of B), that the first argument x of the kernel belongs to the fundamental domain spanned by the basis vectors $\ell_1,\ldots,\ell_n$, and write the second argument in the form $y = y' + \ell$ with $\ell \in \mathcal{L}$ and y', too, in the fundamental domain. Then

$$\begin{aligned} B(x,y) &= \sum_{m=1}^{\infty}\int_{\mathbb{T}^*}\rho_B(m,k)\bar{\psi}_{m,k}(x)\psi_{m,k}(y')\exp(ik\ell)\frac{\mathrm{d}k}{|\mathbb{T}^*|} \\ &= \frac{1}{|\mathbb{T}^*|}\sum_{m=1}^{\infty}\sum_{\ell'\in\mathcal{L}}\ \tilde{\rho}_{B,m}(\ell-\ell')\ \mathcal{F}_{x,y',m}(\ell'), \end{aligned}$$

since Fourier transform converts the product into convolution. By the above decay properties and uniformity of estimates for x and y' in the compact fundamental domain, we obtain

$$B(x,y) = \mathcal{O}(\|x-y\|^{-n-1}) \qquad (\|x-y\| \to \infty) \tag{142}$$

and a similar estimate for $B^{1/2}(x,y)$, using (140).

The estimate of the r.h.s. of (139) is now performed for the first term, the second being of the same kind.

First we need the following geometrical statement on regions $\Lambda \subset \mathbb{R}^n$, using our definition $\Lambda^-(a) = \{q \in \Lambda \mid \mathrm{dist}(q, \mathbb{R}^n - \Lambda) \geq a\}$
The function

$$a \mapsto \left|\Lambda^-(a)\right| \qquad (a \geq 0)$$

is convex, and $\mathrm{d}^2 \left|\Lambda^-(a)\right| / \mathrm{d}a^2 \geq 0$ in the smooth case.
This need only be proved at a=0, since $(\Lambda^-(a_1))^-(a_2) = \Lambda^-(a_1+a_2)$.

Here for Λ being ∂-manifolds, one has by Steiner's formula [19]

$$\left.\frac{d^2\left|\Lambda^-(a)\right|}{da^2}\right|_{a=0} = \int_{\partial\Lambda} (k_1(x) + \ldots + k_n(x)) d\sigma(x)$$

where $k_1, \ldots k_n$ are the principal curvatures of the boundary manifold. This integral over the mean curvature of the boundary manifold is known to be bounded below by the surface area of S^{n-1}. Thus in this case our assertion holds true. Using this uniform bound, we may prove it in the general case by an approximation argument.

Now we use the convexity property to prove that

$$\mathrm{Tr}\,\left(\chi_\Lambda \hat{B} \chi_{\mathbb{R}^n\setminus\Lambda} \hat{B} \chi_\Lambda\right) \leq C\left|\partial\Lambda\right|$$

for

$$C := \sup_{x\in\mathbb{R}^n} \int_0^\infty \left(\int_{\|y-x\|\geq r} B^2(x,y) d^n y\right) dr.$$

Because of periodicity we need to take the sup only for x within the compact fundamental domain, so that the constant C is finite.

$$\begin{aligned}
&\mathrm{Tr}\,\left(\chi_\Lambda \hat{B} \chi_{\mathbb{R}^n\setminus\Lambda} \hat{B} \chi_\Lambda\right) \\
&= \int_\Lambda \left(\int_{\mathbb{R}^n\setminus\Lambda} B^2(x,y) d^n y\right) d^n x \\
&= \int_0^\infty \left(\int_\Lambda \delta\left(\mathrm{dist}(x, \mathbb{R}^n\setminus\Lambda) - a\right) \left(\int_{\mathbb{R}^n\setminus\Lambda} B^2(x,y) d^n y\right) d^n x\right) da \\
&\leq -\int_0^\infty \frac{d\left|\Lambda^-(a)\right|}{da} \cdot \left(\sup_{x\in\Lambda} \int_{\|y-x\|\geq a} B^2(x,y) d^n y\right) da \\
&\leq -\int_0^\infty \left.\frac{d\left|\Lambda^-(r)\right|}{dr}\right|_{r=0} \cdot \left(\sup_{x\in\mathbb{R}^n} \int_{\|y-x\|\geq a} B^2(x,y) d^n y\right) da \\
&= C\left|\partial\Lambda\right|.
\end{aligned}$$

In the last inequality we used the above convexity property (this was also implicitly used before since it allowed us to integrate over $\frac{d|\Lambda^-(a)|}{da}$ which is then defined for almost all a).

The last equality is another application of Steiner's formula, which yields

$$-\left.\frac{d\,|\Lambda^-(r)|}{dr}\right|_{r=0} = |\partial\Lambda|\,. \ \square$$

5.4.2 Mean Entropy

In order to calculate the local (finite-volume) dynamical entropy of a lattice shift, we have to consider the mean entropy $s(\omega)$ (introduced in (132)) for the $\mathcal{L}$-invariant quasifree state $\omega \equiv \omega_\rho$ of the form (118).

By (120)

$$s(\omega) < \infty \tag{143}$$

since $\eta_F(\rho) \leq c_\varepsilon \rho^{1-\varepsilon}$.

$s(\omega)$ can be interpreted as the entropy per unit volume of our electron gas, since it turns out to be the *van Hove* limit of the von Neumann entropy for a configuration space region Λ, divided by the volume $|\Lambda|$.

For $a > 0$ such a bounded measurable region $\Lambda \subset \mathbb{R}^n$ is contained in

$$\Lambda^+(a) := \{q \in \mathbb{R}^n \mid \mathrm{dist}(q, \Lambda) \leq a\}$$

and contains

$$\Lambda^-(a) := \{q \in \Lambda \mid \mathrm{dist}(q, \mathbb{R}^n - \Lambda) \geq a\}\ .$$

so that

$$\delta\Lambda(a) := \Lambda^+(a) \setminus \Lambda^-(a)$$

is a thickened boundary region.

Definition 5.24 *A sequence $\{\Lambda_j\}_{j\in\mathbb{N}}$ of bounded measurable subsets $\Lambda_j \subset \mathbb{R}^n$ tends to infinity in the sense of* **van Hove** *if [12]*

$$\lim_{j\to\infty} |\Lambda_j| = \infty \quad \text{and} \quad \lim_{j\to\infty} \frac{|\delta\Lambda_j(a)|}{|\Lambda_j|} = 0.$$

For simplicity we use the shorthand

$$\omega\restriction_\Lambda := \omega\restriction_{\mathcal{A}(\Lambda)}$$

for the restriction of our quasi-free state to the local CAR algebra over Λ.

Proposition 5.25 *Let the density function ρ meet the above estimates. Then mean entropy $s(\omega)$ equals the van Hove limit*

$$\lim_{\Lambda\to\infty} \frac{S(\omega\restriction_\Lambda)}{|\Lambda|} = s(\omega) \tag{144}$$

of the von Neumann entropy density. The deviation

$$\left|\frac{S(\omega\restriction_\Lambda)}{|\Lambda|} - s(\omega)\right| \tag{145}$$

has an upper bound depending on Λ only through the quotient $\dfrac{|\delta\Lambda(a)|}{|\Lambda|}$.

Proof. Following Park and Shin [39], Prop. A.1, from the definition of the quasi-free state ω, of the single-particle operator $\hat{A}$ in (128 and of its restriction $\hat{A}_\Lambda$ in Remark 5.21.1 , we have

$$S(\omega\restriction_\Lambda) = \operatorname{Tr}\left(\eta_F(\hat{A}_\Lambda)\right) . \tag{146}$$

We first consider parallelotopes $\Lambda_r \subset \mathbb{R}^n$. So let $(\ell_1,\ldots,\ell_n)$ be a basis of $\mathcal{L}$ and for $r\in\mathbb{N}$

$$\Lambda_r := \left\{ \sum_{j=1}^n x_j\ell_j \mid x_j\in[0,r) \right\} . \tag{147}$$

We claim that (144) holds for the van Hove sequence $\{\Lambda_r\}_{r\in\mathbb{N}}$. By subadditivity of entropy and $\mathcal{L}$-invariance of $\hat{A}$

$$\inf_r \frac{S(\omega\restriction_{\Lambda_r})}{|\Lambda_r|} = \lim_{r\to\infty} \frac{S(\omega\restriction_{\Lambda_r})}{|\Lambda_r|} . \tag{148}$$

The first observation is that

$$\hat{A}_{\Lambda_r} = |\Lambda_r|\cdot \sum_{m\in\mathbb{N}} \int_{\mathbb{T}^*} \rho(m,k)|\psi^r_{m,k}\rangle\langle\psi^r_{m,k}| \frac{\mathrm{d}k}{|\mathbb{T}^*|} \tag{149}$$

with the truncated rescaled Bloch functions

$$\psi^r_{m,k} := \frac{\chi_{\Lambda_r}\cdot\psi_{m,k}}{\sqrt{|\Lambda_r|}}$$

of L^2-norm one. Moreover by Def. (112)

$$\begin{aligned} |\Lambda_r|\langle\psi^r_{m,k}\,,\,\psi^r_{m,k'}\rangle_{L^2(\Lambda_r)} &= \int_{\Lambda_r} \bar{u}_{m,k}(q)u_{m,k'}(q)e^{i(k'-k)q}d^nq \\ &= \int_{\Lambda_1} \bar{u}_{m,k}(q)u_{m,k'}(q)e^{i(k'-k)q}f_r(k'-k)d^nq \end{aligned}$$

with

$$f_r(s) := \sum_{m_1,\ldots,m_n=0}^{r-1} \exp\left(is \cdot (\sum_{j=1}^{n} m_j \ell_j) \right) \qquad (s \in \mathbb{T}^*).$$

As $r \to \infty$, f_r tends weakly to the delta function. Thus

$$|\Lambda_r| \langle \psi^r_{m,k} \, , \, \psi^r_{m,k'} \rangle_{L^2(\Lambda_r)} \to \delta(k-k') \ \ |\mathbb{T}^*| \ \ , \tag{150}$$

too.

We evaluate the trace w.r.t. the basis

$$\psi^r_{m,k} \qquad (m \in \mathbb{N}, k \in G^*_r), \tag{151}$$

the group

$$G^*_r := \mathcal{L}^*/(r\mathcal{L})^* \equiv \left\{ \left(\sum_{j=1}^{n} c_j \ell^*_j \right) \Big/ r \ \middle| \ c_j \in \{0, r-1\} \right\}$$

being isomorphic to $\mathbb{Z}^n_r$. These vectors coincide with the (orthonormalized) eigenfunctions of the Schrödinger operator $-\frac{\hbar^2}{2}\Delta + V$ on $L^2(\Lambda_r)$ with periodic boundary conditions.

We substitute (149) and expand η_F in

$$\frac{S(\omega\restriction_{\Lambda_r})}{|\Lambda_r|} = \sum_{m\in\mathbb{N}} |\Lambda_r|^{-1} \sum_{k \in G^*_r} \langle \psi^r_{m,k} \, , \, \eta_F(\hat{A}_{\Lambda_r}) \psi^r_{m,k} \rangle \ .$$

By (150) we obtain

$$\lim_{r\to\infty} \frac{S(\omega\restriction_{\Lambda_r})}{|\Lambda_r|} = s(\omega) \ ,$$

and by (148) the lower bound

$$\frac{S(\omega\restriction_{\Lambda_r})}{|\Lambda_r|} \geq s(\omega). \tag{152}$$

We denote the deviation from mean entropy by

$$\delta_1(r) := \frac{S(\omega\restriction_{\Lambda_r})}{|\Lambda_r|} - s(\omega) \ .$$

From now on we consider a general bounded measurable $\Lambda \subset \mathbb{R}^n$ and more or less follow the strategy of proof which was used in the lattice case in [12], Prop. 6.2.38. However, we need an *apriori bound* of the following form which makes up for the lack of monotonicity of von Neumann entropy.

We claim that there exists a $C \geq 0$ independent of r such that for all measurable $\Lambda \subset \Lambda_r$

$$S(\omega\restriction_\Lambda) \leq C|\Lambda_r|. \tag{153}$$

To prove (153), we remark that, since $\Lambda \subset \Lambda_r$, the positive operator $\hat{A}_\Lambda$ meets the operator inequality $0 \leq \hat{A}_\Lambda \leq \hat{A}_{\Lambda,r} \leq \hat{\mathbb{1}}$. Thus, by the minmax theorem, the number of eigenvalues of $\hat{A}_\Lambda$ in the interval $[\frac{1}{2}, 1]$ is smaller than the number $c'(r)$ of corresponding eigenvalues of $\hat{A}_{\Lambda_r}$. Therefore,

$$\mathrm{Tr}\,(\eta_F(\hat{A}_\Lambda)) \leq \mathrm{Tr}\,(\eta_F(\hat{A}_{\Lambda_r})) + c'(r)\ln(2),$$

which, using (146), (149) and the fact that, for suitable $1 > \epsilon > 0$ and $c_\epsilon > 0$, $\eta_F(\rho) \leq c_\epsilon\, \rho^{1-\epsilon}$, we derive (153) for $r = 1$.

For the sublattice $r\mathcal{L}$ the set of shifted parallelotopes

$$\Lambda_{r,\ell} := \{q + \ell \mid q \in \Lambda_r\} \qquad (\ell \in r\mathcal{L})$$

forms a tesselation of $\mathbb{R}^n$.

We show (153) for arbitrary $r \in \mathbb{N}$ by dividing the parallelotope Λ_r into r^n shifted parallotopes $\Lambda_{1,l}$ and using subadditivity. Thus we control $\Lambda \subset \Lambda_r$ by estimating

$$S(\omega\restriction_\Lambda) \leq \sum_{c_1,\ldots,c_n=0}^{r-1} S\left(\omega\restriction_{\Lambda\cap\Lambda_{1,\sum_j c_j l_j}}\right) \leq r^n C \cdot |\Lambda_1| = C \cdot |\Lambda_r|\ ,$$

proving (153).

For a general bounded measurable $\Lambda \subset \mathbb{R}^n$ we denote by

$$A^+_{\Lambda,r} := \{\ell \in r\mathcal{L} \mid \Lambda_{r,\ell} \cap \Lambda \neq \emptyset\}$$

and

$$A^-_{\Lambda,r} := \{\ell \in r\mathcal{L} \mid \Lambda_{r,\ell} \subset \Lambda\}$$

the index sets of those shifted parallelotopes which have intersection with resp. are contained in Λ. Then for $a \geq \mathrm{diam}(\Lambda_r) = r \cdot \mathrm{diam}(\Lambda_1)$

$$\bigcup_{\ell\in A^+_{\Lambda,r}} \Lambda_{r,\ell} \subset \Lambda^+(a)\ , \qquad \bigcup_{\ell\in A^-_{\Lambda,r}} \Lambda_{r,\ell} \supset \Lambda^-(a)\ . \tag{154}$$

and

$$\bigcup_{\ell \in A^+_{\Lambda,r} - A^-_{\Lambda,r}} \Lambda_{r,\ell} \subset \delta\Lambda(a) := \Lambda^+(a) \setminus \Lambda^-(a) \ . \tag{155}$$

By subadditivity, translation invariance of ω and (153) we get from (154) and (155)

$$\begin{aligned} S(\omega\restriction_\Lambda) &\leq \sum_{\ell \in A^+_{\Lambda,r}} S(\omega\restriction_{\Lambda_{r,\ell}\cap\Lambda}) \leq |A^-_{\Lambda,r}| \cdot S(\omega\restriction_{\Lambda_r}) + C \cdot |\Lambda_r| \cdot |A^+_{\Lambda,r} - A^-_{\Lambda,r}| \\ &\leq |\Lambda| \cdot \frac{S(\omega\restriction_{\Lambda_r})}{|\Lambda_r|} + C \cdot |\delta\Lambda(a)|. \end{aligned} \tag{156}$$

On the other hand by subadditivity (155) implies

$$\begin{aligned} S(\omega\restriction_\Lambda) &\geq S\left(\omega\restriction_{\bigcup_{\ell\in A^+_{\Lambda,r}} \Lambda_{r,\ell}}\right) - \sum_{\ell \in A^+_{\Lambda,r} - A^-_{\Lambda,r}} S\left(\omega\restriction_{(\Lambda_{r,\ell}\setminus\Lambda)}\right) \\ &\geq S\left(\omega\restriction_{\bigcup_{\ell\in A^+_{\Lambda,r}} \Lambda_{r,\ell}}\right) - C \cdot |\delta\Lambda(a)|. \end{aligned} \tag{157}$$

We use *strong subadditivity* [51]

$$S\left(\omega\restriction_{\Lambda_I\cup\Lambda_{II}\cup\Lambda_{III}}\right) - S\left(\omega\restriction_{\Lambda_I\cup\Lambda_{II}}\right) \leq S\left(\omega\restriction_{\Lambda_I\cup\Lambda_{III}}\right) - S\left(\omega\restriction_{\Lambda_I}\right) \tag{158}$$

of von Neumann entropy for obtaining a lower bound for the first term in (157).

We denote by Γ_j ($j = 1, \ldots, |A^+_{\Lambda,r}|$) the union of the first j translates $\Lambda_{r,l}$ w.r.t. lexicographic ordering of $\ell \in A^+_{\Lambda,r}$ and want to prove for all j

$$S\left(\omega\restriction_{\Gamma_{j+1}}\right) - S\left(\omega\restriction_{\Gamma_j}\right) \geq s(\omega) \cdot |\Lambda_r|. \tag{159}$$

Assume to the contrary that for some j and $\varepsilon > 0$

$$S\left(\omega\restriction_{\Gamma_{j+1}}\right) - S\left(\omega\restriction_{\Gamma_j}\right) < (s(\omega) - \varepsilon) \cdot |\Lambda_r|.$$

For $t \in \mathbb{N}$ let Δ_k denote the union of the first k translates (in lexicographic order) of parallelotopes Λ_r contained in the large parallelotopes $\Lambda_{r\cdot t}$. Then, by (158) and the invariance of ω under lattice-translations

$$S\left(\omega\restriction_{\Delta_{k+1}}\right) - S\left(\omega\restriction_{\Delta_k}\right) < (s(\omega) - \varepsilon) \cdot |\Lambda_r|$$

for all k such there exists a translation of Γ_{j+1} into Δ_{k+1} which maps $\Gamma_{j+1} \setminus \Gamma_j$ to $\Delta_{k+1} \setminus \Delta_k$. This is possible if the distance between $\Delta_{k+1} \setminus \Delta_k$ and the boundary of $\Lambda_{r\cdot t}$ is larger than the diameter of Γ_j. For the remaining set of indices k subadditivity gives the a priori estimate

$$S\left(\omega\upharpoonright_{\Delta_{k+1}}\right) - S\left(\omega\upharpoonright_{\Delta_k}\right) \le S\left(\omega\upharpoonright_{\Lambda_r}\right).$$

This subset is of order $\mathcal{O}(t^{n-1})$. Thus for t large

$$S\left(\omega\upharpoonright_{\Lambda_{rt}}\right) = \sum_{k=0}^{t^n-1} S\left(\omega\upharpoonright_{\Delta_{k+1}}\right) - S\left(\omega\upharpoonright_{\Delta_k}\right) \le |\Lambda_{rt}| \cdot \left(s(\omega) - \frac{\varepsilon}{2}\right) ,$$

contradicting our above proof of the van Hove limit for the parallelotopes.

Thus we may use (159) to estimate the first term in (157) by

$$S\left(\omega\upharpoonright_{\bigcup_{\ell\in A^+_{\Lambda,r}}\Lambda_{r,\ell}}\right) \ge s(\omega)\cdot|A^+_{\Lambda,r}|\cdot|\Lambda_r| \ge s(\omega)\cdot|\Lambda|. \tag{160}$$

To collect our estimates, we set

$$\delta_2(a) := \frac{|\delta\Lambda(a)|}{|\Lambda|}.$$

Then (156) and (152) gives us an upper bound

$$\frac{S\left(\omega\upharpoonright_{\Lambda}\right)}{|\Lambda|} - s(\omega) \le \delta_1(r) + \delta_2(a)\ C$$

for the deviation from mean entropy. (157) and (160) give the lower bound

$$s(\omega) - \frac{S\left(\omega\upharpoonright_{\Lambda}\right)}{|\Lambda|} \le \delta_2(a)\ C\ .$$

We couple a and r by setting $a := \mathrm{diam}(\Lambda_1)\cdot r$ and choose $r\in\mathbb{N}$ so that $\delta_1(r) + \delta_2(a)\ C$ is minimized. This shows our proposition. $\square$

5.4.3 Volume Estimates

We now consider a bounded, not necessarily convex, configuration space region $B\subset\mathbb{R}^n$ of the form (129).

For $v\in\mathbb{R}^n$, $v\neq 0$ we denote by

$$\mathrm{Pr}_v : \mathbb{R}^n \to E_v^\perp$$

the orthogonal projection to the subspace $E_v^\perp := \{x\in\mathbb{R}^n \mid x\cdot v = 0\}$. For a Borel subset $B\in\mathbb{R}^n$ we consider the volume $|\mathrm{Pr}_v(B)|$ of its *shadow* $\mathrm{Pr}_v(B)$ (and set $|\mathrm{Pr}_v(B)| := 0$ if $v = 0$).

After $t\in\mathbb{Z}$ time steps the region $\lambda B\subset\mathbb{R}^n$ is shifted to

$$B_\lambda^t := \lambda B + t\cdot v,$$

and we are interested in estimates of the regions

$$B_\lambda^{<T} := \bigcup_{t=0}^{T-1} B_\lambda^t \ .$$

Lemma 5.26 *Let the new volume at time $t \in \mathbb{N}$ be*

$$\Delta_\lambda^t := B_\lambda^{<t+1} \setminus B_\lambda^{<t}.$$

Then $t \mapsto |\Delta_\lambda^t|$ is monotone decreasing,

$$|\Delta_\lambda^t| = |v| \cdot \mathcal{O}(\lambda^{n-1}) \tag{161}$$

and for $t \geq t_0 := [\lambda \cdot \mathrm{diam}(B)/|v|] + 1$

$$\Delta_\lambda^t = \Delta_\lambda^{t_0} + (t - t_0) \cdot v \tag{162}$$

(so that $|\Delta_\lambda^t|$ becomes independent of t), with

$$|\Delta_\lambda^t| \leq |v| \cdot \lambda^{n-1} \cdot |\mathrm{Pr}_v(B)| \tag{163}$$

and

$$|\Delta_\lambda^t| - |v| \cdot \lambda^{n-1} \cdot |\mathrm{Pr}_v(B)| = \mathcal{O}(\lambda^{n-2}). \tag{164}$$

Thus uniformly in $t \in \mathbb{N}$

$$|B_\lambda^{<t}| = t \cdot |v| \cdot \lambda^{n-1} \cdot \big(|\mathrm{Pr}_v(B)| + \mathcal{O}(\lambda^{-1})\big) + \mathcal{O}(\lambda^n). \tag{165}$$

Proof.

$$\Delta_\lambda^t = B_\lambda^t \setminus \bigcup_{i=1}^{t} \big(B_\lambda^t \cap B_\lambda^{t-i}\big)$$

from which one sees that $t \mapsto |\Delta_\lambda^t|$ is monotone decreasing, and for $t \geq t_0$

$$\Delta_\lambda^t = B_\lambda^t \setminus \bigcup_{i=1}^{t_0} \big(B_\lambda^t \cap B_\lambda^{t-i}\big)$$

so that (162) is valid.

For a bounded ∂-manifold B_j the set $\delta B_j(a) = B_j^+(a) \setminus B_j^-(a)$ of points of distance $\leq a$ from ∂B_j is of volume

$$|\delta B_j(a)| = \mathcal{O}(a) \qquad (a \searrow 0),$$

and the same holds for $B = B_1 \cap \ldots \cap B_l$. Thus

$$|\delta(\lambda B)(|v|)| = \lambda^n |\delta B(|v|/\lambda)| = |v| \cdot \mathcal{O}(\lambda^{n-1}) \qquad (\lambda \to \infty),$$

which implies (161), since $|\Delta_\lambda^t| \le |\Delta_\lambda^1|$ and $\Delta_\lambda^1 = (\lambda B + v) \setminus \lambda B \subset |\delta(\lambda B)(|v|)|$. (163) follows from (162). Namely the sets Δ_λ^t are disjoint, so that for each $s \in S := \mathrm{Pr}_v(B)$ (the shadow of B) the intersection between the line $\mathrm{Pr}_v^{-1}(s)$ and Δ_λ^t must be of total length $\le |v|$.

To prove (164), we consider for $\varepsilon > 0$ the subset S_ε of the shadow given by

$$S_\varepsilon := \left\{ s \in S \mid \mathrm{Pr}_v^{-1}(s) \cap B \text{ contains an interval of length } \ge \varepsilon \right\}.$$

For $s \in S_\varepsilon$, $\varepsilon \ge |v|/\lambda$ and $t \ge t_0$ the set

$$\mathrm{Pr}_v^{-1}(\lambda s) \cap B_\lambda^{<t}$$

contains an interval of length $\ge (t - t_0) \cdot |v|$, since the shifted intervals overlap. Together with the translation property (162) this implies that for $t \ge t_0$

$$\mathrm{Pr}_v^{-1}(\lambda s) \cap \Delta_\lambda^t$$

is of length $|v|$. Otherwise, due to the fixed and finite length of the intersections with the volume $\Delta_\lambda^{t_0}$, intersections of length $\le |v|$ could not make for intervals of length $\ge (t - t_0)|v|$ when $t >> 1$.

This implies that

$$\left|\mathrm{Pr}_v^{-1}(\lambda S_\varepsilon) \cap \Delta_\lambda^t\right| = |v| \cdot |\lambda S_\varepsilon| = |v| \cdot \lambda^{n-1} \cdot |S_\varepsilon|.$$

Next we show that most points of Δ_λ^t project to the subset λS_ε of the shadow. The main step is to see that for $\varepsilon > 0$ small

$$|B - \mathrm{Pr}_v^{-1}(S_\varepsilon) \cap B| = \mathcal{O}(\varepsilon^2). \tag{166}$$

To prove (166), we first claim that

(P) There exists a $L > 1$ such that for $\varepsilon > 0$ small and all $s \in S - S_\varepsilon$ the end points $b_0, b_1 \in \partial B$ of each interval in $\mathrm{Pr}_v^{-1}(s) \cap B$ can be connected by a curve of length $\le \varepsilon \cdot L$ lying on the boundary ∂B.

By definition of S_ε these end points have a distance $|b_1 - b_0| < \varepsilon$.

By compactness of ∂B we could otherwise find a limit point $b \in \partial B$ of such pairs of end points which is isolated in $\mathrm{Pr}_v^{-1}(\mathrm{Pr}_v(b))$.

1. If $b \in \partial B_i \cap \partial B_j$ with $i \neq j$, then the nonexistence of a common L would contradict transversality of intersections of the ∂-manifolds B_j, $j = 1, \ldots, l$.

2. Otherwise there is only one $j \in \{1, \ldots, l\}$ with $b \in \partial B_j$, that is, b is contained in a smooth component of the boundary ∂B. But in that case the curvature of ∂B in a neighbourhood of b is bounded, so that for some $L > 1$ any two points b_0, b_1 in that neighbourhood can be connected by a curve of length $\leq L \cdot |b_1 - b_0|$ in that neighbourhood.

Now having proved property **(P)**, we consider the end points $b_0, b_1 \in \partial B$ of such an interval in $\mathrm{Pr}_v^{-1}(s) \cap B$.

1. If $b_0 \in \partial B_i$ and $b_1 \in \partial B_j$ with $i \neq j$, the points of the interval between b_0 and b_1 belong to a $(L+1) \cdot \varepsilon$-neighbourhood Y_1^ε of the codimension two (dimension $n-2$) subset

$$X_1 := \{x \in \partial B \mid x \in \partial B_i \cap \partial B_j \text{ with } i \neq j\}.$$

   The size of that neighbourhood is thus $|Y_1^\varepsilon| = \mathcal{O}(\varepsilon^2)$, compatible with (166).

2. Otherwise $b_0, b_1 \in \partial B_j$. Then uniformly for all points b on these interval

$$\mathrm{dist}(b, \partial B) \leq C \cdot \varepsilon^2 \tag{167}$$

   for a suitable $C > 0$.

   To prove (167), we take a curve $c : [0,1] \to \partial B_j$ of length $\leq L \cdot \varepsilon$ which connects $c_0 = b_0$ with $c_1 = b_1$ on the boundary component ∂B_j. If $n(b)$ denotes the unit normal at a point $b \in \partial B_j$, then the sign of $n(b_0) \cdot v$ is different from $\mathrm{sign}(n(b_1) \cdot v)$, since b_0 and b_1 are the end points of a interval on a line parallel to v (more precisely, $\mathrm{sign}(n(b_0) \cdot v) \cdot \mathrm{sign}(n(b_1) \cdot v) \neq +1$).

   Thus by continuity there is a $t \in [0,1]$ with $n(c(t)) \perp v$. By compactness the curvature of ∂B_j and thus the change of the normal vector n along c is bounded. Thus be remembering the length estimate $L\varepsilon$ for c, we obtain $n(b_i) \cdot v = \mathcal{O}(\varepsilon)$, $i = 0, 1$. In words, at b_i the interval between b_0 and b_1, (which by assumption is of length $\leq \varepsilon$) makes an small angle of order ε with a suitable tangential direction in $T_{b_i}(\partial B_j)$.

   But this implies that each point $b \in B$ of the interval has only a distance of order ε^2 from the boundary, proving (167). The measure of these points

$$Y_2^\varepsilon := \left\{b \in B \setminus Y_1^\varepsilon \mid \mathrm{dist}(b, \partial B) \leq C\varepsilon^2\right\}$$

   is thus $|Y_2^\varepsilon| = \mathcal{O}(\varepsilon^2)$, too.

This shows (166). But (166) implies that for λ large and $\varepsilon := |v|/\lambda$

$$\left|\Delta_\lambda^t - \mathrm{Pr}_v^{-1}(\lambda S_\varepsilon) \cap \Delta_\lambda^t\right| = \lambda^n \left|\Delta_1^t - \mathrm{Pr}_v^{-1}(S_\varepsilon) \cap \Delta_1^t\right| = \mathcal{O}(\lambda^{n-2})$$

and thus (164). $\square$

Remark 5.27 *If B is* convex, *then (162) holds for $t_0 = 1$, since then*

$$B_\lambda^t \cap B_\lambda^{t-i} \subset B_\lambda^t \cap B_\lambda^{t-1}.$$

The volume of $\Delta_\lambda^t = B_\lambda^t \setminus (B_\lambda^t \cap B_\lambda^{t-1})$ then equals

$$\left|\Delta_\lambda^t\right| = \tfrac{1}{2}\left|B_\lambda^0 \Delta B_\lambda^1\right|,$$

where Δ denotes the symmetric difference.

Our next task is to control under which conditions the above sets form van Hove sequences as the scaling λ goes to infinity.

Remark 5.28 *Analytically one problem consists in controlling the shadow*

$$S := \mathrm{Pr}_v(M) \subset E_v^\perp \cong \mathbb{R}^{n-1}$$

of a subset $M \subset \mathbb{R}^n$.

In our case $M := \mathrm{int}(B)$. If B is a strictly convex ∂-manifold, then it follows from a transversality argument that the topological boundary $\partial S \subset E_v^\perp$ of its shadow is an $(n-2)$-dimensional smooth submanifold.

If one does not assume convexity, ∂S may loose smoothness (think of the similar geometrical situation of the V-shaped skyline between two the contours of two smooth mountains).

If B is a manifold with boundary ∂B, then ∂S is contained in the set of critical values of $(\mathrm{Pr}_v)\restriction_{\partial B}$, Thus in that case it follows from the Morse-Sard Theorem that ∂S has ($n-1$-dimensional) measure zero (see, e.g., Hirsch [22]).

In [29] one of us shows the following theorem:

'Let $M \subset \mathbb{R}^n$ be a closed embedded $(n-1)$-dimensional manifold with maximal exterior curvature $R > 0$. Then the $(n-2)$-dimensional measure

$$|\partial S(M)| := \lim_{s \searrow 0} \tfrac{1}{2} \frac{|U_\varepsilon|}{\varepsilon} \tag{168}$$

of the shadow boundary is bounded above by

$$|\partial S(M)| \le \left|\partial S(S_R^{n-1})\right| \cdot \frac{\mathrm{Vol}(M)}{\mathrm{Vol}(S_R^{n-1})},$$

where $S_R^{n-1} \subset \mathbb{R}^n$ is a sphere with radius R.'

In particular this geometrical estimate implies that $|\partial S(M)| < \infty$.

In order to obtain the lower bound in our theorem on shifts, we rescale speed, that is, we go from v to rv, with $r \in \mathbb{N}$. So we consider for time $t \in \mathbb{N}$ the sets

$$\Delta_\lambda^{r,t} := B_\lambda^{r,<t+1} \setminus B_\lambda^{r,<t} \tag{169}$$

where

$$B_\lambda^{r,<T} := \cup_{t=0}^{T-1} B_\lambda^{rt} \ , \quad B_\lambda^{rt} := \lambda B + rtv \ ,$$

are the configuration space subsets for rv (compare Lemma 5.26). By (162) for $t \ge t_0' := [t_0/r] + 1$, where t_0 has been defined in Lemma 5.26, these sets are shift-related:

$$\Delta_\lambda^{r,t+l} = \Delta_\lambda^{r,t} + lr \cdot v \ .$$

For simplicity we enforce shift invariance for all $t \in \mathbb{N}_0$ by setting

$$\begin{aligned} &\tilde{\Delta}_\lambda^{r,t} := \Delta_\lambda^{r,t} \quad \text{if } t \ge t_0' \\ &\tilde{\Delta}_\lambda^{r,t} := \tilde{\Delta}_\lambda^{r,t_0'} - (t_0' - t) r \cdot v \quad \text{otherwise} \ . \end{aligned} \tag{170}$$

Then for all $t \in \mathbb{N}_0$

$$\tilde{\Delta}_\lambda^{r,t} \subset B_\lambda^{rt} \setminus B_\lambda^{r(t-1)} \ .$$

Lemma 5.29 *As $\lambda \to \infty$ the family of sets $B_\lambda^{<T}$ forms a van Hove sequence. More precisely for all $a > 0$*

$$\frac{\left|\delta\left(B_\lambda^{<T}\right)(a)\right|}{\left|B_\lambda^{<T}\right|} = \mathcal{O}(\lambda^{-1}) \tag{171}$$

uniformly in $T \in \mathbb{N}$.

For $t = 0$ (and thus for all $t \in \mathbb{N}_0$) and $a \ll r \ll \lambda$ the family of sets $\tilde{\Delta}_\lambda^{r,0}$ forms a van Hove sequence, with

$$\frac{\left|\delta\left(\tilde{\Delta}_\lambda^{r,0}\right)(a)\right|}{\left|\tilde{\Delta}_\lambda^{r,0}\right|} = \mathcal{O}(r^{-1}) \tag{172}$$

for all $a > 0$.

Proof. In both cases the volumes go to infinity in the $\lambda \to \infty$ limit. So we need only check the second condition in (5.24). This clearly follows from (171) resp. (172).

We now prove (171) and start by rescaling. So equivalently we must show that for $\varepsilon > 0$ small

$$\frac{\left|\delta\left(B_1^{\varepsilon,<T}\right)(a\varepsilon)\right|}{\left|B_1^{\varepsilon,<T}\right|} = \mathcal{O}(\varepsilon). \tag{173}$$

Now we use a property of B which follows from its definition (129):
$B = B_1 \cap \ldots \cap B_l$, the boundaries ∂B_i intersecting transversally.

Each point b on ∂B which belongs to a unique ∂B_i has a unique outward normal vector $n(b) \equiv n_i(b)$. On the other hand, by transversality of intersections, also for the points $b \in \partial B$ belonging to different boundaries ∂B_i, $i \in I(b)$, there exists a normal vector $n(b)$ which has positive scalar product $n(b) \cdot n_i(b) > 0$ with each $n_i(b)$, $i \in I(b)$.

By compactness for some minimal cosine $C > 0$ we may cover ∂B by finitely many neighbourhoods $U_1, \ldots, U_s$ and choose unit vectors $\mathbf{n}_1, \ldots, \mathbf{n}_s$ such that

$$n_i(b) \cdot \mathbf{n}_j > C \qquad (j = 1, \ldots, s;\ b \in U_j;\ i \in I(b)).$$

We thus may obtain an upper estimate of the surface areas $|U_j|$ by dividing the area $|\mathrm{Pr}_{\mathbf{n}_j}(U_j)|$ by C.

Now we consider the subsets V_j, $j = 1, \ldots, s$ of points on the surface $\partial B_1^{\varepsilon,<T}$ which belong to U_j or one of its translates. Again we can estimate from above the areas of the V_j by $|\mathrm{Pr}_{\mathbf{n}_j}(V_j)|/C$. But for some $c_1 > 0$

$$|\mathrm{Pr}_{\mathbf{n}_j}(V_j)| \leq |\mathrm{Pr}_{\mathbf{n}_j}(B_1^{\varepsilon,<T})| \leq c_1(1 + \varepsilon T)$$

By the rescaled version of (165) we see that

$$\left|B_1^{\varepsilon,<T}\right| \geq c_2(1 + \varepsilon T) \tag{174}$$

so that we obtain (173).

To prove (172), we use the estimate

$$\left|\tilde{\Delta}_\lambda^{r,0}\right| = r\lambda^{n-1}|\mathrm{Pr}_v(B)| \cdot (1 + \mathcal{O}(r/\lambda))$$

which is obtained from (164) by rescaling v and using $|\tilde{\Delta}_\lambda^{r,0}| = |\Delta_\lambda^{r,t}|$ for t large. Thus (172) follows from an estimate of the form

$$\left|\delta\left(\tilde{\Delta}_\lambda^{r,0}\right)(a)\right| = \mathcal{O}(\lambda^{n-1})$$

for each $a > 0$. After rescaling, this is a consequence of

$$\lim_{\rho \searrow 0} \frac{\left|\delta\left(\tilde{\Delta}_1^{\varepsilon,0}\right)(\rho)\right|}{\rho} = \mathcal{O}(\varepsilon^0), \tag{175}$$

that is, uniform boundedness w.r.t. ε of the surface area of $\partial\tilde{\Delta}_1^{\varepsilon,0}$. By Def. (170)

$$\tilde{\Delta}_1^{\varepsilon,0} = \Delta_1^{\varepsilon,t_0'} - (t_0' - 1)\varepsilon v$$

for $t_0' = [t_0/\varepsilon] + 1$ so that we may instead estimate the surface of $\Delta_1^{\varepsilon,t}$. But according to Def. (169)

$$\Delta_1^{\varepsilon,t_0'} = B_1^{\varepsilon,<t_0'+1} - B_1^{\varepsilon,<t_0'}$$

so that

$$\left|\partial\Delta_1^{\varepsilon,t_0'}\right| \leq \left|\partial B_1^{\varepsilon,<t_0'+1}\right| + \left|\partial B_1^{\varepsilon,<t_0'}\right|$$

By (174) the r.h.s. is bounded by $2c_2(1 + \varepsilon(t_0' + 1)) < 2c_2(1 + (t_0 + 1))$ so that we have shown (175). $\square$

5.4.4 Upper Bound for the Shift

Proposition 5.30 *For $v \in \mathcal{L}$*

$$\lim_{\lambda\to\infty} \frac{1}{\lambda^{n-1}}\, h_{\omega_\rho,\lambda B}(\alpha_v) \leq s(\omega)\cdot|\mathrm{Pr}_v(B)|\cdot|v|\ .$$

Proof. As assumed at the beginning of this section, the state ω is locally normal. That is the restriction $\omega\restriction_{\lambda B}$ corresponds to a density matrix $\hat{\rho}_\lambda$ belonging to the local CAR algebra $\mathcal{A}(\lambda B)$. We shall write its eigenvalues ρ_i^λ in decreasing order and denote by $\hat{P}_\lambda^{\leq N}$ the orthogonal projection onto the Hilbert space spanned by the first N eigenvectors $|\Psi_i^\lambda\rangle$. That is

$$\hat{\rho}_\lambda|\Psi_i^\lambda\rangle = \rho_i^\lambda|\Psi_i^\lambda\rangle\ , \quad \hat{P}_\lambda^{\leq N} = \sum_{i=1}^{N}|\Psi_i^\lambda\rangle\langle\Psi_i^\lambda|\ ,$$

where the vectors $|\Psi_i^\lambda\rangle$ belong to the Fock space $\mathbb{H}_F^\lambda$ built over the single-particle Hilbert space $L^2(\lambda B)$. These eigenvectors are obtained by acting on the Fock vacuum with creation operators $\hat{a}(\psi_i^\lambda)$, where the $|\psi_i^\lambda\rangle$ are the eigenvectors of the restriction A_λ of the operator A in (128) to the given volume λB. The eigenvectors $|\psi_i^\lambda\rangle$ are thus supported within λB and

$$\sum_{i=1}^{\infty} |\psi_i^\lambda\rangle\langle\psi_i^\lambda| = \chi_{\lambda B} \ ,$$

namely, the characteristic function of the considered volume λB.

Using the orthogonal projections $P^\lambda_{N]}$ we construct the finite dimensional subalgebra

$$\mathcal{A}_\lambda^{\leq N} := \hat{P}_\lambda^{\leq N} \mathcal{A}(\lambda B) \hat{P}_\lambda^{\leq N} \bigoplus \mathbb{C}(\hat{1\!\!1} - \hat{P}_\lambda^{\leq N})$$

that form an increasing sequence uniformly converging to $\mathcal{A}(\lambda B)$.

As shown by Park and Shin in [39], Prop. 4.4 (compare also the proof of Thm. 3.2), the finite volume *CNT* entropy of the translation automorphism is given by

$$h_\omega\left(\alpha_v, \mathcal{A}(\lambda B)\right) = \lim_N h_\omega\left(\alpha_v, \mathcal{A}_\lambda^{\leq N}\right) \ .$$

So we can continue to use this finite-dimensional subalgebra. The join

$$\bigvee_{t=0}^{T-1} \alpha_v^t(\mathcal{A}_\lambda^{\leq N}) \subseteq \mathcal{A}(B_\lambda^{<T})$$

generated by the first T translates of $\mathcal{A}_\lambda^{\leq N}$ is finite dimensional. In fact, it is contained in the C*–algebra $B(\mathbb{H}_T)$ of bounded operators on the Hilbert space $\mathbb{H}_T := \sum_{t=0}^{T-1} \alpha_v^t(\mathcal{A}^\lambda_{N]})\mathbb{H}^\lambda_F$, which is finite dimensional: $\dim(\mathbb{H}_T) \leq TN$.

Thus

$$\begin{aligned} H_\omega\left(\mathcal{A}_\lambda^{\leq N}, \ldots, \alpha_v^{T-1}(\mathcal{A}_\lambda^{\leq N})\right) &\leq H_\omega\left(\bigvee_{t=0}^{T-1} \alpha_v^t(\mathcal{A}_\lambda^{\leq N})\right) \\ &\leq H_\omega\left(\mathcal{A}\left(B_\lambda^{<T}\right)\right) \leq S\left(\omega\restriction_{B_\lambda^{<T}}\right) \ , \end{aligned}$$

which is a consequence of monotonicity under inclusions, invariance under repetitions and boundedness by the von Neumann entropy of the entropy functionals.

We divide on both sides of the above inequality by T and perform the $T \to \infty$ and $N \to \infty$ limits. Then we obtain

$$h_{\omega,\lambda B}(\alpha_v) \leq \lim_{T\to\infty} \frac{1}{T} S\left(\omega\restriction_{B_\lambda^{<T}}\right) \ .$$

The proposition follows from (165), together with the van Hove estimate (171). $\square$

5.4.5 Lower Bound for the Shift

In this section we shall prove the lower bound

$$\lim_{\lambda\to\infty} \frac{1}{\lambda^{n-1}}\, h_{\omega,\lambda B}(\alpha_v) \geq s(\omega)\cdot|\mathrm{Pr}_v(B)|\cdot|v|$$

for a shift by a lattice vector $v \in \mathcal{L}$.

Let ψ_j^λ, $j \in \mathbb{N}$, be the orthonormal eigenstates of $\hat{A}\restriction_{\tilde{\Delta}_\lambda^{r,0}}$ in decreasing order. We denote by

$$P_j^1 := \hat{a}^\dagger(\psi_j^\lambda)\hat{a}(\psi_j^\lambda) \tag{176}$$

the projection operators on multi-particle states which include the jth eigenfunction, and set

$$P_j^0 := \hat{1\!\!1} - P_j^1 = \hat{a}(\psi_j^\lambda)\hat{a}^\dagger(\psi_j^\lambda).$$

For $I \subset \{1,...,N\}$ let

$$P_I^{\leq N} := \prod_{i\in I} P_i^1 \prod_{i\notin I} P_i^0.$$

Similarly for a finite subset $J \subset \{N+1, N+2, \ldots\}$ let

$$P_J^{>N} := \prod_{i\in J} P_i^1 \prod_{i\notin J} P_i^0\ .$$

More generally we consider for $\mathcal{I} = (I_0, \ldots, I_{T-1})$, $I_t \subset \{1,...,N\}$ the operators

$$P_{\mathcal{I}}^{\leq N} := \prod_{t=0}^{T-1} \alpha_v^{rt}(P_{I_t}^{\leq N}) \tag{177}$$

and for finite $\mathcal{J} = (J_0, \ldots, J_{T-1})$, $J_t \subset \{N+1, \ldots\}$ the operators

$$P_{\mathcal{J}}^{>N} := \prod_{t=0}^{T-1} \alpha_v^{rt}(P_{J_t}^{>N}). \tag{178}$$

Since the regions $\tilde{\Delta}_\lambda^{r,t_1}$ and $\tilde{\Delta}_\lambda^{r,t_2}$ are disjoint for $t_1 \neq t_2$, the operators in the products (177) and (178) commute so that the $P_{\mathcal{I}}^{\leq N}$ and $P_{\mathcal{J}}^{>N}$ form a family of commuting orthoprojectors.

Observe that we do not only have the resolution of identity

$$\sum_{\mathcal{I}, I_t\subset\{1,\ldots,N\}} P_{\mathcal{I}}^{\leq N} = \hat{1\!\!1}\ ,$$

but also

$$\sum_{\mathcal{J},J_t\subset\{N+1,\dots\}} P_{\mathcal{J}}^{>N} = \hat{\mathbb{1}}\ ,$$

with the convention of summing only over *finite* $\mathcal{J}$, since our construction is based on Fock space: That is, only finitely many single-particle states are occupied.

The operators $P_I^{\leq N}$, $I \subset \{1,...,N\}$, generate a 2^N–dimensional Abelian subalgebra $\mathbf{N}_\lambda^{ab}(N) \subset \mathcal{A}(\lambda B)$.

We will use this algebra and its translates in two ways:

- as the subalgebra whose entropy we estimate and
- as a means to decompose the state. Thus we consider the decomposition

  $$\omega = \sum_{\mathcal{I},I_t\subset\{1,\dots,N\}} \omega_{\mathcal{I}}$$

  into the linear functionals

  $$\omega_{\mathcal{I}}(a) := \omega\left(\sigma^{i/2}(P_{\mathcal{I}}^{\leq N})a\right)$$

  where $\sigma^{i/2}$ is the modular automorphism of ω which ensures positivity of the $\omega_{\mathcal{I}}$. So by normalization we obtain the states

  $$\hat{\omega}_{\mathcal{I}} := \frac{\omega_{\mathcal{I}}}{\omega_{\mathcal{I}}(\hat{\mathbb{1}})}.$$

Lemma 5.31 *For all $r, N \in \mathbb{N}$ the local dynamical entropy of the shift is bounded below by*

$$h_{\omega,\lambda B}(\alpha_v) \geq \lim_{T\to\infty} E_\lambda^{r,N}(T) - D_\lambda^{r,N} \tag{179}$$

with

$$E_\lambda^{r,N}(T) := \frac{1}{rT} \sum_{\mathcal{I},I_t\subset\{1,\dots,N\}} \eta\left(\omega(P_{\mathcal{I}}^{\leq N})\right) \tag{180}$$

and

$$D_\lambda^{r,N} := \frac{1}{r} \sum_{I\subset\{1,\dots,N\}} \omega\left(P_I^{\leq N}\right) \cdot \sum_{J\subset\{1,\dots,N\}} \eta\left(\hat{\omega}_I(P_J^{\leq N})\right). \tag{181}$$

Remarks 5.32 *1. The modular group σ^t of the state ω is defined by*

$$\sigma^t(\hat{a}^\natural(f)) = \hat{a}^\natural(e^{-iht}f) \ ,$$

where the modular Hamiltonian is related to the operator $\hat{A}$ in (128) by

$$\hat{A} = \frac{1}{\hat{\mathbb{1}} + e^h} \ .$$

It proves useful to write the positive operator B introduced in 5.21 2. as

$$B = \frac{\hat{A}}{\hat{\mathbb{1}} - \hat{A}} = e^{-\hat{h}} \ ,$$

so that the celebrated KMS-relations

$$\omega(\hat{a}^\dagger(f)\hat{a}(g)) = \omega(\hat{a}(g)\sigma^{-i}(\hat{a}^\dagger(f)))$$

read

$$\omega(\hat{a}^\dagger(f)\hat{a}(g)) = \omega(\hat{a}(g)\hat{a}^\dagger(\hat{B}f)) \ . \tag{182}$$

2. *By considering the positive single-particle operator B^Λ of 5.21 2., we can similarly write*

$$\hat{B}^\Lambda = e^{-\hat{h}_\Lambda} \ ,$$

and thus define a local modular group as at point 1. above (compare [39], Section 4.). Clearly, the eigenvectors of the restricted state $\omega\restriction_\Lambda$ that are all the way used in this section are also eigenstates of $\hat{A}_\Lambda$, $\hat{B}^\Lambda$ and $\hat{h}_\Lambda$.

3. *The term (180) is the entropy of the restriction of the state ω to the Abelian algebra which is the direct sum of $\mathbf{N}^{ab}_\lambda(N)$ and its translates. It will be shown to be related to mean entropy.*

4. *The entropy defect (181) is a boundary term. This is related to the fact that $\hat{\omega}_I(P^{\leq N}_{\vec{J}}) = \delta_{I,J}$ if the modular automorphism leaves P_I invariant, and the definition of both σ and P_I in terms of the state.*

Proof. We apply the definitions and properties of finite-volume CNT-entropy and of the entropy functionals, in particular the property (26) together with the subalgebra–monotonicity of the entropy (24), to estimate from below as follows:

$$
\begin{aligned}
& h_\omega\left(\alpha_v\,,\,\mathcal{A}(\lambda B)\right) \\
& \geq \frac{1}{r} h_\omega\left(\alpha_v^r\,,\,\mathbf{N}_\lambda^{ab}(N)\right) \\
& \geq \frac{1}{r}\lim_{T\to\infty}\frac{1}{T}\Bigg\{\sum_{\mathcal{I},I_t\subset\{1,\ldots,N\}}\eta(\omega(P_{\mathcal{I}}^{\leq N})) && (183)\\
& -\sum_{t=0}^{T-1}\sum_{I\subset\{1,\ldots,N\}}\eta(\omega(\alpha_v^{rt}(P_I^{\leq N}))) && (184)\\
& +\sum_{t=0}^{T-1} S\left(\omega\restriction\alpha_v^{rt}(\mathbf{N}_\lambda^{ab}(N))\right) && (185)\\
& -\sum_{t=0}^{T-1}\sum_{I\subset\{1,\ldots,N\}}\omega(\alpha_v^{rt}(P_I^{\leq N}))\; S\left(\frac{\omega(\sigma^{i/2}(\alpha_v^{rt}(P_I^{\leq N}))\ \cdot\ )}{\omega(P_I^{\leq N})}\restriction\alpha_v^{rt}(\mathbf{N}_\lambda^{ab}(N))\right)\Bigg\} && (186)
\end{aligned}
$$

So the first term (183) coincides with $\lim_{T\to\infty} E_\lambda^{r,N}(T)$.

Moreover, ω is α_v-invariant, and $\mathbf{N}_\lambda^{ab}(N)$ is Abelian. Thus,

$$
\omega(\alpha_v^{rt}(P_I^{\leq N})) = \omega(P_I^{\leq N})
$$

and

$$
S\left(\omega\restriction\alpha_v^{tr(\lambda)}(\mathbf{N}_\lambda^{ab}(N))\right) = -\sum_{I\subset\{1,\ldots,N\}}\omega(P_I^{\leq N})\log\omega(P_I^{\leq N})
$$

so that (184) and (185) cancel.

By the same argument, and since the automorphism α_v commutes with the modular automorphism $\sigma^{i/2}$, (186) reduces to (181), because

$$
\begin{aligned}
& S\left(\frac{\omega(\sigma^{i/2}(\alpha_v^{rt}(P_I^{\leq N}))\ \cdot\ )}{\omega(P_I^{\leq N})}\restriction\alpha_v^{rt}(\mathbf{N}_\lambda^{ab}(N))\right)\Bigg\} \\
& \quad = \sum_{J\subset\{1,\ldots,N\}}\eta\left(\frac{\omega(\sigma^{i/2}(\alpha_v^{rt}(P_I^{\leq N}))\alpha_v^{rt}(P_J^{\leq N}))}{\omega(P_I^{\leq N})}\right) \\
& \quad = \sum_{J\subset\{1,\ldots,N\}}\eta\left(\frac{\omega(\sigma^{i/2}(P_I^{\leq N})P_J^{\leq N})}{\omega(P_I^{\leq N})}\right). \qquad \Box
\end{aligned}
$$

Next we relate the main term $E_\lambda^{r,N}(T)$ in Lemma 5.31 to von Neumann entropy.

Lemma 5.33 *For $\varepsilon > 0$ there is an $N_0(\varepsilon)$ so that for all $N \geq N_0(\varepsilon)$*

$$
E_\lambda^{r,N}(T) \geq \frac{1}{T} S\left(\omega\restriction_{\bigcup_{t=0}^{T-1}\tilde{\Delta}_\lambda^{r,t}}\right) - \varepsilon
$$

Proof. From local normality and the other assumptions on ω we required at the beginning of the section, the restricted state

$$\rho_\lambda^{r,<T} := \omega\restriction_{\bigcup_{t=0}^{T-1}\tilde{\Delta}_\lambda^{r,t}}$$

is a density matrix with finite von Neumann entropy.

The Abelian subalgebra

$$\mathbf{N}_\lambda^{r,<T}(N) := \bigvee_{t=0}^{T-1} \alpha_v^{rt}(\mathbf{N}_\lambda(N)) \subset \mathcal{A}(\bigcup_{t=0}^{T-1} \tilde{\Delta}_\lambda^{r,t})$$

generated by the spectral projections $P_I^{\leq N}$ is not maximally Abelian. Therefore $\omega\restriction_{\mathbf{N}_\lambda^{r,<T}(N)}$ does not coincide with $\rho_\lambda^{r,<T}$, but the difference can be handled exactly as done in [39], Prop. 4.1. □

Our last task is thus to show that under the previous limit the contribution from the *entropy defect* $D_\lambda^{r,N}$ vanishes.

Lemma 5.34 *For scaling factor $\lambda \to \infty$ and $1 \ll r \ll \lambda$ and arbitrarily small $\varepsilon > 0$ the entropy defect is bounded above by*

$$D_\lambda^{r,N} \leq C(\varepsilon)\lambda^{n-1+\varepsilon}/r.$$

uniformly in $N \in \mathbb{N}$.

Proof. Let us rewrite (181) as follows

$$rD_\lambda^{r,N} = \sum_{I\subset\{1,\dots,N\}} \sum_{J\subset\{1,\dots,N\}} \omega(P_I^{\leq N}) \cdot \eta(x_{I,J})$$

with

$$x_{I,J} := \hat{\omega}_I(P_J^{\leq N}) = \frac{\omega(\sigma^{i/2}(P_I^{\leq N})P_J^{\leq N})}{\omega(P_I^{\leq N})} .$$

For a given I we interpret $J \mapsto x_{I,J}$ as a probability measure on the power set of $\{1,\dots,N\}$. For $l \in \{1,\dots,N\}$ and $e \in \{0,1\}$ we set

$$x_{I,l}^e := \hat{\omega}_I(P_l^e)$$

so that

$$x_{I,l}^1 = \sum_{J\subset\{1,\dots,N\}:l\in J} x_{I,J} \quad \text{and} \quad x_{I,l}^0 = \sum_{J\subset\{1,\dots,N\}:l\notin J} x_{I,J} .$$

In particular we have $x_{I,l}^0 + x_{I,l}^1 = 1$. Then by subadditivity of the entropy w.r.t. joins of partitions for all $I \subset \{1,\dots,N\}$

$$\sum_{l=1}^{N}\eta_F(x^1_{I,l})\equiv\sum_{l=1}^{N}\sum_{e=0}^{1}\eta(x^e_{I,l})\geq\sum_{J\subset\{1,\ldots,N\}}\eta(x_{I,J})$$

so that

$$rD^{r,N}_\lambda\leq\sum_{I\subset\{1,\ldots,N\}}\omega(P^{\leq N}_I)\cdot\sum_{l=1}^{N}\eta_F(x^1_{I,l})=\sum_{l=1}^{N}\sum_{e=0}^{1}\left(\sum_{I\subset\{1,\ldots,N\}}\omega(P^{\leq N}_I)\eta(x^e_{I,l})\right)\ .$$

Setting

$$\hat\omega^e_l(\cdot):=\frac{\omega(\sigma^{i/2}(P^e_l)\cdot)}{\omega(P^e_l)}\ ,$$

these states are the convex combinations

$$\hat\omega^1_l=\sum_{I'\subset\{1,\ldots,N\}-\{l\}}\frac{\omega(P^{\leq N}_{I'\cup\{l\}})}{\omega(P^1_l)}\,\hat\omega_{I'\cup\{l\}}\quad\text{and}\quad\hat\omega^0_l=\sum_{I'\subset\{1,\ldots,N\}-\{l\}}\frac{\omega(P^{\leq N}_{I'})}{\omega(P^0_l)}\,\hat\omega_{I'}$$

So by concavity of $x\mapsto\eta(x)$

$$\sum_{I\subset\{1,\ldots,N\}}\omega(P^{\leq N}_I)\eta(x^e_{I,l})\leq\sum_{e'=0}^{1}\omega(P^{e'}_l)\cdot\eta\left(\hat\omega^{e'}_l(P^e_l)\right)\ .$$

Thus we have the N-independent upper bound

$$rD^{r,N}_\lambda\leq\sum_{l=1}^{\infty}\sum_{e=0}^{1}\omega(P^e_l)\left(\eta\left(\hat\omega^e_l(P^e_l)\right)+\eta\left(\hat\omega^e_l(P^{1-e}_l)\right)\right)$$

for the entropy defect.

By convavity of η, $\eta(1)=0$ and $\eta'(1)=-1$ we have

$$\eta(x)\leq 1-x\qquad(x\in[0,1])\ .$$

On the other hand for $0<\beta<1$ and a suitable positive constant c'_β

$$\eta(x)\leq c'_\beta\ x^\beta\quad\text{and}\quad x\leq x^\beta\qquad(x\in[0,1])\ .$$

Thus, with $c_\beta:=2+c'_\beta$,

$$rD^{r,N}_\lambda\leq c_\beta\sum_{l=1}^{\infty}\sum_{e=0}^{1}\omega(P^e_l)\left(\hat\omega^e_l(P^{1-e}_l)\right)\right)^\beta\leq c_\beta\sum_{l=1}^{\infty}\sum_{e=0}^{1}\left(\omega(\sigma^{i/2}(P^e_l)P^{1-e}_l)\right)^\beta\ .$$

Finally the KMS identity (see Remarks 5.32 2. and 5.21 2.)

$$\omega\left(\sigma^{i/2}(P_l^1)P_l^0\right) = \omega\left(\sigma^{i/2}(P_l^0)P_l^1\right)$$

implies

$$rD_\lambda^{r,N} \leq 2c_\beta \sum_{l=1}^{\infty}\left(\omega(\sigma^{i/2}(P_l^1)P_l^0)\right)^\beta \quad .$$

Let $\hat{B}^\lambda$ be the operator associated with the restricted state $\omega\restriction_{\tilde{\Delta}_\lambda^{r,0}}$ according to Remark 5.32 2 and let ψ_l^λ be the eigenvectors of $\hat{A}_\lambda := \hat{A}\restriction_{\tilde{\Delta}_\lambda^{r,0}}$ and thus of $\hat{B}^\lambda$ itself. Then, using Remark 5.32.2,

$$\begin{aligned}
&\omega\left(\sigma^{i/2}(P_l^1)\cdot P_l^0\right) \\
&= \omega\left(\hat{a}(\hat{B}^{1/2}\psi_l^\lambda)P_l^0\hat{a}^\dagger(\hat{B}^{1/2}\psi_l^\lambda)\right) \\
&= \omega\left(\hat{a}\left((\hat{B}^{1/2}-(\hat{B}^\lambda)^{1/2})\psi_l^\lambda\right)P_l^0\hat{a}^\dagger\left((\hat{B}^{1/2}-(\hat{B}^\lambda)^{1/2})\psi_l^\lambda\right)\right) &(187)\\
&= (g_l,\hat{A}g_l)\cdot(\psi_l^\lambda,\hat{A}\psi_l^\lambda)-(g_l,\hat{A}\psi_l^\lambda)\cdot(\psi_l^\lambda,\hat{A}g_l) &(188)\\
&\leq (g_l,g_l)
\end{aligned}$$

with $g_l := (\hat{B}^{1/2}-(\hat{B}^\lambda)^{1/2})\psi_l^\lambda$.

Eq. (187) holds since 1) ψ_l^λ is an eigenvector of $(\hat{B}^\lambda)^{1/2}$, 2) by Def. (176) of $P_l^0 = \hat{a}(\psi_j^\lambda)\hat{a}^\dagger(\psi_j^\lambda)$, and 3) since $\hat{a}(\psi_j^\lambda)\hat{a}(\psi_j^\lambda)=0$.

We now write $\beta = 1-u\varepsilon$, with $u\in(0,\frac{1}{2})$ and $\varepsilon\in(0,1)$. Then trivially

$$\frac{r}{2c_\beta}D_\lambda^{r,N} \leq \sum_{l=1}^{\infty}\omega\left(\sigma^{i/2}(P_l^1)\cdot P_l^0\right)^{(1-\varepsilon)}\cdot\omega\left(\sigma^{i/2}(P_l^1)\cdot P_l^0\right)^{(1-u)\varepsilon}.$$

We use the Hölder inequality $\|fg\|_1 \leq \|f\|_p\cdot\|g\|_q$ with $p,q\geq 1$ and $1/p+1/q=1$, setting $p := 1/(1-\varepsilon)$, $q = 1/\varepsilon$. Thus

$$\frac{r}{2c_\beta}D_\lambda^{r,N} \leq \left(\sum_{l=1}^{\infty}\|(\hat{B}^{1/2}-(\hat{B}^\lambda)^{1/2})\psi_l^\lambda\|^2\right)^{1-\varepsilon}\cdot\left(\sum_{l=1}^{\infty}\omega\left(\sigma^{i/2}(P_l^1)\cdot P_l^0\right)^{1-u}\right)^{\varepsilon}. \quad (189)$$

The first sum in the right hand side of (189) is

$$\sum_{l=1}^{\infty}\|g_l\|^2 = \mathrm{Tr}\left(\chi_\lambda(\ \hat{B}^{1/2}-(\hat{B}^\lambda)^{1/2}\ )^2\chi_\lambda\right),$$

where χ_λ is the characteristic function of the volume $\tilde{\Delta}_\lambda^{r,0}$. So by Lemma 5.23 this gives a contribution of order

$$\left(\sum_{l=1}^{\infty}\|(\hat{B}^{1/2}-(\hat{B}^\lambda)^{1/2})\psi_l^\lambda\|^2\right)^{1-\varepsilon} \leq C_1\cdot\lambda^{(1-\varepsilon)\cdot(n-1)}$$

to (189).

The second sum in (189) is estimated using

$$\omega\left(\sigma^{i/2}(P_l^1)\cdot P_l^0\right) \leq (\psi_l^\lambda, \hat{A}\psi_l^\lambda) = (\psi_l^\lambda, \hat{A}_\lambda\psi_l^\lambda)$$

and the fact that ψ_l^λ is an eigenfunction of $\hat{A}_\lambda$. Thus

$$\sum_{l=1}^\infty \omega\left(\sigma^{i/2}(P_l^1)\cdot P_l^0\right)^{1-u} \leq \sum_{l=1}^\infty (\psi_l^\lambda, (\hat{A}_\lambda)^{1-u}\psi_l^\lambda) = \mathrm{Tr}\,((\hat{A}_\lambda)^{1-u}).$$

Now $\hat{A}_\lambda$ is defined as the restriction of $\hat{A}$ to $\tilde{\Delta}_\lambda^{r,0}$. As long as the scaling of velocity is smaller than the scaling of the region (that is, $r \leq \lambda$), the diameter scales like

$$\mathrm{diam}\left(\tilde{\Delta}_\lambda^{r,0}\right) \leq k\cdot\lambda$$

for a suitable $k > 0$. We can thus find a $k' \in \mathbb{N}$, $k' \geq k$ such that, after shifting $\tilde{\Delta}_\lambda^{r,0}$ with a lattice vector $\ell = \ell(\lambda) \in \mathcal{L}$, if necessary,

$$\tilde{\Delta}_\lambda^{r,0} + \ell \subset \Lambda_s\ ,$$

the parallelotopes $\Lambda_r \subset \mathbb{R}^n$ being defined in (147) and $s := k'[\lambda] \in \mathbb{N}$. The $\mathcal{L}$-invariance of the state guarantees that our estimate is unaffected by the shift. Moreover, we have the operator inequality

$$\chi_{(\tilde{\Delta}_\lambda^{r,0}+\ell)}\hat{A}\chi_{(\tilde{\Delta}_\lambda^{r,0}+\ell)} \leq \chi_{\Lambda_s}\hat{A}\chi_{\Lambda_s}$$

which by monotonic increase of $x \mapsto x^{1-u}$ and positivity of both operators implies

$$\left(\chi_{(\tilde{\Delta}_\lambda^{r,0}+\ell)}\hat{A}\chi_{(\tilde{\Delta}_\lambda^{r,0}+\ell)}\right)^{1-u} \leq \left(\chi_{\Lambda_s}\hat{A}\chi_{\Lambda_s}\right)^{1-u}.$$

Thus

$$\mathrm{Tr}\,((\hat{A}_\lambda)^{1-u}) \leq \mathrm{Tr}\,((\chi_{\Lambda_s}\hat{A}\chi_{\Lambda_s})^{1-u}).$$

But for $(1-u)\cdot(1+2/n) > 1$

$$\lim_{r\to\infty}\frac{\mathrm{Tr}\,\left((\chi_{\Lambda_r}\hat{A}\chi_{\Lambda_r})^{1-u}\right)}{|\Lambda_r|} = \sum_{m=1}^\infty\int_{\mathbb{T}^*}\rho(m,k)^{1-u}\frac{d^nk}{(2\pi)^n} < \infty.$$

The equality is shown by the same argument leading to the limit mean entropy formula (148) for parallelograms. The finiteness of the right hand expression is shown like the finiteness (143) of $s(\omega)$, observing that by our assumption (120) on ρ

$$\sum_{m=1}^{\infty} \int_{\mathbb{T}^*} \rho(m,k)^{1-u} \frac{d^n k}{(2\pi)^n} \leq C \sum_{m=1}^{\infty} m^{-\alpha(1-u)} < \infty.$$

So the second term in (189) is bounded by

$$\left(\sum_{l=1}^{\infty} \omega \left(\sigma^{i/2}(P_l^1) \cdot P_l^0 \right)^{1-u} \right)^{\varepsilon} \leq C_2 \lambda^{n\varepsilon}$$

which together gives an upper estimate

$$\frac{r}{2c_\beta} D_\lambda^{r,N} \ \leq \ C_1(\varepsilon) C_2(\varepsilon) \cdot \lambda^{n-1+\varepsilon}$$

for arbitrarily small $\varepsilon > 0$. $\square$

Thus we conclude with

Proposition 5.35 *For $v \in \mathcal{L}$ the local dynamical entropy of the shift has the lower bound*

$$\lambda^{1-n} \cdot h_{\omega,\lambda B}(\alpha_v) \geq s(\omega) \cdot |\mathrm{Pr}_v(B)| \cdot |v| \ .$$

Proof. We use Lemma 5.31 in order to get a lower bound for the local entropy $h_{\omega,\lambda B}(\alpha_v)$ of the shift. Note that by that lemma

$$h_{\omega,\lambda B}(\alpha_v) \geq \lim_{T \to \infty} E_\lambda^{r,N}(T) - D_\lambda^{r,N} \tag{190}$$

for all N and r. However, the estimate reduces to the trivial statement

$$h_{\omega,\lambda B}(\alpha_v) \geq 0$$

if $r \gg \lambda$, whereas the D-term can only be made small if $r \gg 1$. Thus we couple $r := r(\lambda)$ to λ so that $1 \ll r \ll \lambda$.

In Lemma 5.33 the E-term is related to von Neumann entropy: For $\varepsilon > 0$ and $N \geq N_0(\varepsilon)$

$$E_\lambda^{r,N}(T) \geq \frac{1}{T} S \left(\omega \restriction_{\bigcup_{t=0}^{T-1} \tilde{\Delta}_\lambda^{r,t}} \right) - \varepsilon. \tag{191}$$

By Def. (170) of $\tilde{\Delta}_\lambda^{r,t}$ for $T > t_0'$ the region

$$X(\lambda, r) := B_\lambda^{r,<T} \setminus \bigcup_{t=0}^{T-1} \tilde{\Delta}_\lambda^{r,t} \subset \mathbb{R}^n$$

becomes independent of T. The size of this region is of order

$$|X(\lambda, r)| = \mathcal{O}(\lambda^n),$$

using the inclusions $X(\lambda, r) \subset B_\lambda^{r,<t'_0} \subset B_\lambda^{<t_0+1}$ (since $t'_0 = [t_0/r] + 1$) and the volumes estimate (165) with the def. $t_0 := [\lambda \cdot \mathrm{diam}(B)/|v|] + 1$.

By subadditivity of S we have

$$S\left(\omega\restriction_{\bigcup_{t=0}^{T-1}\tilde{\Delta}_\lambda^{r,t}}\right) \geq S(\omega\restriction_{B_\lambda^{r,<T}}) - S(\omega\restriction_{X(\lambda,r)}). \tag{192}$$

Another application of (165) gives us by the van Hove property (171) and Prop. 5.25

$$S(\omega\restriction_{B_\lambda^{r,<T}}) = \left(rT \cdot |v| \cdot \lambda^{n-1} \cdot \left(|\mathrm{Pr}_v(B)| + o(\lambda^0)\right) + \mathcal{O}(\lambda^n)\right) \cdot s(\omega). \tag{193}$$

The a priori upper bound (153) for von Neumann entropy gives us

$$S(\omega\restriction_{X(\lambda,r)}) = \mathcal{O}(\lambda^n). \tag{194}$$

Putting (192), (193) and (194) together, and performing the time $T \to \infty$ limit, we get for the first term in (190)

$$\lim_{T\to\infty} E_\lambda^{r,N}(T) \geq |v| \cdot \lambda^{n-1} \cdot \left(|\mathrm{Pr}_v(B)| + o(\lambda^0)\right) \cdot s(\omega) - \varepsilon.$$

We make ε vanish by performing the $N \to \infty$ limit. Finally this gives the result

$$\lim_{\lambda\to\infty} \lambda^{1-n} \lim_{N\to\infty} \lim_{T\to\infty} E_\lambda^{r,N}(T) \geq |v| \cdot |\mathrm{Pr}_v(B)| \cdot s(\omega).$$

In the $\lambda \to \infty$ limit with $1 \ll r \ll \lambda$ the contribution

$$\lim_{\lambda\to\infty} \lambda^{1-n} \lim_{N\to\infty} D_\lambda^{r,N}$$

vanishes, using Lemma 5.34. □

A The Classical Discretized Electron Gas

Similar to [35] we consider now a caricature of the quantum electron gas which is classical in the sense that the C^*–algebra is one of functions on a phase space, but quantum in the sense that this phase space is discretized, the discretization depending implicitly on $\hbar$.

In fact we have a family of these caricatures, the elements being indexed by r and connected with the sublattices $r\mathcal{L}$. The C^*–algebras of these classical discretized electron gases will then turn out to coincide with maximal Abelian subalgebras $\mathcal{A}^r \subset \mathcal{A}$ generated by $\hat{a}^\dagger(\phi^r_{s,l})\hat{a}(\phi^r_{s,l})$ and $\hat{a}(\phi^r_{s,l})\hat{a}^\dagger(\phi^r_{s,l})$.

Below we introduce a family $r \mapsto H^r$ of operators converging in norm resolvent sense to H. Their Bogoliubov automorphism

$$\alpha_{r^2 H^r} : \mathcal{A} \to \mathcal{A}$$

restricts to $\mathcal{A}^r$.

Since the potential is also $r\mathcal{L}$-periodic, we obtain a decomposition of each original band into r^n subbands. However, in order not to introduce additional points of non-analyticity of the band functions, we do not order these subbands with increasing energy. Instead we remember that the Brillouin zone $\mathbb{T}^*$ can be identified with a domain of the form

$$\left\{ k \in \mathbb{R}^{n,*} \;\middle|\; k = \sum_{j=1}^{n} x_j \ell_j^*,\ x_j \in [0,1) \right\},$$

$\ell_1^*, \ldots, \ell_n^* \in \mathbb{R}^{n,*}$ being the basis dual ($\ell_j^*(\ell_k) = 2\pi\delta_{jk}$) to a basis $\ell_1, \ldots, \ell_n \in \mathbb{R}^n$ of $\mathcal{L}$. Then we define the subbands E_s^r of E_m using the r^n subsets

$$\left\{ k \in \mathbb{R}^{n,*} \;\middle|\; k = \sum_{j=1}^{n} x_j \ell_j^*,\ x_j \in [a_j/r, (a_j+1)/r) \right\},$$

indexed by $a := (a_1, \ldots, a_n)$, $a_j \in \{0, \ldots, r-1\}$. We order the bands by energy, and the subbands lexicographically w.r.t. a, so that E_s^r is a subband of E_m if $r^2(m-1) < s \leq r^2 m$.

We denote the Wannier functions of the sublattice $r\mathcal{L}$ by $\phi_{s,\ell}^r$. They are centered in space near $\ell \in r\mathcal{L}$, their delocalisation in configuration space growing asymptotically linearly with r. But as the sizes of the subbands are bounded above by λ/r, λ being the Lipschitz constant of the original band, and the band function is real-analytic, up to a measure zero set, the variation of the group velocities $\hbar^{-1}\nabla_k E_s^r(k)$ in those subbands which do not contain a point of nonanalyticity is of the order r^{-1}.

The set of nonanalyticity of E_m is an analytic variety of degree $\leq n-1$ (see [52]) in the Brillouin zone $\mathbb{T}^*$. Thus the subbands which meet that measure zero set are of density zero (compared to their total number r^n) as $r \to \infty$.

Conversely the group velocity of a density one subset of *nice* subbands has a variation smaller than C/r as $r \to \infty$.

We now attribute to the subbands certain mean group velocities, starting with the true mean

$$\bar{v}_s^r := \int_{\mathbb{T}^{*,r}} \hbar^{-1} \nabla_k E_s^r(k) dk / |\mathbb{T}^{*,r}|.$$

We want instead a velocity vector which is rational w.r.t. the lattice $\mathcal{L}$. Let $L = (\ell_1, \ldots, \ell_n)$ be the matrix composed of a basis of $\mathcal{L}$

Then the discretization

$$\hat{v}_s^r := r^{-1} L \left[r L^{-1} \bar{v}_s^r \right], \tag{195}$$

$[\cdot]$ denoting the componentwise integral part, is $\mathcal{L}$-rational, the denominators dividing r, and $\|\hat{v}_s^r - \bar{v}_s^r\| \leq \sqrt{n}\|L\|/r$.

So there exists an r-independent constant $c \equiv c(m) > 0$ such that for the nice subbands of the mth band

$$\max_{k \in \mathbb{T}^{n,*}} \left| \hbar^{-1} \nabla_k E_s^r(k) - \hat{v}_s^r \right| \leq c/r.$$

Instead of considering directly the Schrödinger operator

$$H_\hbar = U^{-1} \int_{T^{*,r}}^{\oplus} H_\hbar(k) dk \; U$$

with

$$H_\hbar(k) = \sum_{s=1}^{\infty} E_s^r(k) P_{s,k}^r,$$

we consider its approximation

$$H_\hbar^r := U^{-1} \int_{T^{*,r}}^{\oplus} H_\hbar^r(k) dk \; U \tag{196}$$

with

$$H_\hbar^r(k) := \sum_{s=1}^{\infty} \left(E_s^r(0) + \hbar \hat{v}_s^r \cdot k \right) P_{s,k}^r.$$

The useful property of the Hamiltonian $H_\hbar^r$ is that its time evolution permutes the Wannier functions:

$$\exp\left(-i H_\hbar^r t/\hbar\right) \phi_{s,l}^r = \exp(-i E_s^r(0) t/\hbar) \phi_{s,l+t\hat{v}_s^r}^r \tag{197}$$

if $t\hat{v}_s^r \in r\mathcal{L}$, as can be seen from Def. (196). The latter condition holds certainly true if t is a multiple of r^2.

We consider the one-particle classical dynamical system

$$(P^r, \Sigma^r, \mu^r, \Phi^r)$$

whose phase space $P^r := \mathbb{N} \times r\mathcal{L}$ enumerates the Wannier functions of the sublattice, the σ–algebra Σ^r being the power set of P^r. The ℓ-independent measure $\mu^r(s,\ell)$ of a phase space point $(s,\ell) \in P^r$ is given by the expectation

$$\mu^r(s,\ell) := \omega(\hat{a}^\dagger(\phi^r_{s,\ell})\hat{a}(\phi^r_{s,\ell})) = \tilde{\rho}^r_s(0) \tag{198}$$

of $\phi^r_{s,l}$, see (125). The motion $\Phi^{r,t} : P^r \to P^r$, at times $t \in \mathbb{Z}$ is defined by

$$\Phi^{r,t}(s,l) := (s, l + tr^2 \hat{v}^r_s).$$

Here we rescaled time by a factor r^2 in order to stay in accordance with (197).

The many–particle system is described as a Poisson system in the sense of Def. (5.12) built over $(P^r, \Sigma^r, \mu^r, \Phi^r)$. However, the Poisson construction automatically takes the Pauli principle into account, since the one–particle phase space P^r is discrete (and thus the non-atomicity assumption does not hold). That is, we consider

$$(\overline{P^r}, \overline{\Sigma^r}, \overline{\mu^r}, \overline{\Phi^r})$$

with multi–particle phase space $\overline{P^r} := \{A \subset P^r\}$. $A \in \overline{P^r}$ is interpreted as the set of phase space cells occupied by electrons. We set

$$\overline{\mu^r}\left(\mathcal{P}_{(A,B)}\right) := \prod_{a \in A} \mu^r(a) \cdot \prod_{b \in B} (1 - \mu^r(b)).$$

The non–interacting dynamics is given by

$$\overline{\Phi^r}^{\,t}(A) := \{\Phi^{r,t}(x) \mid x \in A\} \qquad (A \in \overline{P^r}).$$

The C^*-algebra $C(\overline{P^r})$ of phase space functions is generated by the orthogonal projections

$$\mathcal{P}_{(A,B)} \in C(\overline{P^r}),$$

indexed by finite disjoint subsets $A, B \subset P^r$, whose value at a phase space point $C \in \overline{P^r}$ is given

$$\mathcal{P}_{(A,B)}(C) := \begin{cases} 1, & A \subset C, B \cap C = \emptyset \\ 0, & \text{otherwise} \end{cases}.$$

So $\mathcal{P}_{(A,B)}(C) = 1$ iff the phase space region A is fully occupied by electrons, whereas there is no electron in B.

We define the isomorphism

$$\mathcal{I}^r : C(\overline{P^r}) \to \mathcal{A}^r$$

on the projections by

$$\mathcal{I}^r\left(\mathcal{P}_{(A,B)}\right) := \prod_{(s,\ell)\in A} \hat{a}^\dagger(\phi^r_{s,\ell})\hat{a}(\phi^r_{s,\ell}) \prod_{(s',\ell')\in B} \hat{a}(\phi^r_{s',\ell'})\hat{a}^\dagger(\phi^r_{s',\ell'})$$

and then extend linearly. Here the orthonormality property of the Wannier functions $\phi^r_{s,\ell}$ is used.

As $r \to \infty$, the measure $\overline{\mu^r}$ becomes more and more related to the restriction of the state ω to $\mathcal{A}^r$. This may be seen as follows:
The expression

$$A = \sum_{s\in\mathbb{N}} \sum_{\ell_1,\ell_2\in r\mathcal{L}} \tilde{\rho}^r_s(\ell_1-\ell_2)|\phi^r_{s,\ell_1}\rangle\langle\phi^r_{s,\ell_2}|$$

with the Fourier coefficients

$$\tilde{\rho}^r_s(\ell) := \int_{\mathbb{T}^{*,r}} \exp(+ik\cdot\ell)\rho^r(s,k)\frac{dk}{|\mathbb{T}^{*,r}|} \qquad (\ell \in r\mathcal{L})$$

shows that, similar to (125) the two-point function

$$\omega\left(\hat{a}^\dagger(\phi^r_{s_1,\ell_1})\hat{a}(\phi^r_{s_2,\ell_2})\right) = \delta_{s_1,s_2}\cdot\tilde{\rho}^r_s(\ell_1-\ell_2). \tag{199}$$

Now if we assume ρ to be smooth (C^1 suffices here), then by partial integration the non-zero Fourier coefficients are seen to decay:

$$\tilde{\rho}^r_s(r\ell) = \mathcal{O}(r^{-1}), \qquad (\ell \in \mathcal{L}\setminus\{0\}),$$

whereas $\tilde{\rho}^r_s(0)$ is bounded below by $\min_{k\in\mathbb{T}^*}\rho(m,k)$ if s enumerates a subband of band m.

The higher moment formula (4) for the quasifree state ω together with (199) then shows as $r \to \infty$ that

$$\overline{\mu^r}\left(\mathcal{P}_{(A,B)}\right) \sim \omega\left(\mathcal{I}^r\left(\mathcal{P}_{(A,B)}\right)\right).$$

A finite phase space region $R \subset P^r$ carries an $2^{|R|}$–dimensional subalgebra $\mathcal{A}_R \subset \mathcal{A}^r$ generated by the family $\{\mathcal{P}_{(A,R-A)} \mid A \subset R\}$ of projections. Clearly

$$\mathcal{A}_{R_1} \vee \mathcal{A}_{R_2} = \mathcal{A}_{R_1\cup R_2}.$$

The entropy of such a partition equals

$$S_{\overline{\mu^r}}(\mathcal{A}_R) = \sum_{x\in R} \eta_F(\mu^r(x)). \tag{200}$$

Since the algebra $\mathcal{A}^r$ is Abelian, the CNT and KS definitions of dynamical entropy coincide and can be easily calculated by lattice counting.

In particular for a phase space region

$$R := \{(s,\ell) \in P^r \mid \ell \in B\}$$

over a *convex* observation region B one has for the automorphism

$$\sigma^r := \alpha_{r^2 H^r} \restriction_{\mathcal{A}^r}$$

the expression

$$h_{\overline{\mu^r}}(\sigma^r, \mathcal{A}_R) = S_{\overline{\mu^r}}(\mathcal{A}_{R\setminus\Phi^{r\,1}(R)}), \tag{201}$$

since by Remark 5.27 one has the geometrical contraction

$$R \setminus \left(\cup_{t=1}^n \Phi^{r,t}(R)\right) = R \setminus \Phi^{r,1}(R). \tag{202}$$

The r.h.s. of (201) can then be calculated using (200).

Non-convex region B can also be treated, although then more effort is needed.

The above classical caricature of the Fermi gas can (at least) be used as a testing ground for ideas which one would like to apply to the non-Abelian case.

One idea to prove our conjectured formula (134) for the local entropy of the Fermi gas is the following. The automorphisms α_H and α_{H^r}, $r \in \mathbb{N}$ all commute, since the one-particle Hamiltonians H and H^r have this property. So **if** a triangle inequality

$$h_{\omega,B}(\alpha_1 \circ \alpha_2) \leq h_{\omega,B}(\alpha_1) + h_{\omega,B}(\alpha_2) \tag{203}$$

for commuting automorphisms would hold, we could estimate (using time inversion invariance)

$$|h_{\omega,B}(\alpha_H) - h_{\omega,B}(\alpha_{H^r})| \leq h_{\omega,B}(\alpha_H \circ \alpha_{-H_r}).$$

It is known (see Sinai [43]) that (203) does not hold in general.

For our classical caricature one can prove (203) using (202) if B is convex.

However as the following example shows, no weakened form $h_{\omega,B}(\alpha_1 \circ \alpha_2) \leq C(h_{\omega,B}(\alpha_1) + h_{\omega,B}(\alpha_2))$ of (203) with $C \geq 1$ holds for general non-convex B.

Example. By a theorem of Hurwitz there exist irrational numbers $\xi \in (0,1)$ which are badly approximable by rationals in the sense that for $c > 0$ small there exists no rational approximation p/q with

$$\left|\xi - \frac{p}{q}\right| \leq \frac{c}{q^2}.$$

The best example is the golden mean $\xi = \frac{1}{2}(\sqrt{5}-1)$.

We now consider planar shifts with velocities $v_1 := \binom{1}{0}$ and $v_2 := \binom{0}{\xi}$ and regions

$$B_N := \sum_{l_1,l_2=1}^{N} D_{(l_1,l_2)}(r)$$

with $r := c/(\sqrt{8}N)$, where $D_a(r)$ is the disk of radius r centered at $a \in \mathbb{R}^2$.

Now the shadow of B_N in the v_1– and in the v_2–direction is of size $2rN$. In the v_1+v_2–direction it is of size $2rN^2$, since by the above property of ξ no disk shadows any other disk.

Thus the entropy for the shift in the v_1+v_2–direction is (at least, since the speed is augmented) N times larger then each of the entropies in the v_1– and v_2–direction.

This counterexample shows that one needs good geometrical control if one wants to compare two time evolutions.
Another idea for proving formula (134) is to compare the algebras

$$\alpha_H^t(A), \qquad (A \subset \mathcal{A}(\lambda B))$$

at time t with the algebra C^t generated by the set of Wannier functions

$$\left\{\phi_{s,\ell}^r \mid s \in \mathbb{N}, \ell \in r\mathcal{L} : \ell - t\hat{v}_s^r \in \lambda B\right\} \tag{204}$$

for some r with $1 \ll r \ll \lambda$ (technically one introduces an energy cutoff, use an enlarged region λB_ε in (204) etc.).

Then as λ and r go to infinity, one expects a δ-inclusion of the algebra $\alpha_H^t(A)$ by C^t, since the deviation of the group velocity $\hbar^{-1}\nabla_k E_s(k)$ from the mean velocity $\hat{v}_s^r$ on the subbands with Brillouin zone $\mathbb{T}^{*,r}$ becomes smaller so that the direction of the moving particle is fixed with higher precision.

The basic idea here is to have some algebraic version of phase space microlocalization.

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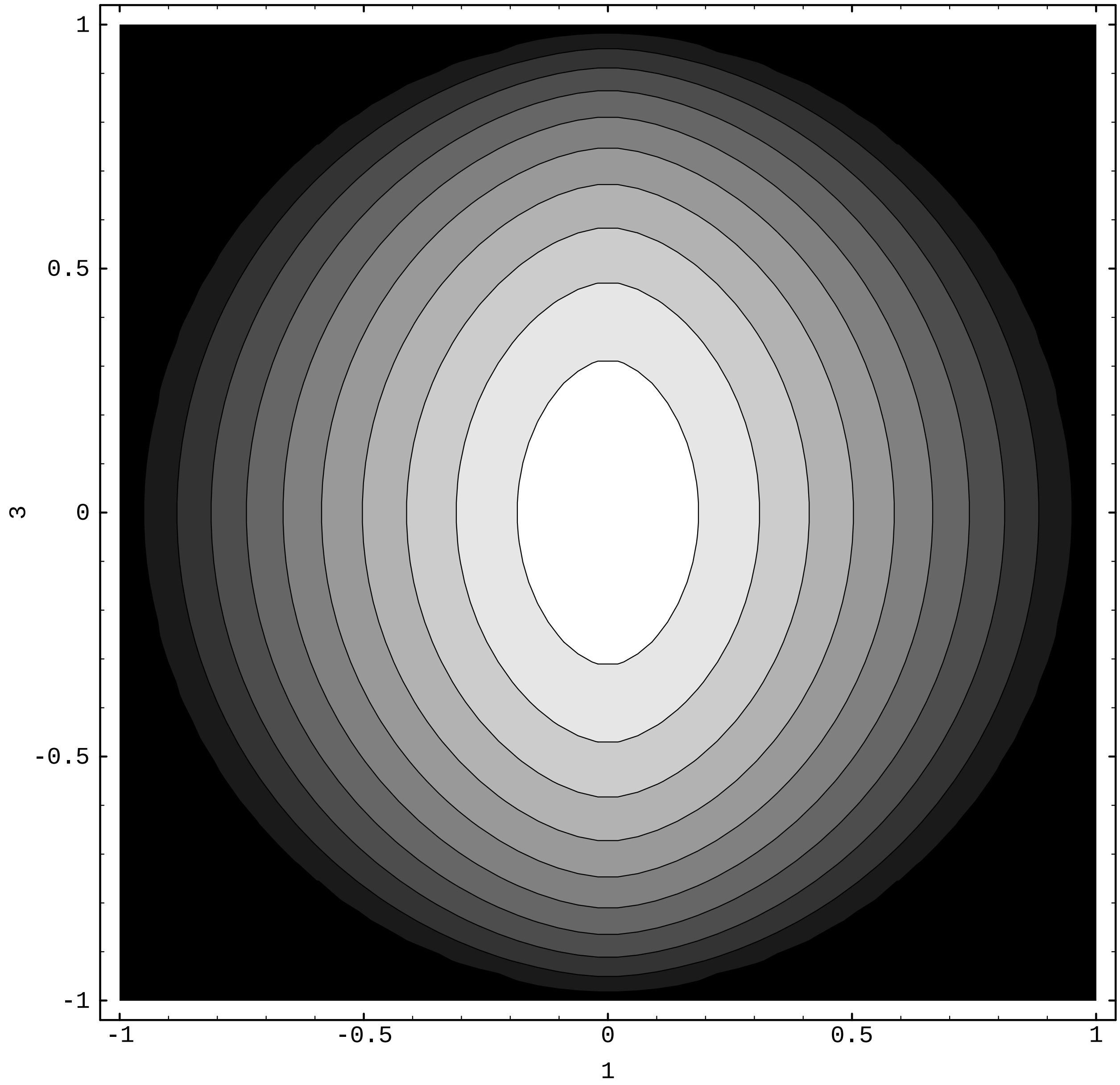

Figure 1: Entropy of the subalgebra **A** for a spin $\frac{1}{2}$ particle as a function of the parameters b_1 and b_3 of the density matrix $\hat{\rho}_{\vec{b}} = \frac{1}{2}(\hat{\mathbb{1}} + \vec{b} \cdot \vec{\sigma})$, with $b_2 = 0$