An extension of the Kac ring model

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Abstract

We introduce a unitary dynamics for quantum spins which is an extension of a model introduced by Mark Kac to clarify the phenomenon of relaxation to equilibrium. When the number of spins gets very large, the magnetization satisfies an autonomous equation as function of time with exponentially fast relaxation to the equilibrium magnetization as determined by the microcanonical ensemble. This is proven as a law of large numbers with respect to a class of initial data. The corresponding Gibbs-von Neumann entropy is also computed and its monotonicity in time discussed.

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1 Relaxation to equilibrium

The Kac ring model was introduced by Mark Kac to clarify how manifestly irreversible behaviour can be obtained from an underlying reversible dynamics, [2, 6, 8]. It explains via a simple model some of the conceptual subtleties in the problem of relaxation to equilibrium as for example are present in the derivation and the status of the Boltzmann equation for dilute gases. In particular, the Kac dynamics shares some basic features with a Hamiltonian time-evolution like being deterministic and dynamically reversible. In the present paper we extend that dynamics to a unitary evolution on a finite quantum spin system. Again, the dynamics remains far from realistic but it allows a precise formulation and discussion of some features of relaxation to equilibrium for a quantum dynamics. That is especially useful and relevant as, in the quantum domain, the problem of relaxation is beset with even greater conceptual difficulties. In our framework, relaxation to equilibrium becomes visible if one can select a small number of macroscopic variables that typically evolve via autonomous deterministic equations to take on values that correspond to equilibrium. Typical refers to a law of large numbers with respect to the initial data. Paradoxes are avoided by taking serious the fact that relaxation is a macroscopic phenomenon, involving a huge amount of degrees of freedom whose evolution is monitored over a realistic time-span. A more general introduction to this and various related problems can be found in the recent [7].

In section 2 we introduce the model and we state the basic result. Section 3 is devoted to a discussion of related issues. The proofs are postponed to the final section 4.

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2 Model and results

2.1 The model

Consider N sites on a ring (periodic boundary conditions). Between any two neighboring sites there is a fixed *scattering* mechanism to be specified below, and at each site, we find a spin 1/2 particle. Time is discrete and at each step the ring rotates in a fixed direction over one ring segment. Depending on the segment that each spin crosses, it is scattered to another state.

For the Hilbert space $\mathcal{H}_N$ we take the N-fold product of copies of $\mathbb{C}^2$, the state space at each site:

$$\mathcal{H}_N \equiv \bigotimes_{j=1}^{N} \mathbb{C}_j^2$$

with the standard inner product that defines the Hermitian conjugate for matrices denoted by the superscript *. We write the elements of $\mathcal{H}_N$ as vectors in $\mathbb{C}^{2N}$, denoted by η or η' with components η_j indicating the state of the spin at site j.

2.1.1 Dynamics and observables

We fix an arbitrary Hermitian matrix $H \in \mathbb{C}^{2\times 2}$, called single site Hamiltonian and we construct the unitary matrix

$$U \equiv e^{iH}, \;\; U^\star = e^{-iH} \tag{2.1}$$

To each segment on the ring connecting the two nearest neighbors $(j, j+1)$ there is associated a scattering variable $\epsilon_j \in \{0,1\}$. The configuration of scatterers is denoted by $\epsilon \equiv (\epsilon_1, \dots, \epsilon_N)$ and does not change in time. We define the unitary matrix $U_j^{\epsilon_j}$ on $\mathbb{C}_j^2$ as

$$U_j^{\epsilon_j} \equiv \begin{cases} \mathbb{1} & \text{for } \epsilon_j = 0 \\ U & \text{for } \epsilon_j = 1 \end{cases}$$

The superscript ϵ_j can thus be read as a power and $U_j^{\epsilon_j} = e^{i\epsilon_j H_j}$ with H_j a copy of H working on $\mathbb{C}_j^2$. This defines the scattering mechanism.

The rotation of the ring is implemented by the operation R on $\mathcal{H}_N$ which transforms every vector $\eta = (\eta_1, \eta_2, \dots, \eta_N)$ into

$$R\eta \equiv (\eta_N, \eta_1, \dots, \eta_{N-1}) \in \mathcal{H}_N$$

and $R^\star = R^{-1}$, rotation in the opposite direction. Combining that with the scattering mechanism finally gives rise to the unitary operator $U_N \equiv U_N(\epsilon)$ on $\mathcal{H}_N$ via

$$U_N \equiv R \bigotimes_{j=1}^{N} U_j^{\epsilon_j}$$

To be specific we look at positive times and the state at time $t = 1, 2, \dots$ is then obtained from the state $\eta_0 \in \mathcal{H}_N$ at time $t = 0$ from

$$\eta_t \equiv U_N(t)\, \eta_0 = U_N(t-1) U_N\, \eta_0$$

This unitary dynamics on the finite-dimensional $\mathcal{H}_N$ is rather simple. For many observables (like the total magnetization) the dynamics is entirely equivalent with leaving the spins in place and rotating instead the scatterers. We therefore work with the more convenient

$$U_N(t) = \bigotimes_{j=1}^{N} U_j^{k_j(\epsilon,t)} \tag{2.2}$$

with $k_j(\epsilon, t) \equiv \sum_{n=1}^{t} \epsilon_{j-n}$ (modulo N). The updating of the spins is independent modulo the fact that they may have a scattering mechanism in common.

The Hamiltonian is a sum of single site contributions,

$$H_N \equiv \sum_{j=1}^{N} H_j \tag{2.3}$$

with $H_j \equiv \mathbb{1} \otimes \ldots \otimes H \otimes \ldots \otimes \mathbb{1}$ (on the j-th site) and for concreteness, we decompose the single-site Hamiltonian in the Pauli basis

$$H = h_1\,\sigma_x + h_2\,\sigma_y + h_3\,\sigma_z = \vec{h}\cdot\vec{\sigma} \qquad\qquad 0 \neq \vec{h} \in \mathbb{R}^3 \tag{2.4}$$

The eigenvalues are $e_+ = \|\vec{h}\|$ and $e_- = -e_+$. (We can of course ignore adding a constant to this Hamiltonian.) Our observables are also built up by adding one-site contributions. We are given a Hermitian matrix $A \in \mathbb{C}^{2\times 2}$ and we construct the system operators

$$A_N \equiv \sum_{j=1}^{N} \mathbb{1} \otimes \ldots \otimes A \otimes \ldots \otimes \mathbb{1} \tag{2.5}$$

where the A is at the j-th position. We will consider the magnetization $M_N \equiv A_N$ defined through $A = \sigma_z$, the third Pauli matrix.
The restriction of looking only at one-site observables will be discussed in Section 3.4.

2.1.2 Equilibrium

The dynamics depends non-trivially on the scatterers but the equilibrium properties are independent of them. That is similar to the situation in the Boltzmann-Grad limit where the hard core matters dynamically but does not enter in the computations of energy or pressure.
Energy is conserved in the sense that the Hamiltonian commutes with the time evolution: $[U_N(t), H_N] = 0$.

Equilibrium is characterized by the microcanonical distribution. Let ψ_+, ψ_- be the two eigenvectors of H with eigenvalues $e_+ \geqslant e_-$ and spectral projectors P_{e_+} and P_{e_-} respectively. For arbitrary $e \in [e_-, e_+]$ we select an energy space by

$$P_e^N \equiv \frac{1}{Z_e^N} \sum_e P_{e_1} \otimes \ldots \otimes P_{e_N} \tag{2.6}$$

where, in $\sum_e$, we sum over all (e_j) with fixed $\sum_j e_j$ satisfying $Ne \leqslant \sum_j e_j < e_+ - e_- + Ne$; the normalization Z_e^N ensures that $\mathrm{Tr}[P_e^N] = 1$. Alternatively, we could have summed in (2.6) over all (e_j) with $\sum_j e_j/N$ in a certain interval around e and at the very end let the interval shrink to zero. The average

$$\langle A_N \rangle_e^N \equiv \mathrm{Tr}[P_e^N\, A_N] \tag{2.7}$$

for a Hermitian matrix A_N on $\mathcal{H}_N$ defines the (finite volume) microcanonical ensemble.

The (infinite volume) equilibrium magnetization corresponding to an energy e is then defined from (2.7) to be the limit

$$m_e \equiv \lim_{N\uparrow+\infty} \frac{1}{N} \langle M_N \rangle_e^N \tag{2.8}$$

This limit exists and can easily be computed: it equals

$$m_e = e\, \frac{h_3}{\|\vec{h}\|^2} \tag{2.9}$$

2.1.3 Initial data

Initial data are determined by a density matrix ρ_0^N on $\mathcal{H}_N$ and by the choice of the scatterers ϵ. Concerning the state of the spins, we keep in mind an initial preparation with a particular magnetization, not in equilibrium. Let Q_+ and Q_- be the projectors on spin up and spin down respectively, with $\sigma_z = Q_+ - Q_-$, to define

$$Q_m^N \equiv \sum_m Q_{m_1} \otimes \ldots \otimes Q_{m_N} \qquad\qquad m \in \{-1,+1\} \tag{2.10}$$

where, as in (2.6), in $\sum_m$, we sum over all (m_j) with fixed $\sum_j m_j$ satisfying $Nm \leqslant \sum_j m_j < 2 + Nm$. Equation (2.10) gives the projector on the magnetization space with magnetization converging to m as $N \uparrow +\infty$. A possible initial density matrix is then $(0 < d(m,N) < +\infty$ is a normalization)

$$\rho_0^N = \frac{1}{d(m,N)}\, Q_m^N \tag{2.11}$$

Another (but thermodynamically equivalent) choice would be the grand-canonical

$$\rho_0^N = \frac{1}{Z_N(\lambda)} \exp\big(\lambda M_N\big) \tag{2.12}$$

A more general class of initial density matrices ρ_0^N will be introduced at the beginning of section 2.2. Most important is that they satisfy a law of large numbers for observables of the form (2.5) and that the single site marginal remains well-defined in the thermodynamic limit.

Now the dynamics starts and the density matrix at time t is defined from (2.2):

$$\rho_t^N \equiv \rho_t^N(\epsilon) \equiv U_N(t)\rho_0^N U_N(t)^\star \tag{2.13}$$

and now also depends on the scatterers ϵ_j.
We are interested in the magnetization in ρ_t^N and in its limiting behavior as (first) $N \uparrow +\infty$ and (then) $t \uparrow +\infty$. In order to take these limits, we also need to specify the initial (and unchanging) condition of the scatterers. For this we introduce the set

$$\Omega_\mu^N \equiv \left\{ \epsilon \in \{0,1\}^N \,\middle|\, \sum_{j=1}^N \epsilon_j = \lceil \mu N \rceil \right\} \tag{2.14}$$

with $\lceil \mu N \rceil$ the smallest integer not smaller than μN. The constraint fixes the fraction of *active* scatterers to be about μ. The probability to select one particular ϵ in Ω_μ^N is uniform:

$$\mathbb{P}_\mu^N(\epsilon) \equiv \frac{1}{\binom{N}{\lceil N\mu \rceil}} \tag{2.15}$$

All limits will involve that probability distribution. We say that a sequence of functions G_N on Ω_μ^N typically takes the value g_μ, written

$$\epsilon\text{-}\lim_{N\uparrow+\infty} G_N = g_\mu \qquad \text{iff} \qquad \lim_{N\uparrow+\infty} \mathbb{E}_\mu^N[(G_N - g_\mu)^p] = 0, \quad p = 1, 2 \tag{2.16}$$

where the expectation refers to the probabilities (2.15). Via the Chebyshev inequality one can reformulate (2.16) as a statement about the fraction of scatterers in Ω_μ^N for which $G_N \simeq g_\mu$. The last $\simeq$ is made stronger if higher p's in (2.16) are obtained. For simplicity, we restrict us here to the average ($p = 1$) and to the variance ($p = 2$).

2.1.4 Entropy

To evaluate the Gibbs-von Neumann entropy as a function of time, we decompose the Hilbert space $\mathcal{H}_N$ in linear subspaces

$$\mathcal{H}_N = \bigoplus \mathcal{H}_\alpha^N \tag{2.17}$$

with $\mathcal{H}_\alpha^N \equiv Q_\alpha^N \mathcal{H}_N$ along the projections

$$Q_\alpha^N \equiv \sum_{\sum_j m_j = N\alpha} Q_{m_1} \otimes \ldots \otimes Q_{m_N}, \quad N\alpha = -N, -N+2, \ldots, N$$

on different eigenvalues of the magnetization M_N/N. We denote by d_α^N the dimension of $\mathcal{H}_\alpha^N$. The (quantum) entropy $S_N(\rho)$ of a density matrix ρ on $\mathcal{H}_N$ is, see e.g. [3]:

$$S_N(\rho) \equiv \sum_\alpha \mathrm{Tr}[Q_\alpha^N \rho] \log d_\alpha^N - \sum_\alpha \mathrm{Tr}[Q_\alpha^N \rho] \log \mathrm{Tr}[Q_\alpha^N \rho] \tag{2.18}$$

We insert $\rho = \rho_t^N$ from (2.13) and put, if the limit exists,

$$s(t) \equiv \epsilon\text{-}\lim_{N\uparrow+\infty} \frac{1}{N} S_N(\rho_t^N) \tag{2.19}$$

The more frequently considered von Neumann entropy -Tr $[\rho_t^N \log \rho_t^N]$ does not change in time and is therefore here less relevant.

2.2 Results

The conditions for our main result on the dynamics (2.13) are on the level of initial data, see section 2.1.3. We ask that ρ_0^N is a density-matrix that is dispersionless in the sense that for all observables (2.5) and for all continuous f

$$\lim_{N\uparrow+\infty} \left| \mathrm{Tr}\left[f\left(\frac{A_N}{N}\right) \rho_0^N \right] - f\left(\mathrm{Tr}\left[\frac{A_N}{N} \rho_0^N \right] \right) \right| = 0 \tag{2.20}$$

Furthermore, we need the existence of the thermodynamic limit of the system-averaged one-site marginal

$$\nu_0 \equiv \lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \mathrm{Tr}_j \left[\rho_0^N\right] \tag{2.21}$$

with Tr_j the reduced density matrix at site j. Finally, the sequence ρ_0^N must satisfy a technical condition. We write

$$\rho_0^N = \sum_{w=1}^{r(N)} \bigotimes_{j=1}^{N} \chi_{j,w}^N$$

the initial density matrix as a sum of products of 2×2 matrices and we assume that

$$\sup_{N\in\mathbb{N}} \sup_{\substack{w=1,..,r(N)\\ j=1,..,N}} \|\chi_{j,w}^N\| \equiv C < \infty \tag{2.22}$$

These three conditions are obviously satisfied by (2.12). That (2.20) is also satisfied for (2.11) needs an argument given in the example after the proof of Lemma 4.3.

The initial magnetization is denoted by $m_0 \equiv \mathrm{Tr}[\sigma_z \nu_0]$ and the equilibrium magnetization m_e is defined in (2.8). The initial energy e is found from $e \equiv \mathrm{Tr}[H\nu_0]$. Finally, we denote by α_0 an initial overlap between the Hamiltonian (2.4) and the magnetization:

$$\alpha_0 \equiv m_0 - m_e + \frac{1}{\|\vec{h}\|}(\mathrm{Tr}[H\nu_0\sigma_z] - h_3) \tag{2.23}$$

α_0 varies in a bounded complex domain but its real part always equals $\mathrm{Re}(\alpha_0) = m_0 - m_e$. Furthermore, $\alpha_0 = 0$ if and only if H and σ_z commute or H and ν_0 commute. If ν_0 is obtained from (2.11) or from (2.12), then $\alpha_0 = m_0 - m_e$ is real.

Theorem 2.1
For all continuous functions f and for initial ρ_0^N satisfying the above conditions,

$$\epsilon\text{-}\lim_{N\uparrow\infty} \mathrm{Tr}\left[f\left(\frac{M_N}{N}\right)\rho_t^N\right] = f\big(m_t\big) \tag{2.24}$$

with

$$m_t \equiv m_e + \mathrm{Re}\left(\alpha_0\big(1-\mu+\mu\exp[i(e_+ - e_-)]\big)^t\right) \tag{2.25}$$

In particular for $f(x) = x$, the magnetization

$$\lim_{t\uparrow+\infty} \epsilon\text{-}\lim_{N\uparrow+\infty} \frac{1}{N}\mathrm{Tr}\left[M_N\,\rho_t^N\right] = m_e \tag{2.26}$$

converges exponentially fast to its equilibrium value, for all $\mu \in (0,1)$ when $e_+ - e_-$ is not a multiple of 2π.
The entropy (2.19) equals

$$s(t) = -\frac{1+m_t}{2}\log\frac{1+m_t}{2} - \frac{1-m_t}{2}\log\frac{1-m_t}{2} \tag{2.27}$$

Similar to (2.21), we can also define the time-evolved version of ν_0, i.e.,

$$\nu_t \equiv \epsilon\text{-}\lim_{N\uparrow+\infty} \frac{1}{N}\sum_{j=1}^{N} \mathrm{Tr}_j \left[\rho_t^N\right] \tag{2.28}$$

and a corresponding overlap

$$\alpha_t \equiv m_0 - m_e + \frac{1}{\|\vec{h}\|}(\mathrm{Tr}[H\nu_t\sigma_z] - h_3) \tag{2.29}$$

We then have

Proposition 2.1

$$\alpha_t = m_0 - m_e + i\,\mathrm{Im}\left(\alpha_0\big(1-\mu+\mu\exp[-i(e_+ - e_-)]\big)^t\right) \tag{2.30}$$

Together, (2.25) and (2.30) constitute an autonomous set of equations, discussed in Section 3.3, in the sense that (m_t, α_t) determines (m_{t+1}, α_{t+1}) once we know $e, \vec{h}$ and μ.

3 Discussion

3.1 Kac ring model

The Kac ring model in [6], p.99, can be recovered by the appropriate choice of the Hamiltonian (2.4). Identifying $\eta_i = 1$ or $|\uparrow\rangle$ with a white ball and the state $\eta_i = -1$ or $|\downarrow\rangle$ with a black ball in the original ring model, the switching between a white and a black ball corresponds to a spin flip. This is accomplished by the single-site Hamiltonian (written out in the σ_z base):

$$H = \frac{\pi}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \qquad \Rightarrow \qquad U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which, up to an irrelevant constant, corresponds to the choice $\vec{h} = -(\frac{\pi}{2}, 0, 0)$ in (2.4). The eigenvalues of this Hamiltonian satisfy $(e_+ - e_-) = \pi$ and the equilibrium magnetization is $m_e = 0$. We start from randomly sampling the balls (or spins) with a fixed overall color (or magnetization) in (2.11) so that $\alpha_t = m_0$ for all t. Substitution in (2.25) yields:

$$m_t = m_0(1-2\mu)^t$$

That coincides with the relaxation formula in the original Kac model. It is interesting to observe that the relaxation to equilibrium gets slower for all the extensions that we have considered here.

3.2 Molecular chaos

The Stoßzahlansatz, or *repeated randomization* hypothesis consists in replacing the real dynamics by an effective dynamics in which the scattering mechanism is not kept fixed but gets replaced with an average. In that way, memory is being erased of where the scatterers are. Since the fraction of active scatterers equals μ, one would then conclude that in the dynamics the original density matrix on $\mathcal{H}_N$ is either copied with probability $(1-\mu)$ or is replaced with a scattered density matrix with probability μ. More precisely:

$$\Lambda^\star(\rho) \equiv (1-\mu)\rho + \mu\, V_N\, \rho\, V_N^\star \qquad\qquad V_N = U \otimes U \otimes \ldots \otimes U \tag{3.1}$$

defines a completely positive map (the quantum equivalent of a discrete time stochastic dynamics, see [1]), which is the dual of a map Λ. The unitary U should be substituted from (2.1). We will write Λ_t for the map Λ applied t times. Using this effective dissipative dynamics instead of the real unitary evolution (2.2), amounts to replacing the time evolution $U_N(t) \cdot U_N(t)^\star$ (depending on the scatterers ϵ_j) by $\Lambda_t^\star$ (only depending on μ) and expectations at time t become

$$\mathrm{Tr}\left[\Lambda_t(A_N)\ \rho_0^N\right]$$

Computations are now even simpler and one easily verifies that this approach reproduces the correct result (see Lemma 4.2):

$$\epsilon\text{-}\lim_{N\uparrow+\infty} \frac{1}{N}\,\mathrm{Tr}\left[M_N\,\rho_t^N\right] = \lim_{N\uparrow+\infty}\frac{1}{N}\,\mathrm{Tr}\left[\Lambda_t(M_N)\ \rho_0^N\right] = \mathrm{Tr}\left[\Lambda_t(\sigma_z)\nu_0\right] \tag{3.2}$$

Similarly, for the entropy

$$\epsilon\text{-}\lim_{N\uparrow+\infty} \frac{1}{N}\,S_N\left(\rho_t^N\right) = \lim_{N\uparrow+\infty} S_N\left(\Lambda_t^\star(\rho_0^N)\right) \tag{3.3}$$

However, this substitution with Λ_t is false if the observable under consideration is not a macroscopic observable of the form (2.5). Hence, we do not have propagation of molecular chaos in the sense that here the state does not remain a product state when started from one.

One can further ask whether there is propagation of constrained equilibrium in the sense that, when starting from (2.11), the density matrix ρ_t^N at later times t would approximately be of the same form (2.11) with m replaced by m_t. The answer is again no because even though α_0 is now real (and equal to m_0), α_t need not be real. That means that the microcanonical states (giving equal probability to any microstate that realizes a certain magnetization) do not propagate in time, but get infected with off-diagonal elements. In that sense our model is more quantum than could be expected in the real world where a source of decoherence would eliminate the off-diagonal elements.

As stated in Theorem 2.1, as in the original Kac ring model (or as for the rigorous derivation of the Boltzmann equation), one really does not need this assumption of molecular chaos to get relaxation. It is replaced with statistical assumptions on the level of the initial conditions for the scatterers — they are typical with respect to the probability (2.15) — and for the spins — they are e.g. randomly sampled with a fixed magnetization in (2.11). In that case we think of both the η (wavefunction) ànd the ϵ (classical scattering centers) as dynamical variables.

3.3 Autonomous equation and $H-$theorem.

If α_0 is real (e.g. in case of (2.11) or (2.12)), then knowing m_t gives m_0 and hence we can predict m_{t+1} from m_t from the knowledge of $\mu, \|\vec{h}\|$ and the energy e. (If $h_3 = 0$ in (2.4), then $m_e = 0$ and we don't even need to know e.) In that case (α_0 real) the relaxation formula (2.25) for m_t can be called autonomous. That remains also generally true when $e_+ + e_-$ is an integer multiple of π because $\mathrm{Re}(\alpha_t) = m_0 - m_e$ always. In other cases however we also need to know the initial overlap $\mathrm{Tr}[H\nu_0\sigma_z]$. To get a set of autonomous equations, we must then complement (2.25) with the closing equation (2.30) for α_t. A simple computation gives first (m_0, α_0) as function of (m_t, α_t) from which (m_{t+1}, α_{t+1})

is obtained as function of (m_t, α_t). Obviously, similar equations can be derived for the magnetization in the other ($x-$ and $y-$) spin directions. Instead of concentrating on the magnetization in the $z-$direction and closing the autonomy with (2.30), the same can be achieved directly by working with the three magnetizations.

One can verify from substituting (2.25) in (2.27) that in general the entropy will not increase monotonically. This has again to do with the infection by off-diagonal elements as discussed already under Section 3.2. By a proper choice of μ and $e_+ - e_-$ (and even in the case of (2.11) or (2.12) and with $h_3 = 0$) one can produce $m_t = m_e$ and $s(t) < s(t-1)$ for an infinite sequence of times t. One can also have a situation where for a certain choice of H and $\rho_0^N, m_0 = 0$ and $m_e > 0$. On the other hand, there remains an open set of choices for μ and $e_+ - e_-$ for which the entropy $s(t)$ does satisfy an $H-$theorem and we have that $s(t) > s(0)$ for all t sufficiently large when $h_3 = 0$ and $m_0 \neq 0$.

3.4 Relaxation to equilibrium?

The relaxation formula (2.25) is that of a damped oscillator. For initial (2.11) or (2.12) we have from (2.25)

$$m_t = m_e + (m_0 - m_e) r^t \cos \omega t$$

with $r^2 \equiv (1-\mu)^2 + \mu^2 + 2\mu(1-\mu)\cos(e_+ - e_-)$ and $\tan(\omega) \equiv \mu \sin(e_+ - e_-)/(1 - \mu + \mu \cos(e_+ - e_-))$. The frequency is maximal for $e_+ - e_- = \pi/2$ and the damping is maximal for $e_+ - e_- = \pi$.

The model does however not show the full glory of relaxation to equilibrium. That is already true in the original Kac ring model. As an example, consider a macroscopic variable which involves a two-spin function, in contrast with the single site observables that we introduced in (2.5):

$$A_N = \sum_j \sigma_{z,j}\sigma_{z,j+1}$$

It is easy to verify that A_N/N does not show relaxation. This is not surprising given the fact that two neighboring spins live exactly the same history and thus they do not decorrelate. This seriously restricts the usefulness of the model for studies of relaxation but it remains possible to study the phenomenon of relaxation for the special macroscopic observables of (2.5).

On the other hand, the fact that we consider relaxation in terms of macroscopic observables should not be considered as a restriction. After all, equilibrium is characterized by a maximal entropy condition given macroscopic constraints. In particular, relaxation is not be read off from the Liouville-von Neumann evolution for all microscopic details of the density matrix. The fact that we first let $N \uparrow +\infty$ (before time) avoids the presence of (quasi-)periodicities or of Poincaré-recurrence.

A final useful comparison concerns the notion of ergodicity which is quite universal, see e.g. [5, 4]. Consider a quantum mechanical system with a discrete non-degenerate energy spectrum (E_n) with (ϕ_n) a complete set of orthonormal energy eigenfunctions. The wavefunction at time t is denoted by $\psi(x,t) = \exp[-iHt]\psi(x)$ for initial $\psi(x) = \sum_n c_n \phi_n(x)$. The time-average of the expectation value of a Hermitian A is

$$\bar{A} \equiv \lim_{T\uparrow+\infty} \frac{1}{T}\int_0^T dt \int dx\, \psi^\star(x,t) A \psi(x,t)$$

It is rather easy to see in that case (but it remains true in a much broader context) that

$$\bar{A} = \sum_n |c_n|^2 \int dx\, \phi_n^\star(x) A \phi_n(x) \tag{3.4}$$

which could be argued to correspond to the microcanonical ensemble. Note however that no use was made in the above of the fact that N is large nor of the fact that we consider macroscopic variables. The result (3.4) is equally not very satisfactory: we are interested in the typical manifest behavior over realistic time-spans for large systems while (3.4) gives trivial information about an infinite time-average that cannot be identified with relaxation phenomena. There is in fact no relaxation to equilibrium on a microscopic scale even though (3.4) always holds.

3.5 Higher spins

Instead of considering spin 1/2 particles, it is also possible to set up exactly the same problem as above for a Hilbertspace $\mathcal{H}_N = \bigotimes_{j=1}^N \mathbb{C}_j^n$. We are then dealing with $n \times n$ matrices but there is little difference in the computations except for one extra complication: there is a larger class of conserved quantities. To explain that, we split the single-site observable A (a Hermitian matrix in $\mathbb{C}^{n\times n}$) in a part that commutes with the Hamiltonian H, and its orthogonal complement:

$$A = A_H \oplus A_\perp \tag{3.5}$$

with $[A_H, H] = 0$ and with respect to the scalar product

$$\langle A|B\rangle = \mathrm{Tr}\left[A^\star B\right] \tag{3.6}$$

The set of commuting observables $\mathcal{A}_H$ is a vector space with dimension

$$\dim\bigl(\mathcal{A}_H\bigr) = n$$

If $n > 2$ there is more than just the $\mathbb{1}$ and $H \in \mathcal{A}_H$ (e.g. not all functions of H can be expressed as linear combinations of $\mathbb{1}$ and H).
Because of the triviality of the dynamics as was discussed in the previous section, these extra conserved quantities give rise to conserved quantities for the full system dynamics and none of them disappear as the size of the system grows. For more realistic systems, truly interacting, we expect that, in the thermodynamic limit, essentially only such physical quantities as particle number and total energy remain conserved. In that respect, the case $n = 2$ is more physical and that is the reason why we have concentrated on it since the beginning. The mathematical theory can however be completed if we change the definition of the microcanonical ensemble (2.7) to include the extra conserved quantities.

4 Proof of results

Since it is important for physical interpretation that the relaxation curve (2.25) is obtained for almost all choices of scatterers ϵ drawn from (2.14), we must first remind in Lemma 4.1 of the thermodynamic equivalence with a grand-canonical set-up. Next, in Lemma 4.2 is shown that an effective dynamics reproduces the time-evolution of our macroscopic observables. Using that, and from Lemma 4.3, the propagation of the dispersionless condition (2.20) is obtained. It is therefore sufficient to derive (2.25) to get (2.24). That computation is introduced by Lemma 4.4. The entropy (2.27) can then also be computed using the obtained law of large numbers. The relaxation (2.30) is again a straightforward calculation that starts from the elements in Lemma 4.4.

Let $\Omega \equiv \{0,1\}$ and $\epsilon \in \Omega^N$. We have already defined the "canonical" measure $\mathbb{P}_\mu^N$ in (2.15) on Ω_μ^N of (2.14). Define now its "grand-canonical" version, the probability measure $\mathbb{P}_\mu$ on $\Omega^{\mathbb{N}}$, as the Bernoulli measure with density $\mathbb{P}_\mu(\epsilon_j = 1) = \mu$. $\mathbb{E}_\mu^N(\cdot)$ and $\mathbb{E}_\mu(\cdot)$ denote the expectation values with respect to $\mathbb{P}_\mu^N$ and $\mathbb{P}_\mu$ respectively. The following equivalence is standard.

Lemma 4.1 *For all functions $g \equiv g(\epsilon_1, \ldots, \epsilon_k)$ on Ω^k*

$$\Big| \mathbb{E}_\mu^N(g) - \mathbb{E}_\mu(g) \Big| \leqslant \frac{2^{2k+1}k}{N} \|g\| \qquad \text{if} \quad 2k \leqslant N$$

with

$$\|g\| \equiv \max_{\xi \in \Omega^k} |g(\xi)|$$

Proof:

$$\Big| \mathbb{E}_\mu^N(g) - \mathbb{E}_\mu(g) \Big| \leqslant \sum_{\xi \in \Omega^k} |g(\xi)| \left| \mathbb{P}_\mu^N(\xi) - \mathbb{P}_\mu(\xi) \right|$$

The right-hand side can be bounded by developing $\mathbb{P}_\mu^N(\xi)$ in conditional expectations. By explicit calculation

$$\left| \mathbb{P}_\mu^N \big(\xi_{k+1} = 1 \mid (\xi_1, \ldots, \xi_k) = \xi \big) - \mu \right| \leqslant \frac{k+1}{N-k}$$

after which a simple calculation finishes the proof. ■

We define for fixed j and matrix element per element

$$\Lambda_t(A_j) \equiv \mathbb{E}_\mu A_j(t, \epsilon) = \epsilon\text{-}\lim_{N \uparrow +\infty} \mathbb{E}_\mu^N A_j(t, \epsilon)$$

where the last equality follows from the previous Lemma 4.1.

Lemma 4.2 *For macroscopic observables $A_N = \sum_j A_j$ and continuous functions f, the dynamics is typically equivalent to the semigroup dynamics Λ_t,i.e.,*

$$\epsilon\text{-}\lim_{N \uparrow +\infty} \operatorname{Tr} \left[f\left(\frac{A_N}{N} \right) \rho_t^N \right] = \lim_{N \uparrow +\infty} \operatorname{Tr} \left[f\left(\Lambda_t \left(\frac{A_N}{N} \right) \right) \rho_0^N \right]$$

Proof:

The proof is for all monomials. By the Stone-Weierstrass theorem, this proves the theorem for all continuous functions f.

Let

$$D(n) \equiv \{1, \ldots, N\}^n$$

$$T(n, t) \equiv \Big\{ K \in D(n) \Big| \, \forall i, j \leqslant n : i \neq j \quad \Rightarrow \quad |K_i - K_j| > t \Big\}$$

and

$$A(K) \equiv A_{j(1)}^{k(1)} \otimes \ldots \otimes A_{j(l)}^{k(l)}$$

where

$$K = \{\underbrace{j(1), \ldots, j(1)}_{k(1)}, \ldots, \underbrace{j(l), \ldots, j(l)}_{k(l)}\}$$

We also need the index set $J(K) \equiv \{j \mid \exists p : K_p = j\}$.

We begin by calculating the ϵ-average. Denote $A_N(t,\epsilon) \equiv U_N(t)^\star A_N U_N(t)$, and similarly for the one-site observables A_j.

$$\mathrm{Tr}\left[\left(\frac{A_N}{N}(t,\epsilon)\right)^n \rho_0^N\right] = \frac{1}{N^n}\sum_w \sum_{K\in T(n,t)} \prod_{j\in J(K)}^{n} \mathrm{Tr}\left[A_j(t,\epsilon)\chi_{j,w}^N\right] \prod_{j\notin J(K)} \mathrm{Tr}\left[\chi_{j,w}^N\right]$$
$$+ \frac{1}{N^n}\sum_{K\in D(n)\setminus T(n,t)} \mathrm{Tr}\left[A(K)(t,\epsilon)\rho_0^N\right]$$

The last term can be dropped because

$$\left|\frac{1}{N^n}\sum_{K\in D(n)\setminus T(n,t)} \mathrm{Tr}\left[A(K)(t,\epsilon)\rho_0^N\right]\right| \le \frac{1}{N^n}\sum_{K\in D(n)\setminus T(n,t)} \|A(K)\| = \mathcal{O}\left(\frac{\|A\|^n}{N}\right)$$

We apply Lemma 4.1 with $g_{K,w}(\epsilon) \equiv \prod_{j\in K} \mathrm{Tr}\left[A_j(t,\epsilon)\chi_{j,w}^N\right]$ as function on Ω^{tn}. For $K \in T(n,t)$,

$$\left|\mathbb{E}_\mu^N \prod_{j\in K} \mathrm{Tr}\left[A_j(t,\epsilon)\chi_{j,w}^N\right] - \left(\mathbb{E}_\mu^C \mathrm{Tr}\left[A_j(t,\epsilon)\chi_{j,w}^N\right]\right)^n\right| \leqslant \frac{2^{2tn}2(tn)}{N} C^n \|A\|^n$$

We replace $\mathbb{E}_\mu \mathrm{Tr}[A_j(t,\epsilon)\chi_{j,w}^N]$ by $\mathrm{Tr}[\Lambda_t(A_j)\chi_{j,w}^N]$ and we add terms of order N^{-1} (essentially the ones we first subtracted) to arrive at the average from the lemma.

For the variance, we similarly write

$$\mathbb{E}_\mu^N\left(\mathrm{Tr}\left[\left(\frac{A_N}{N}(t,\epsilon)\right)^n \rho_0^N\right]\right)^2$$

as

$$\frac{1}{N^{2n}}\sum_{K,L\in T(n,t)} \mathbb{E}_\mu^N(\mathrm{Tr}\left[A(K)(t,\epsilon)\rho_0^N\right] \mathrm{Tr}\left[A(L)(t,\epsilon)\rho_0^N\right]) + \mathcal{O}(N^{-1})$$

Also the contribution of sets K and L that are within a distance less than t are of lower order. We apply Lemma 4.1 just as above.

■

Lemma 4.3 *For all continuous functions f and macroscopic observables A_N,*

$$\epsilon\text{-}\lim_{N\uparrow+\infty} \mathrm{Tr}\left[f\left(\frac{A_N}{N}\right)\rho_t^N\right] = \lim_{N\uparrow+\infty} f\left(\mathrm{Tr}\left[\Lambda_t\left(\frac{A_N}{N}\right)\rho_0^N\right]\right)$$

at all times t.

Proof:

By Lemma 4.2 we can replace $\mathbb{E}_\mu^N(A_j(t,\epsilon))$ by $\Lambda_t(A_j)$ in these expressions. Then the condition about the initial state applied to the observable $\sum_j \Lambda_t(A_j)$ yields the proof.

■

As an illustration of the lemma above, we show that it can be applied for the state ρ_0^N given by (2.11).

Example:

Call P_a^N the projector on the eigenvalue a of the macroscopic variable A_N/N. Let I^N be the spectrum of A_N/N and $I = \overline{\cup I^N}$. We want to establish a large deviations property for the probability measures W^N:

$$W^N(K) \equiv \sum_{a \in I^N \cap K} \mathrm{Tr}\left[P_a^N \rho_0^N\right] \tag{4.1}$$

The product $P_a^N \rho_0^N$ can be written as a sum over 1-dimensional projections and (4.1) can be developed and written in terms of

$$\mathrm{Tr}[P_{a_j} Q_{m_j}]$$

which takes four possible values depending on (p_j, m_j). The problem amounts therefore to estimate the probability that at the same time $\sum_j p_j, \sum_j m_j$ and $\sum_j m_j p_j$ take on specific values when the (p_j, m_j) are independent and identically distributed with uniform weights. That can be found from the multinomial distribution and Stirling's formula gives the large deviation rate function corresponding to (4.1). As a consequence, a law of large numbers is satisfied and in the thermodynamic limit the state (2.11) concentrates on only one eigenvalue of A_N/N.

♢

We now come back to (2.21) defining the marginal ν_0 and the overlap α_0 defined in (2.23). We split $\sigma_z = \sigma_H + \sigma_\perp$ as in (3.5) and parameterize:

$$\nu_0 = \begin{pmatrix} p & \beta \\ \bar\beta & 1-p \end{pmatrix} \qquad \sigma_\perp = \begin{pmatrix} 0 & \theta \\ \bar\theta & 0 \end{pmatrix}$$

A straightforward calculation yields $\alpha_0 = 2\beta\bar\theta$.
Lemma 4.4

$$m_t \equiv \epsilon\text{-}\lim_{N\uparrow+\infty} \mathrm{Tr}\left[\frac{M_N}{N}\rho_t^N\right] = m_e + \mathrm{Re}\left[\alpha_0(1-\mu+\mu\exp[i(e_+ - e_-)])^t\right] \tag{4.2}$$

Proof:

σ_H is invariant under the time-evolution and it is easy to verify that

$$\lim_{t\uparrow+\infty} \mathrm{Tr}\left[\Lambda_t(\sigma_z)\nu_0\right] = \mathrm{Tr}\left[\sigma_H \nu_0\right] = m_e$$

Fixing t, we write $k(\epsilon) \equiv \sum_{j=1}^t \epsilon_j$ and we obtain

$$\Lambda_t(\sigma_\perp) = \mathbb{E}_\mu\left[U^{k(\epsilon)\star}\sigma_\perp U^{k(\epsilon)}\right] = \begin{pmatrix} 0 & z(t) \\ \bar z(t) & 0 \end{pmatrix}$$

with

$$z(t) \equiv \theta(1-\mu+\mu\exp[i(e_+ - e_-)])^t \tag{4.3}$$

from which (4.2) follows at once.

■

The asymptotics (2.26) is trivial and the proof of Theorem 2.1 is thus completed if we add the equation (2.27) for $s(t)$.

Proof:

Consider

$$\frac{1}{N} S_N(\rho_t^N) = \frac{1}{N} \sum_\alpha \mathrm{Tr}\left[Q_\alpha^N \, \rho_t^N\right] \log d_\alpha^N - \frac{1}{N} \sum_\alpha \mathrm{Tr}\left[Q_\alpha^N \, \rho_t^N\right] \, \log \mathrm{Tr}\left[Q_\alpha^N \, \rho_t^N\right] \tag{4.4}$$

Rewrite the first term as

$$\sum_\alpha \mathrm{Tr}\left[s(\alpha) Q_\alpha^N \, \rho_t^N\right] - \sum_\alpha \left(s(\alpha) - \frac{\log d_\alpha^N}{N}\right) \mathrm{Tr}\left[Q_\alpha^N \, \rho_t^N\right] \tag{4.5}$$

In this expression the second term is in fact

$$\int d\nu_t^N(\alpha) \left(s(\alpha) - \frac{\log d_\alpha^N}{N}\right) \tag{4.6}$$

with ν_t^N a discrete probability measure on $[-1, 1]$. We choose

$$s(\alpha) \equiv -\frac{1+\alpha}{2} \log \frac{1+\alpha}{2} - \frac{1-\alpha}{2} \log \frac{1-\alpha}{2}$$

Now use that $\lim_N N^{-1} \log d_\alpha^N = s(\alpha)$ so that (4.6) vanishes. Use the spectral theorem and apply Lemma's 4.2 and 4.3 on the first term in (4.5) to obtain

$$\epsilon\text{-}\lim_{N\uparrow+\infty} \ \mathrm{Tr}\left[s\left(\frac{M_N}{N}\right)\rho_t^N\right] = s(m_t)$$

On the other hand, the second term in (4.4) is the Shannon entropy of the probability measure ν_t^N divided by N. Since that Shannon entropy is bounded by $\log N$, this term always vanishes.

■

The proof of (2.30) is a simple consequence of (4.3) and can be completed by explicit computation.

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