Approach to Microcanonical Equilibrium for Nonisolated Systems

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Abstract

The approach to equilibrium for systems interacting with their environment by being regularly exposed to low energy, low intensity pulses of some type of quanta is studied. Assuming a randomness condition on the interaction of these quanta with the system, but making no assumptions about the accessible states of the system, we show that microcanonical equilibrium is reached. Although the intensity of the pulses is assumed to be weak the interactions are treated exactly, with no recourse to perturbation theory. The origin of time asymmetry and the absence of recurrence is discussed.

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I. INTRODUCTION

For over a 100 years various approaches have been used to study the foundations of statistical mechanics. That this subject continues to be of interest \[1\] indicates that no completely satisfactory description exists; this is true, both, for classical and quantum statistical mechanics. The question of how macroscopic irreversibility arises from reversible microscopic dynamics continues to be of a topic of discussion and is reviewed in Ref. \[1\].

For quantum statistical mechanics the goal to show that a system can be described by a microcanonical density matrix, which for some given energy $E$ is

$$\rho_{i,j}(E) = \frac{\delta_{i,j}}{N(E)}, \quad (1)$$

where $N(E)$ is the number of degenerate eigenstates with energy $E$. It would be desirable to obtain the completely mixed state represented by the density matrix of eq. (1) as a time development of a pure initial state; this is of course impossible under unitary time evolution and one has to resort to various averaging assumptions. In the most straightforward ensemble “derivation” of this result one essentially assumes the answer by postulating random phases and equal \textit{à priori} probabilities for the eigenstates of some Hamiltonian. More recently developments in the theory of chaotic systems have lead to a different ways of obtaining quantum statistical mechanics \[2\]. An old approach to (1) is through the Pauli master equation \[3\],

$$\frac{dP_i(t)}{dt} = \sum_n [t_{i\leftarrow n} P_n(t) - t_{n\leftarrow i} P_i(t)], \quad (2)$$

where $P_i(t)$ is the probability at time $t$ of the system being in the state $i$ and $t_{i\leftarrow n}$ is the rate per unit time to go from state $n$ to state $i$. In order to obtain eq. (2) certain assumptions have to hold \[3\):

(i) A repeated randomness assumptions insuring that the off diagonal elements of $\rho_{i,j}$ vanish. This is an assumption on the states that are accessible as the system evolves.
(ii) The interaction potential that causes the mixing of states is assumed to be weak as to permit the use of first order perturbation theory.

(iii) There is an inherent clash in that the $P_i$'s refer to discrete states and yet one has to use continuum normalization in order to obtain a Dirac delta function in the energies. Conditions (i) and (ii) can be weakened for certain classes of interactions [4] (also see L. Van Hove’s in Ref. [3]).

In this presentation we shall consider a nonisolated, finite but large, system that is allowed to interact with its environment; by this we mean that from time to time the system is exposed to a low energy, low intensity packet of some quanta. These quanta are spatially unconstrained (continuum normalized) and after a certain characteristic interaction time $\tau$ the system settles into a new state or density matrix. After intervals larger than this characteristic time, this process is repeated. The above qualitative terms, low intensity, low energy and time interval, will be made precise and summarized in Sec. V. The quanta in these pulses will be referred to as “photons”. We shall show that with one assumption on the interaction of these packets with the system, but independent of any assumptions on the accessibility of the system itself, microcanonical equilibrium, eq. (1), will be reached. Contrary to the approach to equilibrium for isolated systems, in this case equilibrium is attained by “entangling” the system with photons and then looking at expectation values of operators that are diagonal in the photon variables. Even though we may start out with a pure system-photon state, the system itself will be in a mixed state after the interactions have ceased. No recourse is made to perturbation theory; the interactions are treated exactly.

The system, its interactions and time evolution are presented in Sec. II while the time evolution of density matrices is discussed in Sec. III; an assumption on the randomness of phases of certain amplitudes is presented and discussed in this section. How the system approaches equilibrium is shown in IV; although we do not get a master equation the approach to equilibrium is Markovian [3], governed by a Chapman-Kolmogorov [3] equation. The relations among various energy and time scales that the system and perturbing quanta
have to satisfy are given in Sec. V where the origin of time irreversibility and the absence of recurrence is discussed.

II. INTERACTIONS AND TIME EVOLUTION OF STATES

The energy levels $E_\alpha$ of the system are highly degenerate with states $|\alpha, i\rangle$. The energies of the photons in the packets are taken to be too small to cause transitions between states of different energy; these interactions can, however, cause transitions between the degenerate levels within a given $E_\alpha$; for convenience we take the energy $E_\alpha = 0$ and drop the quantum number $\alpha$ in the description of the states. As usual the total Hamiltonian will be split into two parts, $H = H_0 + H_1$; eigenstates of $H_0$ that are of interest are $|i, k\rangle$ with

$$H_0|i, k\rangle = \omega(k)|i, k\rangle;$$

the specific dispersion relation for $\omega(k)$ is unimportant. $H_1$ induces transitions between $|i, k\rangle \leftrightarrow |j, k'\rangle$. Whether this Hamiltonian is time reversal invariant or not is immaterial to subsequent developments.

Let $|i, k\rangle_H$ be that eigenstate of the total Hamiltonian that approaches $|i, k\rangle$ for large negative times; we use the notation $| \rangle_H$ for an eigenstate of the total Hamiltonian, whereas $| \rangle$, without the subscript $H$, for an eigenstate of $H_0$. This state satisfies the Lippmann-Schwinger equation

$$|i, k\rangle_H = |i, k\rangle + \frac{1}{\omega(k) - H_0 + i\epsilon}H_1|i, k\rangle_H.$$

The overlap with an eigenstate of the free Hamiltonian is

$$\langle j, p|i, k\rangle_H = \delta_{ij}\delta(k - p) + \frac{1}{\omega(k) - \omega(p) + i\epsilon}\mathcal{T}_{j,i}(p, k),$$

where

$$\mathcal{T}_{j,i}(p, k) = \langle j, p|H_1|i, k\rangle_H$$

(4)
is the scattering amplitude for the transition \(|i, k\rangle \rightarrow |j, p\rangle\) and satisfies the off shell unitarity relations

\[ T_{j,i}(p, k) - T_{i,j}^*(k, p) = \int dq \left[ \frac{1}{\omega(q) - \omega(p) + i\epsilon} - \frac{1}{\omega(q) - \omega(k) - i\epsilon} \right] T_{j,n}(p, q) T_{i,n}^*(k, q) , \]

\[ = \int dq \left[ \frac{1}{\omega(q) - \omega(p) + i\epsilon} - \frac{1}{\omega(q) - \omega(k) - i\epsilon} \right] T_{n,i}(q, k) T_{n,j}^*(q, p) . \]  

We want to describe the time evolution of a state that at \(t = 0\) started out as \(|i, k\rangle\); more specifically we want the overlap at time \(t\) with the state \(|j, p\rangle\).

\[ \langle j, p | e^{-iHt} | i, k \rangle = [\delta_{i,j} \delta(p - k) + iR_{j,i}(p, k; t)] e^{-i\omega(p)t} ; \]  

in the above

\[ iR_{j,i}(p, k; t) = \frac{1}{\omega(p) - \omega(k) - i\epsilon} [ -T_{j,i}(p, k) e^{i[\omega(p) - \omega(k)]t} + T_{i,j}^*(k, p) ] \]

\[ + \int dq e^{i[\omega(p) - \omega(q)]t} \frac{T_{j,n}(p, q)}{\omega(q) - \omega(p) + i\epsilon} \frac{T_{i,n}^*(k, q)}{\omega(q) - \omega(k) - i\epsilon} . \]  

For the definition of \(R\) in eq. (8) we have pulled out the factor \(\exp [-i\omega(p)]\) for later convenience. Eq. (7) or (8) implies unitarity relations for \(R\)

\[ -i \left[ R_{j,i}(k', k; t) - R_{i,j}^*(k, k'; t) \right] = \sum_n \int dq R_{j,n}(k', q; t) R_{i,n}^*(k, q; t) , \]

\[ = \sum_n \int dq R_{n,i}(q, k; t) R_{n,j}^*(q, k'; t) . \]  

III. TIME EVOLUTION OF THE DENSITY MATRIX

We shall be interested in operators \(O\) be that have off diagonal matrix elements between the different \(|i\rangle\)'s and are diagonal in the photon subspace. For any state

\[ |S\rangle = \sum_i \int dq \phi_i(q) |i, q\rangle , \]  

the expectation value of \(O\) is

\[ \langle S | O | S \rangle = \sum_{i,j} \langle j | O | i \rangle \rho_{i,j} , \]  

with a density matrix

\[ \rho_{i,j} = \int dq \phi_i(q) \phi_j^*(q) . \]
A. Evolution of $\rho$ entangled with a wave packet of photons

Suppose that at time $t = 0$ our system, described by a density matrix $\rho_{j,i}(0)$, is exposed to a photon state. The total density matrix, for the system plus photons is

$$\rho_T = \sum_{i,j} \int dk \, dk' \psi(k)\psi^*(k') |j,k\rangle \rho_{j,i}(0) \langle i,k'|,$$

where $\psi(k)$ describes the photon wave packet scattered of the mixed state at $t = 0$; $\int dk|\psi(k)|^2 = 1$. Using eq. (8) and eq. (9) the density matrix at time $t$, after summing over the photon states, is

$$\rho_{j,i}(t) = \rho_{j,i}(0) + \int dk \, dk' \psi(k)\psi^*(k') \left[ i \sum_n R_{j,n}(k',k; t) \rho_{n,i}(0) ight.$$

$$- i \sum_m R^*_{i,m}(k',k; t) \rho_{jm}(0) + \left. \int dp \sum_{n,m} R_{j,n}(p,k; t) R^*_{i,m}(p,k'; t) \rho_{n,m}(0) \right].$$

In subsequent discussions we shall need some randomness condition on the phases of the $R$’s. It is unlikely that such a condition could be valid for all times; we shall try for ones that may hold at large times. For short duration pulses we expect that after some characteristic collision time $\tau$, as for example the inverse of the width of a resonance in resonance dominated scattering [6], the system will settle down and

$$\lim_{t \to \infty} \int dk \psi(k) R_{j,i}(p,k; t) = R_{j,i}(p); \quad (16)$$

$R_{j,i}(p)$ depends implicitly on the wave function $\psi$ and, using the definition in eq. (9) we find

$$R_{j,i}(p) = \int dk \psi(k) \frac{-i}{\omega(p) - \omega(k) - i\epsilon} T_{i,j}^*(k,p). \quad (17)$$

For further developments, this explicit form will not be needed. We also define

$$R_{j,i} = \int dk \psi^*(k') R_{j,i}(k'). \quad (18)$$

These, in turn, satisfy the unitarity relations.
\[-i \left( R_{j,i} - R^*_{i,j} \right) = \sum_n \int dp R_{n,i}(p) R^*_{n,j}(p). \quad \text{(19)}\]

In particular, we find
\[
\text{Im} \ R_{j,j} > 0. \quad \text{(20)}
\]

The evolution of the density matrix, eq. (15), may be expressed as
\[
\rho_{j,i}(t) = \rho_{j,i}(0) + i \sum_n \left[ R_{j,n} \rho_{n,i}(0) - R^*_{i,n} \rho_{j,n}(0) \right] + \sum_{m,n} \int dp R_{j,n}(p) R^*_{i,m}(p) \rho_{n,m}(0). \quad \text{(21)}
\]

**B. Randomness Assumption**

In order to proceed further we must impose a crucial condition on the \( R \)'s:
\[
\int dp R_{j,n}(p) R^*_{i,m}(p) = 0 \quad \text{for} \ i \neq j \quad \text{and} \ m \neq n. \quad \text{(22)}
\]

This results from the assumption that, as we integrate over \( p \), the phases of \( R_{j,n}(p) \) fluctuate rapidly. *It should be emphasized that this is an assumptions on the dynamics of the system and not on states or density matrices of the system at any particular time.*

The above and unitarity relation, eq. (19), lead to
\[
\left( R_{j,i} - R^*_{i,j} \right) = 0 \quad \text{for} \ i \neq j; \quad \text{(23)}
\]

which together with eq. (20) implies
\[
R = R_H + iD \quad \text{(24)}
\]

with \( R_H \) Hermitian and \( D \) a diagonal matrix with positive elements. As a matter of fact, there always exists a basis of the states \( |i\rangle \) where such a decomposition of \( R \) holds. Any matrix can be written as a sum of a Hermitian and an anti-Hermitian one and we go to the basis where the anti-Hermitian part is diagonal. Although eq. (22) implies eq. (24), the inverse is not true and eq. (22) remains an assumption. We work in the basis where this decomposition holds. The time evolution of the density matrix becomes
\[
\rho_{j,i}(t) = \rho_{j,i}(0) + i \left[ R_H, \rho(0) \right]_{j,i} - \left[ D, \rho(0) \right]_{j,i} + \delta_{i,j} \sum_n \int dp \left| R_{i,n}(p) \right|^2 \rho_{n,n}(0); \quad \text{(25)}
\]

\([A, B]\) is the commutator of the matrices \( A \) and \( B \).
IV. APPROACH TO EQUILIBRIUM

At this point we have to require the $R_{j,i}$’s to be small; how this is achieved will be made precise in Sec. V. We solve eq. (25) to first order in the $R$’s by first rewriting it as

$$\tilde{\rho}_{j,i}(t) = \rho_{j,i}(0) - \left[ D, \rho(0) \right]_{j,i} + \delta_{i,j} \sum_n \int dp |R_{i,n}(p)|^2 \rho_{n,n}(0),$$

with

$$\tilde{\rho}_{j,i}(t) = \sum_{n,m} [1 - iR]_{j,n} \rho_{n,m}(t) [1 + iR]_{m,i}.$$

To the order we are working $1 - iR$ is a unitary matrix and $\tilde{\rho}_{j,i}(t)$ is the density matrix in a basis rotated from the one we started out at $t = 0$.

Let us first look at eq. (26) for $i \neq j$.

$$\tilde{\rho}_{j,i}(t) = [1 - (D_{i,i} + D_{j,j})] \rho_{j,i}(0).$$

The off diagonal elements of the unitarily rotated density matrix at time $t$ are smaller than the corresponding matrix element at $t = 0$;

$$|\tilde{\rho}_{j,i}(t)| \leq |\rho_{j,i}(0)|.$$  \hspace{1cm} (29)

For the case $i = j$ we have

$$\tilde{\rho}_{i,i}(t) = \rho_{i,i}(0) + i \left( R_{i,i} - R_{i,i}^* \right) \rho_{i,i}(0) + \sum_n \int dp |R_{i,n}(p)|^2 \rho_{n,n}(0).$$

The coefficient of $\rho_{n,n}(0)$ in the last term of this equation may be identified with the transition probability for $|n\rangle$ to evolve into $|i\rangle$,

$$\mathcal{W}_{i\leftarrow n} = \int dp |R_{i,n}(p)|^2.$$  \hspace{1cm} (31)

Using the unitarity relation, eq. (19), we find

$$i(R_{i,i} - R_{i,i}^*) = -\sum_n \mathcal{W}_{n\leftarrow i}$$  \hspace{1cm} (32)

and the evolution equation for this case becomes

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\[ \tilde{\rho}_{i,i}(t) = \rho_{i,i}(0) - \sum_n W_{n\leftarrow i} \rho_{i,i}(0) + \sum_n W_{i\rightarrow n} \rho_{i,i}(0). \]  

(33)

Even if we include the unitary rotations this equation is of the Chapman-Kolmogorov type and for the \( W_{i\rightarrow n} \)'s not too large, will directly yield microcanonical equilibrium. This follows from the observation that the matrix

\[ M_{i,j} = -\delta_{i,j} \sum_n W_{n\leftarrow i} + W_{i,j} \]  

(34)

has one eigenvalue equal to zero and all others are negative which in turn is obtained by showing the function \( H(\tau) = -\sum_i P_i(\tau) \ln P_i(\tau) \) satisfies a Boltzmann H-theorem, \( dH/d\tau \geq 0 \) with the probabilities being functions of the auxiliary variable \( \tau \) and (c.f. eq (3))

\[ \frac{dP_i}{d\tau} = \sum_j M_{i,j} P_j. \]  

(35)

Let \( v_i^{(0)} \sim (1, 1, \ldots, 1) \) be the eigenvector of \( M_{i,j} \) with eigenvalue zero and \( v_i^{(\alpha)} \) be all the others.

\[ \rho_{i,i} = c_0 v_i^{(0)} + \sum_\alpha c_\alpha v_i^{(\alpha)}. \]  

(36)

At the end of the interval \( t \) \( c_0 \) hasn’t changed and the other \( c_\alpha \)'s have all decreased in magnitude. We find that repeated pulses will drive off diagonal elements to zero and the diagonal ones to the same constant or the final density matrix will be as in eq. (1).

\section{V. CONCLUDING REMARKS}

We have to consider three characteristic energies: (i) \( \Delta_\alpha \), the difference in the energy levels \( E_\alpha \) of the system, (ii) \( \delta_\omega \), the energy spread of the impinging wave packets, and (iii) \( \gamma \), the inverse of the interaction time \( \tau \). These quantities have to satisfy

\[ \Delta_\alpha \gg \delta_\omega \gg \gamma. \]  

(37)

The first of these inequalities insures that there will be no transitions between the different energy levels of the system; for such transition the energy denominator in eq. (1) would have
a typical magnitude of $\Delta_\alpha$ as opposed to $\delta_\omega$ for intra level transitions. Due to the second inequality the “arrival period” of the pulse is much shorter than the interaction time and for times greater than $\tau$ the system and the photons propagate separately. In addition the repetition time of these pulses, $T$, must satisfy

$$T \gg \frac{1}{\gamma};$$

(38)

this guarantees that as a new packet interacts with the system it is unencumbered by photons from the previous pulses; for example $T$ must be large enough to allow any possible system-photon resonances to decay.

Till now, all this has been worked out for the system interacting with a one photon packet; the random impulses from the outside are likely to contain many photons and we extend our results to $N$ photons where the states are $\int \prod_{n=1}^{N} d\mathbf{k}_n \psi_n(\mathbf{k}_n)|i; \mathbf{k}_1, \mathbf{k}_2 \cdots \mathbf{k}_N\rangle$. In the case the packets $\psi_n(\mathbf{k})$ are different for different $n$’s this expression should be appropriately symmetrized; doing this explicitly would just lead to unnecessary notational complications. The scattering amplitude is not necessarily a sum of two body amplitudes and the rest of the development is as the previous one. We identify a weak, or low intensity pulse as one with few photons and an intense one with a large number. We require that $N$ be sufficiently small that the $R_{j,i}$’s are small compared to one; $N$ should not be too small as the time to reach equilibrium would become very large.

With these conditions and the assumption about interactions made in eq. (22) satisfied, repeats interactions of the system with external quanta will drive it to equilibrium. Time irreversibility is built in right at the start in the choice of the sign of the $i\epsilon$ term in eq. (4). The continuous energy levels of the photons preclude any recurrences; had the photons also been quantized in a finite volume the limit considered in eq. (16) would not have existed.
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[6] We ignore the very small nonexponential terms that behave as $t^{-\frac{5}{2}}$; see Ref. [5].