Entropy production in a quantum Kac model

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10 July 2006

1 von Neumann entropy

von Neumann defined the entropy $S(\rho)$ of a quantum system in the state [=density operator] ρ to be

$$S(\rho) := -k_B \mathsf{tr}[\rho \log \rho]. \tag{1}$$

He knew that, when $\rho \mapsto \rho(t)$ is the dynamics given by unitary transformations of ρ, then $S(t) := S(\rho(t))$ is independent of time. The same thing happens in classcal dynamics for the differential entropy defined as

$$S_c(\rho) = -k_B \int_\Gamma \rho(q,p) \log \rho(q,p) d^n p d^n q. \tag{2}$$

Here, Γ is the phase space of n degrees of freedom, and ρ is a classical probability on Γ; the dynamics $\rho \mapsto \rho(t)$ is given by Hamilton's equations. It is Liouville's theorem, that $d^n p d^n q$ is invariant under Hamiltonian motion, that causes S_c to remain invariant under time-evolution.

Lebowitz argued as follows; macroscopically we measure very few variables. Since entropy is associated with uncertainty, the entropy we detect omits all the uncertainty associated with the variables we have omitted to measure: thermodynamic entropy is much less than S, and could increase with time. However, it seems to me that, in that case, we lose the calculation from first principles, involving k_B, that is so successful in the theory of equilibrium. In his book, von Neumann suggested that thermodynamic entropy requires a different formula, related to the measurements made on the system. Such an entropy, say $s(t)$, might increase in time, due to the disturbances of the system, that occur in quantum measurement. The trouble is, how large an increase then seems to depend on what is being measured. Nevertheless, Maes, De Roeck, Jacobs and Netočńy take this up [1]. They define a quantum version of the Kac spin model, and show that the new entropy, $s(t)$, increases with time under the dynamics, with probability going to 1 as the volume of the system increases. We show that the increase in $s(t)$ under the Schrödinger dynamics, obtained by Maes et al. can be regarded as the increase in von Neumann's original entropy, S, under an approximate dynamics; indeed, $s(t)$ is equal to $S(t)/N$, where N is the number of spins.

Let $\mathcal{A} = \mathcal{M}^n$, the algebra of complex $n \times n$ matrices. Suppose that the dynamics, with discrete time, is given by a group of automorphisms

$$A \mapsto A(t), \qquad t \in \mathbf{Z}, A \in \mathcal{A}. \tag{3}$$

This dynamics can be transferred to the states by duality; a state ρ is a positive normalised linear form on $\mathcal{A}$, and its time evolution $\rho(t)$, is defined by

$$\rho(t)(A) := \rho(A(-t)). \tag{4}$$

Then it is well known that von Neumann's definition of entropy eq. (1) is constant in time. The trouble is, thermodynamics involves taking the thermodynamic limit, Volume, $V \longrightarrow \infty$; in the limit, the von Neumann entropy S diverges to infinity, and only the entropy-density S/V remains finite. We take the view that V should remain finite, but is large, and that S IS the correct thermodynamic entropy, but is evaluated for an approximate dynamics, $\rho \mapsto T(t)\rho$. The dynamics $T(t)$ is usually non-linear, and it increases the von Neumann entropy of the state.

In the recent paper on the quantum Kac model, [1], the authors show that a version of entropy does increase under the true dynamics, with a high probability, which converges to 1 as the volume tends to infinity. I show in this paper that one can rewrite their theorem to show that the von Neumann entropy, eq. (1), increases under a suitable approximate dynamics

$$\rho(t) \mapsto T^*\rho$$

involving changing only the macrovariables of the state, and is the limit (in probability) to infinite V of the true, invertible dynamics of the model.

2 Entropy Increase in Quantum Mechanics

In macroscopic physics, we have a large system, and can only observe the slow variables, the macrovariables. Let us use the word *thermodynamics* to refer to the limit dynamics of the macrovariables, of the model. Each expectation value of the macrovariables defines an approximate state of the system, which is the state of greatest entropy, eq. (1), having these values for the mean macrovariables. This approximate state cannot be separated from the true state $\rho(t)$, if we limit ourselves to the measurement of only the macrovariables. I claim that (in the quantum Kac model) the von Neumann entropy of eq. (1) of the approximate dynamics increases in time.

Acting on observables, a linear map T is said to be *stochastic* if

1. T is a positive map: T maps the cone of positive operators to itself;
2. TI=I.

A stochastic map does not necessarily increase the entropy; its iteration does not always converge. If we impose *detailed balance* on a stochastic map T, then its iteration often converges to the Gibbs state determined by the temperature arising in the detailed balance. I claim that this situation arises in isothermal theory, when a system is placed in a heat-bath. The free energy decreases, but the von Neumann entropy may increase or decrease. To increase (or leave the same) the entropy of a system requires a *bistochastic map*: a stochastic map T is bistochastic if it preserves the trace:

$$Tr(TA) = Tr(A) \qquad \text{for all } A \text{ of trace class.} \tag{5}$$

We throw the action of T onto the states by duality; we then have

Theorem 1 *if T is bistochastic, then*

$$S(T^*\rho) \geq S(\rho). \tag{6}$$

In the classical case we may assume that $\mathcal{A}$ is abelian; then Birkhoff's theorem says that every bistochastic map is a weighted mixture of permutations. In the quantum case one might think that any bistochastic map is a weighted mixture of automorphisms; this is not the case, but one gets a useful class of bistochastic maps by this method; for example, the finite sum

$$TA := \sum_\alpha \lambda_\alpha U_\alpha A U_\alpha^{-1} \tag{7}$$

where $0 < \lambda_\alpha < 1$ and $\sum_\alpha \lambda_\alpha = 1$ hold. In the Kac model, this arises as the mixture of two terms, one the identity automorphism and the other, one time-step of the dynamics given by the conjugation by $U = e^{iH}$, where H is the one-body energy.

Non-linear dynamics can also increase entropy. Consider a system of two particles of spin $\frac{1}{2}$. The algebra of observables is then

$$\mathcal{A} = \mathcal{M}^4 = \mathcal{M}^2 \otimes \mathcal{M}^2. \tag{8}$$

The general state ρ of $\mathcal{A}$ will have entanglement between the spins. These are determined by the *marginal states*

$$\rho_1 := Tr_2\rho \text{ and } \rho_2 := Tr_1\rho. \tag{9}$$

The product state

$$Q\rho := \rho_1 \otimes \rho_2 \tag{10}$$

maximises the von Neumann entropy $S(\rho)$, subject to these values, eq. (9) of its marginals. The map $\rho \mapsto Q\rho$ is non-linear in ρ; it ignores any correlations between the two particles.

For their quantum Kac model, Maes et al. show that the macroscopic dynamics is, in the limit $V \to \infty$ probably given by the bistochastic dynamics of the spin described by a 2×2 density operator σ,

$$T\sigma := (1-\mu)\sigma + \mu U\sigma U^{-1} \tag{11}$$

followed by the tensor product $T\sigma \otimes \ldots \otimes T\sigma$ over the points of V.

3 The Quantum Kac Model

Kac introduced his ring model [2] to show how reversible dynamics can appear to show convergence to equilibrium for most initial states. A quantum version was constructed by de Roeck, Jacobs, Maes and Netočný [1].

The system consists of N atoms, each of spin $\frac{1}{2}$, situated on a ring. The Hilbert space is

$$\mathcal{H}_N = \otimes_{j=1}^N \mathbf{C}_j^2. \tag{12}$$

Fix a hermitian matrix $H = \boldsymbol{h} \cdot \boldsymbol{\sigma} \in \mathcal{M}^2$, the single-site Hamiltonian, and put $U = e^{iH}$. The energy E_N is given by

$$E_N := \sum_{i=1}^N I \otimes \ldots I \otimes H \otimes I \ldots \otimes I \tag{13}$$

where the factor H is in the i$^{\text{th}}$ position. The points $1, \ldots, N$ are placed on a ring; on the segment $(j, j+1)$ is a "scattering variable" ϵ_j, equal to 0 or 1. The configuration $\epsilon = \{\epsilon_1, \ldots, \epsilon_N\}$ does not change with time. We define the unitary matrix on $\mathbf{C}_j^2$ by

$$U_j^{\epsilon_j} := \exp i\epsilon_j H_j = \begin{cases} 1 \text{ for } \epsilon_j = 0 \\ U \text{ for } \epsilon_j = 1 \end{cases} \tag{14}$$

The ring is rotated by the unitary operator R on $\mathcal{H}$, defined by extending the isometric action on product vectors

$$R\left(\eta_1 \otimes \eta_2 \otimes \ldots \otimes \eta_N\right) = \left(\eta_N \otimes \eta_1 \otimes \ldots \otimes \eta_{N-1}\right). \tag{15}$$

One time-step in the dynamics is given by the unitary operator U_N on $\mathcal{H}_N$:

$$U_N := R \otimes_{j=1}^N U_j^{\epsilon_j}. \tag{16}$$

This commutes with the energy-operator, E_n given by eq. (13), which is therefore conserved. Note that the time variable is discrete, and does not need to go to infinity to get the increase in entropy.

The *slow variables* of the model are those of the form of a sum over sites

$$A_N := \sum_{j=1}^{N} I \otimes \ldots \otimes A \otimes \ldots \otimes I \tag{17}$$

for any $A \in \mathcal{M}^2$. When $A = \sigma_\alpha$, $(\alpha = x, y, z)$, then A_N is the total magnetisation; together with the identity, these are the thermodynamic variables.

4 Equilibrium

The energy E_N is conserved by the dynamics and the equilibrium is for example the micro-canonical distribution. Let $P_\pm$ be the projectors onto the eigenvalues $e_\pm$ of the one-body Hamiltonian H, and let $e \in [e_-, e_+]$. Let

$$\rho_e^N := \frac{1}{Z_e^N} \sum_{e_\pm} P_{e_1} \otimes \ldots \otimes P_{e_N}, \tag{18}$$

where the sum runs over all $e_\pm$ satisfying

$$Ne \leq \sum_j e_j < e_+ - e_- + Ne. \tag{19}$$

The average

$$\langle A_N \rangle_e^N := Tr(\rho_e^N A_N) \tag{20}$$

gives the mean of A_N in equilibrium; for example

$$\mathbf{m}_e = \lim_{N\to\infty} \frac{1}{N} \langle \mathbf{M}_N \rangle_e^N \tag{21}$$

is the mean magnetisation. The limit exists and equals

$$\mathbf{m}_e = e \frac{\mathbf{h}}{\|\mathbf{h}\|^2}, \tag{22}$$

which is proportional to the one-body energy.

5 The ϵ-limit

The results of the paper are for unexceptional choices of ϵ. Let $\mu \in (0,1)$ be chosen and put

$$\Omega_\mu^N := \left\{ \epsilon \in \{0,1\} | \sum_1^N \epsilon_j = [\mu N] \right\} \tag{23}$$

where $[\mu N]$ is the integer part of $\mu N + 1$. Ω_μ^N is thus the set of ϵ so that the fraction of active scatterers (those with $\epsilon_j = 1$) is about μ. The authors furnish Ω_μ^N with the uniform distribution, so that, as $C_{[N\mu]}^N$ is the number of points, we get

$$\mathbf{P}_\mu^N(\epsilon) = \left(C_{[N\mu]}^N \right)^{-1}. \tag{24}$$

Limits $N \to \infty$ will often involve this probability; let us say that a sequence of functions G_N on Ω_μ^N typically converges to the value g_μ, written as

$$\epsilon - \lim_{N\to\infty} G_N = g_\mu \tag{25}$$

if and only if

$$\lim_{N\to\infty} \mathbf{E}_{\mathbf{P}_\mu^N}\left[(G_N - g_\mu)^p\right] = 0, \qquad p = 1, 2. \tag{26}$$

In fact, ϵ is fixed, and is not random; but for a given mean value μ, if we can prove that G_N typically converges to g_μ, then the ϵ for which it does not are very rare. The authors show that $M_N^\alpha(t)$ is typically determined by $M_N^\alpha(t-1)$: the slow variables obey an autonomous dynamical law, which give a quantum stochastic process, with discrete time, on the algebra of the slow variables. The dynamics is not unitary, but is given by eq. (11). It does depend on ϵ, but for most choices of ϵ of mean μ, these equations depend only on μ, the average number of ones in ϵ.

6 The Marginals and Entropy

The time-dynamics U_N is unitary, and does not change the von Neumann entropy. The authors define a new entropy S_N,

$$S_N(\rho^N) := -N\,Tr[\nu^N \log \nu^N] \tag{27}$$

where

$$\nu^N = \frac{1}{N}\sum_1^N Tr_j[\rho^N]; \tag{28}$$

here, Tr_j is the reduced density matrix, a 2×2 matrix. This follows von Neumann's suggestion, of the change in entropy when the energy is measured, and it changes in time under the true dynamics as

$$\nu^N(t) = \frac{1}{N}\sum_1^N Tr_j[\rho^N(t)] \tag{29}$$

$$S_N(\rho^N(t)) = -N\,Tr[\nu^N(t)\log\nu^N(t)], \tag{30}$$

and if all goes well, which they show to be true for some technical conditions on the initial state:

$$s(t) = \epsilon - \lim_{N\uparrow\infty}\frac{1}{N}S_N(\rho^N(t)) \tag{31}$$

is an increasing entropy.

7 The Results

Let ρ_0^N obey some technical conditions. Then $\rho^N(t)$ obeys, for any continuous function f:

$$\epsilon - \lim_{N\uparrow\infty} Tr\left[f\left(\frac{M_N^\alpha}{N}\right)\rho^N(t)\right] = f\left(m^\alpha(t)\right) \tag{32}$$

with $m^\alpha(t)$ obeying the autonomous equation

$$\mathbf{m}_t = \mathbf{m}_e + \mathrm{Re}\left[\left(\mathbf{m}_0 - \mathbf{m}_e + i\frac{\mathbf{h}\times\mathbf{m}_e}{\|\mathbf{h}\|}\right)\left(1-\mu+\mu e^{i(e_+-e_-)}\right)^t\right] \tag{33}$$

This converges to $\mathbf{m}_e$, the value at equilibrium, as $t \to \infty$, if $\mu \neq 0, 1$. Eq(32) says that the limit of the mean of any function f of the slow variables is probably equal to the function f of the means.

The entropy equals

$$s(t) = -\frac{1 + \|\mathbf{m}_t\|}{2} \log\left(\frac{1 + \|\mathbf{m}_t\|}{2}\right) - \frac{1 - \|\mathbf{m}_t\|}{2} \log\left(\frac{1 - \|\mathbf{m}_t\|}{2}\right) \tag{34}$$

and increases in time.

8 My Point of View

We can interpret $S(t)$ as the von Neumann entropy of the approximate dynamics as follows. Start with ρ_0 obeying the technical conditions. Then apply the dynamics U^N, and compute the new value of the magnetisation. Change the state to the product of the one-body state with this magnetisation, divided by N. This state has a greater entropy than that of ρ_0, since it is the state of maximum entropy with the given total magnetisation. Now take *this approximate state* and compute its dynamics under U^N. This will be different from what we get from taking the true state at time 1 and applying U^N, but it will give rise to the same new value of $\mathbf{M}$, since (as was shown by the authors) the true value is (in the limit of large N) the same for all states having the previous value of $\mathbf{M}$. Proceed in this way. We get that the state we use has the same value of $\mathbf{M}$ as the true state; and its von Neumann entropy is exactly $Ns(t)$. Indeed, let μ be the average value of the "external field" ϵ. Then in one time step, the change in $s(t+1) - s(t)$ is the same as the if the average value of ϵ had acted at each site. That is

$$T\sigma = (1 - \mu)\sigma + \mu U \sigma U^{-1} \tag{35}$$

where σ is the one-site state, taken to be independent of time, and $U = e^{iH}$ is the unitary time evolution given by the energy operator. After this stochastic map, we then form the product state $T\sigma \otimes \ldots \otimes T\sigma$; its von Neumann entropy is $Ns(t+1)$. Thus, the von Neumann entropy of the approximate dynamics increases in time. Note that there is not enough mixing in the model for the microdynamics to approach the equilibrium state; indeed, the covariances between neighbouring spin vectors, do not converge to zero as $N \to \infty$.

My point of view is expounded in the book [3].

References

[1] De Roeck, W., Jacobs, T., Maes, C., Netočný, K., J. Phys. A, **36**, 11547-11559, 2003

[2] Kac, M., Ch 14, **Probability and Related Topics in Phys Sci**, Interscience, 1959

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