

## Passage from a pure state description to the microcanonical ensemble description for closed quantum systems

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**Abstract.** We have addressed the foundational issue of how a macroscopic quantum system starting off as a pure state tends towards a mixed state described by the microcanonical ensemble. The earlier works of von Neumann and Van Kampen are also reviewed. A simple criterion is given as to when the above mentioned passage can take place.

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### 1. Introduction

According to the basic premises of statistical mechanics, both classical (CSM) and quantum (QSM), a macrosystem starting from an arbitrary initial state *eventually* tends to a state of *thermodynamic equilibrium*. Inherent in this assertion is a certain *irreversibility* and one of the main issues is the reconciliation of this with *reversible* dynamics. In the context of CSM, there are many ways of appreciating this basic conflict. In terms of the Liouville equation, the Liouville operator has *real* eigenvalues and this leads to oscillatory solutions which do not show any one-way approach. The fact that the spectrum of the Liouville operator is *continuous* makes the situation more subtle but it still does not help in getting statistical mechanics out of Hamiltonian dynamics.

This dilemma is also sharpened by the Poincaré recurrence theorem which says that a system, after a sufficiently long time, comes *arbitrarily close* to its initial configuration.

Of course these difficulties were known right from the beginning and the broad contours of their resolutions were also understood even at the time of Boltzmann.

A very important conceptual development was that of *coarse-graining* introduced by Gibbs. The *energy surface* is coarse-grained to a degree determined by the *imprecision* in the measurement of phase space variables. In this view, the distribution function  $\rho$  will spread so finely (while keeping the total volume fixed) that eventually the fraction of the coarse-grained cell (phase cell) that is *occupied* becomes *uniform*. This state also corresponds to *maximum entropy*. Coarse-graining must be such that each phase cell contains a large number of microstates. If the phase cells are too fine, the phase cells are either fully occupied or fully empty leading to *zero entropy*. Interestingly, this is analogous to the *von Neumann entropy* for pure quantum systems. Time averages over reasonable time-scales agree with *ensemble* averages taken with equal *weight* for all the phase cells. This

ensemble distribution (*microcanonical distribution*) has no *memory* of the initial state. In the *Boltzmannian* as well as the *Gibbsian* approaches it is necessary to make *further* assumptions that can be generally interpreted as assumptions about some type of *chaotic* behaviour.

## 2. Foundational issues in quantum statistical mechanics

We now sketch some of the foundational issues in QSM. Unlike classical statistical mechanics, there is no *phase-space description* available. The thermodynamic state in QSM is a *mixed* state. If the initial state is *pure*, the dynamical evolution described by unitary transformations can never yield a mixed state. One faces the same difficulty in the *quantum measurement problem* as well. In classical statistical mechanics the microcanonical distribution is obtained by maximizing the entropy which is a functional of the distribution function. In the quantum case if one uses the von Neumann entropy, this can not work, as the entropy of a *pure state* is *zero*! One can get a *mixed density matrix* by *time-averaging* the density matrix,  $\rho$ . This does not help as the *impurity* ( $\text{tr } \rho^2$ ) is entirely determined by the *initial state* and the *spectrum* of the Hamiltonian. In fact traces of all powers of  $\rho$  are likewise determined and the maximization of entropy will have to be done with all these constraints

$$\text{tr } \bar{\rho}(t)^2 = \sum_{n,m} |\langle n|\rho(0)|m\rangle|^2 \left( \frac{\sin(\Delta E_{nm}T)}{(\Delta E_{nm}T)} \right)^2.$$

### 2.1 Motion in the Hilbert space

Even though there is no phase space available to look at the motion of the system point, the space of all states in QSM is the *Hilbert space* (more precisely it is the *projective Hilbert space*) and we can study the time evolution of the quantum system as a motion in this space.

Let  $E_A$ ,  $|A\rangle$  denote the *exact* eigenvalues and eigenfunctions of the system Hamiltonian  $H$ . We assume that this spectrum is *discrete* and *nondegenerate*. The initial state  $|\psi\rangle$  can then be represented as

$$|\psi\rangle_{t=0} = \sum_A C_A^\psi(t=0)|A\rangle. \quad (1)$$

The state at time  $t$  is

$$|\psi\rangle_t = \sum_A C_A^\psi(t)|A\rangle = \sum_A C_A^\psi(t=0)e^{-iE_A t}|A\rangle. \quad (2)$$

To mimic the discussion in CSM, let  $\sum_A$  include only states such that  $E_0 - \Delta < E_A < E_0 + \Delta$ . Let  $n_A$  be the number of such states. It should be noted that  $|C_A^\psi(t)|^2$  is *independent of time*. In quantum theory  $H$  and  $f(H)$  are independent in the sense that the average value of one does not determine the average value of the other. This is a very important difference

between the classical and quantum cases. It follows from eq. (2) that not only the average energy

$$\bar{E} = \sum_A |C_A^\Psi|^2 E_A, \quad (3)$$

but averages of all functions of the Hamiltonian

$$\bar{f}(E) = \sum_A |C_A^\Psi|^2 f(E_A) \quad (4)$$

are *constants of motion*. In other words, in quantum theory we have as many *independent* conserved quantities as there are energy levels.

Thus the notion of *energy surface* in QSM is replaced by the subspace of the Hilbert space with  $|C_A^\Psi|^2$  fixed for all  $A$ . Unlike the classical case where this surface depends only on the *total energy* of the system, in the quantum case it practically depends on the *initial system itself*. On writing  $C_A^\Psi(t) = r_A^\Psi e^{i\theta_A(t)}$  we see that this subspace is parametrized by the  $n_A$  angles  $\theta_A$  whose time-dependence is given by eq. (2) to be

$$\theta_A(t) = \theta_A(0) - E_A t. \quad (5)$$

We can ask for the circumstances when the motion on this  $n_A$ -torus is *ergodic*. From the works of Kronecker and of Weyl (for all details including references, see [1]), the conditions for such *ergodicity* are *non-degenerate* spectrum of  $E_A$  and *absence of resonances*, i.e.,  $E_A - E_B \neq E_C - E_D$  for all  $A, B, C, D$ . These conditions should hold only generically. In other words, one can tolerate deviations from these conditions of measure zero.

This is considerably weaker than conditions for *quantum chaos* or even for quantum systems that are *classically chaotic*. Even if this ergodicity holds, memory of the initial state is not erased as the subspace is still *state-dependent* and *no statistical mechanics emerges*. In the context of QSM we have so far not addressed the issue of *coarse-graining* which was crucial in CSM. We have to give meaning to the notion of *quantum coarse-graining* and that is one of the main themes considered in this discussion.

Finally, in the classical discussion *chaos* played a central role. The important question to be asked in QSM is: *What, if any, is the role of quantum chaos, in whatever sense it is to be understood?*

### 3. Earlier approaches

#### 3.1 Quantum statistical mechanics of von Neumann

von Neumann's remarkable work *The Proof of the Ergodic Principle and the H-theorem in the New Mechanics* appeared (in German) in 1929 barely a few years after the quantum formalism was developed. We will very briefly sketch the essentials of this paper and refer the reader to [1] for details.

He takes the spectrum of the Hamiltonian  $H$  to be *discrete* and *nondegenerate*. These are the *microstates*.  $\Delta E$  is taken as the resolution with which macroscopic energy measurements can be made. The energy levels are divided into groups of width  $\Delta E$  each.

The energy eigenfunctions within each group span an *energy surface*.  $S_a$  is the number of microstates spanning the energy surface  $a$ . The other important construct in his approach is that of the *macroscopic observables*. The macroscopic observables are all *mutually commuting* and hence have simultaneous eigenfunctions which are labelled by  $\{\lambda, p\}$  ( $\lambda = 1, 2, 0, \dots, s_p$ ). Distinct values of  $p$  denote distinct values of the observables. All states with the same  $p$  but different  $\lambda$  have the same values for all observables. The density matrix for an equal mixture of states for  $p$  fixed but for all possible values of  $\lambda$  is taken as the density matrix for a *phase cell*. It then follows that every macroscopic observable has a spectral decomposition in terms of the density matrices for phase cells. A very important upshot is a *unique partitioning* of all the phase cells among the energy surfaces. The number of phase cells belonging to the energy surface  $a$  is  $N_a$  and they are labelled by  $v, a$ .

The density matrix for the *microcanonical ensemble* is the density matrix for an equal mixture of energy eigenstates belonging to the energy surface  $a$ . If the probability of finding the initial state in the energy surface  $a$  is nonzero for many  $a$ , a *mixture* of microcanonical ensembles with weight factors proportional to the probabilities for finding the initial state in various energy surfaces has to be considered.

In this work von Neumann also clarifies the meaning of the so-called *von Neumann entropy*,  $S = -\text{tr} \rho \ln \rho$ , which is *zero* for *pure* states. According to him, it is *observer-dependent* and is meaningful only to an observer capable of making arbitrary measurements. In the present context observers can only make *macroscopic* measurements. If the probability of finding the system in the phase cell  $v, a$  is  $x_{v,a}$ , von Neumann advocates using in the present context, even for pure states, the entropy

$$S(\psi) = - \sum_a \sum_v^{N_a} x_{v,a} \ln \frac{x_{v,a}}{s_{v,a}}. \quad (6)$$

With these preliminaries and a liberal use of mathematical techniques he establishes that the time average of the entropy as defined above is bounded from above by the entropy of the microcanonical distribution, and furthermore, the difference between the two approaches zero. In the same vein he also shows that the time-averaged rms deviation of the expectation value of any macroscopic observable from its microcanonical average is bounded by a very small number which decreases with the number of phase cells.

### 3.2 *Van Kampen's approach*

In von Neumann's work the physical nature of the macroscopic observables is not very transparent and it does not seem obvious whether one can even find such observables for a *generic* quantum system. Van Kampen through a careful analysis shows how such observables can always be constructed through coarse graining. He then expands the initial state  $|\psi\rangle$  in terms of the simultaneous eigenstates of the coarse-grained observables. The phase cells are again defined by the values of these macroscopic observables. Using the time dependence of the state and some reasonable assumptions about *random phases*, he shows that the time evolution of the probability of finding the system in a phase cell is a *Markov process*. Standard techniques of stochastic processes then guarantee the passage to an equilibrium distribution. He also derives the so-called *master equation* from first principles.

#### 4. Dynamical quantum coarse graining

The quantum coarse graining introduced by both von Neumann and Van Kampen are *kine-matical* in the sense that they are based on the inevitable imprecision in the measurement of macroscopic observables. Our proposal for coarse graining is quite different in that it is *dynamical*. We came to know of the earlier works only after we had finished our work. Our scheme is logically independent of the earlier schemes.

Our point of view is the following: in any macroscopic system there are always what we call *soft states*. The energies of these states are so small that macroscopic measurements of energy cannot distinguish them. Nevertheless they are dynamically coupled to the rest of the system and the combined system follows unitary evolution. But our inability to distinguish these soft states leads to an effective coarse graining of the remainder and it is the purpose of our work to investigate the circumstances wherein this picture leads to quantum statistical mechanics.

We start with a composite Hilbert space  $\mathcal{H}$  which is a *tensor product* of two Hilbert spaces  $\mathcal{H}_i$  and  $\mathcal{H}_a$ . States in  $\mathcal{H}$  are the *microstates* of our system.  $a$  represents the soft degrees of freedom that we are not interested in and possibly over which we have no control.  $i$  are what become the *coarse-grained* microstates. The  $a$  states are taken to constitute a continuum of gap-less excitations, or the gap  $\delta_a$  between two consecutive energy levels of the unperturbed  $a$  system should be *much smaller* than the inverse of the time interval during which we observe the system. There is an *interaction* between the  $i$  and  $a$  degrees which should be understood as a process of resonant absorption and emission. The observables of interest  $O$  are such that

$$\langle i, a | O | j, b \rangle = \delta_{ab} \langle i | O | j \rangle. \quad (7)$$

Next we consider two types of mutually commuting variables  $I, \mathcal{A}$ , where  $I$  acts on  $\mathcal{H}_i$  and  $\mathcal{A}$  on  $\mathcal{H}_a$ . It is assumed that to a very good approximation the  $\mathcal{A}$  variables couple *weakly* to the  $I$ -variables in the total Hamiltonian

$$H_{\text{tot}} = H^{(i)} + H^{(a)} + \lambda H^{(i,a)}, \quad (8)$$

with  $\lambda$  very small. Let  $|A^*\rangle$  be the eigenstates of  $H^{(i)}$  with eigenvalues in the range  $E_0 - \Delta E < E_0 + \Delta$ . Let  $N_i$  be the number of such states in that range. Construct the matrix  $I_{AB}^* = \langle B^* | I | A^* \rangle$  of size  $N_i \times N_i$ . Let  $|i\rangle$  be the eigenstates of  $I^*$ . Choose  $|i, a\rangle = |i\rangle \otimes |a\rangle$ , where  $|a\rangle$  are the eigenstates of  $\mathcal{A}$ . The  $N_i \times N_a$  states  $|i, a\rangle$  form a *basis* for the microcanonical band. Let  $|A\rangle$  be the *exact* energy eigenstates a subset of which reduces to  $|A^*\rangle$  when the coupling  $\lambda = 0$ . Because of the weakness of the coupling  $\lambda$ , the exact energy eigenvalues will also lie in a range that approximates the range of eigenvalues of  $\mathcal{H}_i$ . But the eigenfunctions can be very different from  $|i, a\rangle$ .

Now consider some initial state in this subspace

$$|\psi\rangle = \sum C_A^\psi |A\rangle. \quad (9)$$

The exact eigenstates  $|A\rangle$  can be expanded in terms of the basis  $|i, a\rangle$ ,

$$|A\rangle = \sum_{i,a} C_A^{*ia} |i, a\rangle, \quad |i, a\rangle = \sum_A C_A^{ia} |A\rangle. \quad (10)$$

The coefficients  $C_A^{ia}$  obey the following unitarity conditions:

$$\sum_A C_A^{*ia} C_A^{i'a'} = \delta_{i'i'} \delta_{aa'}, \quad \sum_{ia} C_A^{ia} C_{A'}^{*ia} = \delta_{AA'}. \quad (11)$$

In terms of these definitions we can express the expectation value of any observable  $O$  satisfying eq. (7) as

$$O_{\psi\psi} = \sum_{a,ij} \sum_{A,B} C_B^{*\psi} C_A^\psi C_A^{*ia} C_B^{ja} O_{ij}. \quad (12)$$

Let us now introduce two auxiliary quantities  $P_A^j$  and  $R_{AB}^{jk}$ :

$$\sum_a C_A^{ja} C_B^{*ka} = \delta_{jk} \delta_{AB} P_A^j + R_{AB}^{jk}, \quad (13)$$

where, by definition,

$$P_A^j \equiv \sum_b C_A^{jb} C_A^{*jb}. \quad (14)$$

It should be noted that eq. (13) only amounts to a *diagonal + off-diagonal* split and is completely general. The following important properties of  $P$  and  $R$  are easily proved:

$$\sum_k R_{AB}^{kk} = 0, \quad \sum_k P_A^k = 1, \quad \sum_A P_A^k = N_a, \quad \sum_A R_{AA}^{kj} = 0. \quad (15)$$

One can also expand  $|\psi_t\rangle$  in the  $|i, a\rangle$  basis

$$|\psi(t)\rangle = \sum_{ia} D_{ia}^\psi(t) |ia\rangle. \quad (16)$$

After a lot of algebra, one gets

$$\begin{aligned} O_{\psi_t, \psi_t} = & \frac{1}{N_a} \sum_{A, \xi} [D_{ic}^\psi D_{ic}^{*\psi} P_A^i P_A^k O_{kk} + D_{ic}^\psi D_{jc}^{*\psi} R_{AA}^{ij} P_A^k O_{kk} \\ & + D_{ic}^\psi D_{ic}^{*\psi} P_A^i R_{AA}^{kl} O_{kl}] + \frac{1}{N_a} \sum_{A \neq B, \xi} D_{ic}^\psi D_{jc}^{*\psi} R_{AB}^{ij} R_{AB}^{kl} O_{kl}, \end{aligned} \quad (17)$$

where  $\xi$  stands collectively for all the other indices to be summed over. So far no assumptions have been made and eq. (17) is *completely general*. If, however,  $P_A^j$  have a *weak* dependence on either  $j$  or  $A$ , we can draw additional conclusions. On using eq. (15),

$$P_A^j = \frac{1}{N_i}. \quad (18)$$

Using eq. (18), the unitarity relations eq. (11) and  $\sum_A R_{AA}^{ij} = 0$  from eq. (15), the result one gets is

$$O_{\psi_t, \psi_t} = \frac{1}{N_i} \sum_j O_{jj} + \frac{1}{N_a} \sum_{i,j,k,l,c,A \neq B} D_{ic}^\psi(t) D_{jc}^{*\psi}(t) R_{AB}^{ij} R_{AB}^{kl} O_{kl}. \quad (19)$$

The first term represents the *microcanonical average* while the second term is *time-dependent*. On using *random phase* approximation the second term can be seen to vanish for late times. The second term is very important for determining the *thermalization times*. The *time average* of this second term can be estimated to be of the order of  $1/N_a^{1/2}$ .

One may wonder about the significance of eq. (18). One of the ways of realizing this restriction on  $P_A^i$  is when  $|A\rangle$  states have equal amounts of  $|i, a\rangle$ . This happens trivially for the so-called *random matrix theories*. But this is too *strong* a requirement. The significance of  $P_A^j$  is that it is the *probability* for the exact energy eigenstates  $|A\rangle$  to be found in the *coarse-grained state*  $j$ . It is clear that such a condition on  $P_A^j$  can be expected to be satisfied only when the perturbation  $H^{i,a}$  thoroughly mixes up the *unperturbed eigenstates*.

We have also carried out a first-order perturbation calculation for a two-level system in interaction with a continuum of low frequency harmonic oscillators in either coherent states or in number states (generalization of Feynmann and Hibbs calculations). These calculations support the picture elaborated here. It is noteworthy that no strong assumptions about *chaos* have been invoked in any of the three approaches! The *mathematical formalism* describing our prescription looks very much like von Neumann's approach but there are many important differences. In our case the observables generally *do not commute*, and for this reason von Neumann's method of proving quantum ergodicity does not work. However, van Kampen's derivation of the Markov process works here too. This can be taken as a justification for the restriction on  $P_A^i$ .

## References

- [1] N D Hari Dass, B Sathiapalan and Kalyanarama, *On the emergence of the microcanonical description from a pure quantum state*, cond-mat/0112439