UWThPh-1982-2

ON THE ADIABATIC THEOREM IN QUANTUM STATISTICAL MECHANICS

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Abstract

We show that with suitable assumptions the equilibrium states are exactly the states invariant under adiabatic local perturbations. The relevance of this fact to the problem of ergodicity is discussed.

1. Introduction

P. Ehrenfest [1] was the first to appreciate the importance of adiabatic invariance. At a time when the complete quantum theory was not available he guessed that the quantum laws would only allow motions which are invariant under adiabatic perturbations. He also noted that the adiabatic invariance of the action variables makes Boltzmann's statistically defined entropy adiabatically invariant. Shortly after the discovery of quantum mechanics [2] it was recognized that in the region of the discrete spectrum of the Hamiltonian the adiabatic hypothesis holds. However it took a long time until Kato [3,4] found the complete proof which is now reproduced in the more substantial books on quantum mechanics [5]. The theorem states the following: Let

$$H(t) = \sum_i P_i(t)\, e_i(t)$$

be a time-dependent Hamiltonian, $e_i(t)$ its i-th eigenvalue, $P_i(t)$ the projection onto the corresponding eigenspace and $U(t)$ the time evolution generated by $H(t/T)$, i.e. $\dot{U}_T(t) = -iH(t/T)\, U_T(t)$. Although in general $H(t/T) \neq U_T^{-1}(t)\, H(0)\, U_T(t)$ we have

$$\lim_{T\to\infty} U_T^{-1}(T)\, P_i(0)\, U_T(T) = P_i(1)\ .$$

This result implies in statistical mechanics that the microcanonical density matrix $\rho = \sum_{i=1}^{n} P_i$ is adiabatically invariant (in the nondegenerate case) in the sense

$$\lim_{T\to\infty} (\rho(T) - U_T^{-1}(T)\, \rho(0)\, U_T(T)) = 0\ .$$

The canonical density matrix $\rho = e^{-\beta H}/\mathrm{Tr}\, e^{-\beta H}$ is adiabatically invariant only for those perturbations which are switched off at the end, $H(0) = H(1)$.

An important assumption in the adiabatic theorem is $e_i \neq e_j$ for $i \neq j$, P_i has to project onto all eigenvectors belonging to e_i otherwise one easily constructs counterexamples even in two dimensions:

Example 1

$$H(t) = \begin{pmatrix} 0 & 0 \\ 0 & \pi t \end{pmatrix}, \quad U_T(t) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\pi t/T} \end{pmatrix}. \quad U_T(T) = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$ does not leave the eigenvector $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ of $H(0)$ invariant, $\lim T \to \infty$ does not help.

Since degeneracy causes a problem one might expect difficulties with the adiabatic theorem in the continuous spectrum. It turns out, however, that there things are even better, $H(t)$ does not even have to be differentiable as in the case of the discrete spectrum. The pertinent question in the continuous spectrum is whether the time evolution approaches as free time evolution $U^o(t) = \exp(-iH_o t)$, i.e. whether the Møller operators

$$\Omega_\pm(H,H_o) = \lim_{t\to\pm\infty} U^*(t)\, U^o(t)$$

exist. It turns out, that this is the case, even when $H(t)$ is a step function, for which in the discrete spectrum the sudden and not the adiabatic approximation is applicable.

Example 2

Let $H(t) = \begin{cases} H_1 & \text{for } 0 \le t < \alpha \\ H_2 & \text{for } \alpha \le t \le 1 \end{cases}$ such that $\Omega(H_1,H_o)$ and $\Omega(H_2,H_o)$ exist.

$$U_T^*(T) = \exp(iH_1 T\alpha)\exp(iH_2 T(1-\alpha)),$$

$$\Omega_\pm = \lim_{T\to\infty} \exp(iH_1T\alpha)\exp(iH_2T(1-\alpha))\exp(-iH_oT) =$$

$$= \lim_{T\to\infty} \exp(iH_1T\alpha)\exp(-iH_oT\alpha)\exp(iH_oT\alpha)\exp(-iH_2T\alpha)\exp(iH_2T)\exp(-iH_oT) =$$

$$= \Omega_\pm(H_1,H_o)\,\Omega_\pm^*(H_2,H_o)\,\Omega_\pm(H_2,H_o) = \Omega_\pm(H_1,H_o).$$

We shall not dwell on the finer points of mathematical rigor for the $\lim_{T\to\infty}$ but stress that intuitively the result is clear. If you scatter a particle and change at the time αT the Hamiltonian to H_2 then for large T the particle will be gone and does not feel the change. Thus you get the same scattering as for H_1. Since we could not find a demonstration of this rather trivial fact we shall give as warming up exercise in the next section a general proof of the adiabatic theorem in scattering theory which spots some conditions under which it holds.

Our main concern will be quantum statistics of infinite systems. In thermodynamics some people speak synonymously about adiabatic and reversible changes. We interpret this as follows. Although in principle every time evolution in quantum mechanics is reversible in practice the best thing one can do to undo a perturbation is to switch it off very slowly. If only the equilibrium states admit reversible operations in this sense then they should be characterized by adiabatic invariance. In § 3 we will show that this actually is true in the appropriate setting of infinite quantum systems. There [6,7] the equilibrium states are given by states satisfying the KMS-condition. This state gives the only eigenvector of H, the rest of the spectrum is continuous. Under these circumstances we can easily extend the adiabatic theorem from scattering theory to statistical mechanics. One finds that adiabatic invariance is equivalent to dynamical stability which was shown by Haag, Kastler and Trych-Pohlmeyer to characterize the KMS-condition. Dynamical stability of a stationary state requires that for every small time-independent perturbation a state close by invariant under the perturbed time evolution exists. Since people make linear response theories with impunity one would think that one always has dynamical stability. It turns out, however, that even for simple classical dynamical systems dynamical stability may fail and in this case the state is also not adiabatically invariant.

<u>Example 3</u>

Consider the free motion on the two-dimensional torus T^2 and introduce on its phase-space the canonical coordinates $(\phi_1,\phi_2;L_1,L_2)$; $0 \leq \phi_{1,2} < 2\pi$. The Hamiltonian is $H = \omega_1 L_1 + \omega_2 L_2$ and the time evolution $\phi_i(t) = \phi_i(0) + \omega_i t (\mathrm{mod}\ 2\pi)$, $L_i = \mathrm{const}$. If the frequencies are rationally dependent, $\omega_2 = (g_2/g_1)\omega_1$, $g_i \in Z$, then there exists besides the L_i another constant $f = \sin(g_2\phi_1 - g_1\phi_2)$ and $f^2 \prod_i d\phi_i/(2\pi)^2$ provides a state (i.e. a probability measure) on the submanifolds L_i = const. However for any change of the ω's no matter how small, which renders them rationally independent, there is no similar (on T^2 singlevalued) function. Thus this state is not dynamically stable and we shall now show that it is not adiabatically invariant. For this purpose make the frequencies time-dependent and switch the perturbation off after some time, $\omega_i = \omega g_i(t)$, $g_i(0) = g_i(1) \in Z$. The Hamiltonian $\sum \omega_i(t/T)L_i$ changes $f = \sin(\phi_1 g_2(0) - \phi_2 g_1(0))$ after time T into

$$f(T) = \sin(\phi_1(0)g_2(0) - \phi_2(0)g_1(0) + \omega\int_0^T dt(g_1(\tfrac{t}{T})g_2(0) - g_2(\tfrac{t}{T})g_1(0))).$$

Thus $\lim_{T\to\infty} f(T)$ does not need to exist and if it does it may be different from f(0).

The last example shows the relevance of adiabatic invariance to the question of ergodicity. If a system is not ergodic it has other constants besides H. If the equilibrium states f(H) are the only adiabatically invariant states then the other constants will not be adiabatically invariant. One can now argue, that these other states are actually not stationary if the system is considered in its environment. There will be necessarily some interaction with the environment and even if the time scale of these perturbations is macroscopic they will destroy such a state. Thus those infinite quantum systems for which only the equilibrium states are adiabatically invariant have reasonable ergodicity properties.

2. The Adiabatic Theorem in Scattering Theory

In this section we shall show that the scattering operator is not affected by adiabatic changes of the potential. We shall use the simplest rather than the most refined estimates for proving the existence of the Møller operators [9]. Correspondingly the results are not optimal but typical for what can be achieved by simple means. They cover, however, easily the adiabatic switching on of the potential which one encounters in the folklore.

Theorem 2.1*

Let $H_T(t) = H_o + V(t/T)$ be a one parameter family of Hamiltonians, $0 \le t \le T$, $H_o = p^2/2m$, $V(\alpha)$ are multiplication operators with square integrable functions such that

$$\|V(t)\|_2 \le M < \infty \;\forall\, t, \qquad \int_0^1 \frac{d\alpha}{\alpha^{3/2}} \|V(\alpha)-V(0)\|_2 < \infty ,$$

and

$$\lim_{\alpha\to 0} \|V(\alpha)-V(0)\| \to 0 .$$

Then the time evolution $U_T(t)$ with

$$\frac{d}{dt} U_T(t) = -i\, H_T(t)\, U_T(t) \tag{1}$$

approaches $\exp(-iH_oT)$ in the sense that

$$\lim_{T\to\infty} U_T^*(T) \exp(-iH_oT) = \Omega(H(0),H_o) \equiv \lim_{T\to\infty} \exp(iH(0)T) \exp(-iH_oT) . \tag{2}$$

Proof

The existence of $\Omega(H(0),H_o)$ follows from the well-known argument

$$\|(\exp(iH(0)T_2) \exp(-iH_oT_2) - \exp(iH(0)T_1) \exp(-iH_oT_1))\psi\|_2 = \tag{3}$$

$$= \|i \int_{T_1}^{T_2} dt \exp(iH(0)t)\, V(0) \exp(-iH_ot)\psi\|_2 \le \int_{T_1}^{T_2} dt\, \|V(0) \exp(-iH_ot)\psi\|_2 .$$

Now there is a dense set of functions ψ such that $\|\exp(-iH_ot)\psi\|_\infty < c/t^{3/2}$ and $\|V(0) \exp(-iH_ot)\psi\| \le \|V(0)\|_2 \; \|\exp(-iH_ot)\psi\|_\infty$. Hence

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*) We will use the following notations:

$\|A\|$	operator norm of A
$\|V\|_2$	L_2 norm of a function $= [\int |V(x)|^2 d^\nu x]^{1/2}$
o	composition of maps
*	adjoint operator
[A,B]	commutator = AB - BA
$\|V\|_\infty$	L_∞ norm of a function $= \sup_x |V(x)|$

$$\int_{T_1}^{T_2} dt \,\|\cdot\|_2 \le \|V(0)\|_2\, c \int_{T_1}^{T_2} \frac{dt}{t^{3/2}} = \|V(0)\| c\, 2(T_2^{-1/2} - T_1^{-1/2}) \qquad (4)$$

which guarantees the convergence of the sequence. Next we show that $\forall\, \psi$ of this dense set and $\varepsilon > 0\ \exists\, T_o$ such that

$$\|(U_T^*(T)\exp(-iH_oT) - \exp(iH(0)T)\exp(-iH_oT))\psi\| < \varepsilon \quad \forall\, T > T_o \qquad (5)$$

which proves the existence and the asserted value of the limit. For this purpose we use (with $W = V - V(0)$)

$$U_T^*(t) = \exp(iH(0)t) + i\int_0^t dt'\; U_T^*(t')\; W(\tfrac{t'}{T})\; \exp(iH(0)(t-t')) \qquad (6)$$

and by the same methods one gets

$$U_T^*(T)\exp(-iH_oT) = 1 + i\int_0^T dt[\exp(iH(0)t) + i\int_0^t dt' U_T^*(t')W(\tfrac{t'}{T})\exp(iH(0)(t-t'))]\cdot$$
$$\cdot\,[V(0) + W(\tfrac{t}{T})]\exp(-iH_ot)\,. \qquad (7)$$

This gives the estimate

$$\|(U_T^*(T)\exp(-iH_oT) - \exp(iH(0)T)\exp(-iH_oT))\psi\|_2 \le$$
$$\le \|\int_0^T dt \int_0^t dt' U_T^*(t')W(\tfrac{t'}{T})\exp(iH(0)(t-t'))\,V(\tfrac{t}{T})\exp(-iH_ot)\psi\|_2 +$$
$$+ \|\int_0^T dt\,\exp(iH(0)t)\,W(\tfrac{t}{T})\exp(-iH_ot)\psi\|_2\,. \qquad (8)$$

To show that the first term goes to zero we first note that

$$\|\int_0^t dt' U_T^*(t')\; W(\tfrac{t'}{T})\exp(-iH(0)(t'-t))\| \le 2$$

since it is the difference of two unitary operators. Hence it is $\le 2\int_0^T dt\, \|V(\tfrac{t}{T})\|_2 \|\exp(-iH_ot)\psi\|_\infty$ and $\|\cdot\|_\infty \le c/t^{3/2}$ guarantees that the integral converges for $T \to \infty$. Therefore there is a T_o such that $\int_0^T dt\, \|\cdot\|_2 \le \int_0^{T_o} dt\, \|\cdot\| + \varepsilon/3$. Now

$$\lim_{T\to\infty} \int_0^{T_0} dt \int_0^t dt' \, \|W(\tfrac{t'}{T}) \exp(-iH(0)(t'-t)) \, V(\tfrac{t}{T}) \exp(-iH_0 t)\psi\|_2 \leq \tag{9}$$

$$\leq \lim_{T\to\infty} \sup_{0\leq\alpha\leq T_0/T} \|W(\alpha)\| \int_0^{T_0} dt \; t \, \|V(\tfrac{t}{T}) \exp(-iH_0 t)\psi\|_2 \, .$$

Since by assumption $\lim_{\alpha\to 0} \|W(\alpha)\| = 0$ and the second factor is bounded T-independent this shows that the first term is $\leq \varepsilon/3$ for sufficiently large T. According to the estimates used the second term is

$$\leq c \int_0^T dt \, \|W(\tfrac{t}{T})\|_2 \, t^{-3/2} = c \, T^{-1/2} \int_\alpha^1 \frac{d\alpha}{\alpha^{3/2}} \|W(\alpha)\|_2 \tag{10}$$

and this also tends to zero. □

Remarks

1. As mentioned in § 1 $V(t)$ need not be continuous for all times but only for $t = 0$.
2. The classical meaning of Ω_T is that one follows the free time evolution till $t = T$ and then returns on the actual trajectories back to $t = 0$ [10]. This makes it clear why for $T \to \infty$ only $V(0)$ matters.
3. If one describes scattering by a potential which is switched on and off, $V(0) = V(1) = 0$, one has to make sure that the particle is around when the potential is on. The theorem shows that in this case $U_T^*(T)\exp(-iH_0T)$ converges toward 1 whereas $\exp(-iH_0T/2)U_T^*(T)\exp(-iH_0T/2)$ converges to the S-matrix with $V(1/2)$.

3. The Adiabatic Theorem in Quantum Statistics

The relevance of the adiabatic invariance in statistical mechanics has recently been emphasized by Lochak [11]. However, he considered Hamiltonians with discrete spectrum whereas the thermodynamic behaviour requires an absolutely continuous spectrum. Thus we shall deal in this section with infinite quantum systems. For their description we use the standard setting [6,7]: A C^*-algebra $\mathcal{A}$ of local observables and a one-parameter group τ_t of automorphisms of $\mathcal{A}$ describing the time evolution.

States ω are positive normalized linear functionals over A. A state is stationary if $\omega\circ\tau_t = \omega$ and KMS if $\omega(a\tau_t(b)) = \omega(b\tau_{i\beta}(a))$, a,b $\in$ A, β = 1/temperature. The extremal KMS-states, i.e. those which are not convex combinations of other KMS-states are considered as equilibrium states. The adiabatic theorem states that the extremal KMS-states are exactly the states which are invariant under local adiabatic perturbations. To make a reasonable defirition of adiabatic invariance one has to keep in mind that we are dealing with local observables and that they diffuse with time since we assume that H has an absolutely continuous spectrum. Thus if you take a τ-invariant state and ask how it changes if you switch on a local perturbation adiabatically the answer is trivially that it does not change. The reason is simply that by the time the perturbation becomes effective the observable has diffused and is no longer affected by a local perturbation, similar to what we learned in § 2. So this kind of adiabatic invariance does not characterize any state but is a purely dynamical effect. Furthermore if we want to require that a time-invariant state has not changed we better switch the perturbation off at the end. If a perturbation is switched on adiabatically at t = -T, reaches its full strength at t = 0 and then goes to zero for t = T, then we should ask that the state is unchanged even for those observables which are localized at t = 0. Thus if V(t/T) generates a time development $\tau^T_{t_1,t_2}$ our requirement will be $\lim_{T\to\infty} \omega\circ\tau_{-T}\circ\tau^T_{-T,T}\circ\tau_{-T} = \omega$. Thus we have a situation as in scattering theory and to mimik the proof of § 2 we use $\tau^T_{-T,T} = \tau^T_{-T,0}\circ\tau^T_{0,T}$ and first study $\lim_{T\to\infty} \tau^T_{0,T}\circ\tau_{-T}$ and then get the second half by exchanging τ and τ^T.

The main assumption for our demonstration is that A is asymptotically abelian [6,7] with respect to τ. More precisely we require that for a dense subalgebra A' we have the cluster properties: $\forall$ a,b $\in$ A' $\exists$ M < ∞, ε > 0, such that

$$\|[a,\tau_t(b)]\| \leq \frac{M}{t^{1+\varepsilon}} \quad \forall\, t > 0 \, . \tag{11}$$

For infinite systems the time evolution can be written $\tau_t(a) = e^{iHt}\, a\, e^{-iHt}$ only in some representations, there is no representation

independent Hamiltonian H. To make the following derivation more transparent we shall pretend to start with the assumption that the time evolution has this familiar form, the final result remains valid for the infinite system.
If we have a time dependent Hamiltonian $H_T(t) = H_o + V(t/T)$ it generates a time evolution $\tau^T_{t',t}$ from t' to t such that

$$\frac{d}{dt}\tau^T_{t',t}(a) = i[H_T(t),\tau^T_{t',t}(a)]$$
$$\frac{d}{dt'}\tau^T_{t',t}(a) = -i\tau^T_{t',t}([H_T(t'),a]) \ . \tag{12}$$

Thus

$$\tau^T_{0,T}\circ\tau_{-T}(a) = a - \int_0^T dt \frac{d}{dt}\tau^T_{t,T}\circ\tau_{-(T-t)}(a) =$$
$$= 1 + i\int_0^T dt \ \tau^T_{t,T}([V(\tfrac{t}{T}),\tau_{-(T-t)}(a)]) \ . \tag{13}$$

According to the heuristics given above we think that τ^T should approach the time-evolution $\tau^{V(1)}$ given by $H_o + V(1)$, thus we compare with

$$\tau^{V(1)}_T\circ\tau_{-T}(a) = a + i\int_0^T dt \ \tau^{V(1)}_t([V(1),\tau_{-t}(a)]) \ . \tag{14}$$

As in § 2 we introduce $\tau^{V(1)}$ in (13) by

$$\tau^T_{T-t,T}\, a = \tau^{V(1)}_t(a) + i\int_0^t dt' \ \tau^T_{T-t',T}([W(\tfrac{t'}{T}),\tau^{V(1)}_{t-t'}(a)]) \ ,$$
$$W(\tfrac{t}{T}) = V(\tfrac{T-t}{T}) - V(1) \ , \tag{15}$$

so that the main terms cancel in the difference

$$\tau^T_{0,T}\circ\tau_{-T}(a) - \tau^{V(1)}_T\circ\tau_{-T}(a) = i\int_0^T dt \ \tau^{V(1)}_t([W(\tfrac{t}{T}),\tau_{-t}(a)]) +$$
$$+ i\int_0^T dt\int_0^t dt' \ \tau^T_{T-t',t}([W(\tfrac{t}{T}),\tau^{V(1)}_{t-t'}(V(\tfrac{T-t}{T}),\tau_{-t}(a)])]) \ . \tag{16}$$

In these formulas the Hamiltonian has disappeared and the result remains valid for the infinite system if $V(t) = g(t)h$, $h \in A$ and g a function continuous at 1. Then we can show that the right hand side goes to zero as in § 2. Since by assumption $\|[h,\tau_{-t}(a)]\| \leq M/t^{1+\varepsilon}$ and $\tau^{V(1)}$ as automorphism does not change the norm. The norm of the first term is

$$\leq \int_0^T dt\, \frac{M(g(1) - g(\frac{T-t}{T}))}{t^{1+\varepsilon}} \leq T^{-\varepsilon} \cdot \text{const.}$$

For the second term we argue as before: $\int_0^t dt'$ increases the norm at most by 2, and the decrease of the commutator shows that the integral converges for $T \to \infty$; hence we can restrict the integral to $(0,T_1)$ with T_1 independent of T. But $\int_0^{T_1} dt$ tends to zero for $T \to \infty$ since $W(0) = 0$. Since one knows that $\lim_{T\to\infty} \tau_T^{V(1)} o \tau_{-T}^{o} \equiv \gamma_-$ exist (11) we have shown that $\tau_{0,T}^{T} o \tau_{-T}(a)$ converges in norm for $T \to \infty$ towards $\gamma_-(a)$. The proof of $\tau_{-T} o \tau_{-T,0}^{T}$ proceeds in the same way except that τ and τ^T have exchanged their role and hence we have to require that $\tau^{V(1)}$ is asymptotically abelian. In this case the limits $T \to \mp\infty$: $\gamma_\pm$ are automorphisms and $\lim_{T\to\infty} \tau_{-T} o \tau_{-T,T}^{T} o \tau_{-T} = \gamma_+^{-1} o \gamma_-$.

After these dynamical consideration we can draw on previous results [8] about properties of KMS-states. They state that clustering states [6] (i.e. for $t \to \infty$, $\omega(a\tau_t(b)) \to 0$ sufficiently strongly) the KMS-states are exactly the ones with $\omega o \gamma_+^{-1} o \gamma_+ = \omega$ for a dense set of V's. Thus we can formulate the

<u>Adiabatic Theorem for Infinite Quantum Systems</u>

Let A be the algebra of local observables and its time automorphism asymptotically abelian in the sense: $\forall\, a,b \in A'$, A' dense $\exists\, M < \infty$, $\varepsilon > 0$, such that $\|[a,\tau_t(b)]\| \leq M/t^{1+\varepsilon}$ $\forall\, t > 0$. Furthermore assume that the time evolutions τ^V with all perturbations λV from a set dense in A have the same properties for small λ. Then the extremal KMS-states are exactly those clustering states ω for which $\lim_{T\to\infty} \omega o \tau_{-T} o \tau_{-T,T}^{T} o \tau_{-T} = \omega$ where τ^T is the time evolution perturbed by $g(t/T)V$, $g(-1) = g(1) = 0$.

Remarks

1. The cluster condition reflects the extremality of the states. For suitable systems they are satisfied by extremal KMS-states [6] and more generally by states which generate factor representations. Non-extremal KMS-states are unstable with respect to perturbations which tend spatially to infinity [12].
2. If V generates a discrete spectrum then the γ's will no longer be surjective and $\omega\circ\gamma_+^{-1}$ no longer a KMS-state over A. $\omega\circ\gamma_+^{-1}\circ\gamma_-$ might still be ω but then our adiabatic process does not go over the equilibrium state at $t = 0$.
3. Even if $\gamma_\pm$ are automorphisms $\omega\circ\gamma_+^{-1}\circ\gamma_-$ may give an inequivalent representation. In fact, if ω gives a factor representation it is the only τ_t-invariant state in this representation. As $\omega\circ\gamma_+^{-1}\circ\gamma_-$ is τ-invariant it has to be ω if we stay in the representation. Hence either ω is extremal KMS, in which case $\omega\circ\gamma_+^{-1}\circ\gamma_-$ is always ω or ω is not extremal KMS, in which case $\omega\circ\gamma_+^{-1}\circ\gamma_-$ will give, for some γ, an inequivalent representation [13]. Therefore not equilibrium stationary states are those which can be changed globally by local adiabatic perturbations.
4. Our perturbations are local and do not cover cases like two-body interactions. Hence our results do not substantiate the usual adiabatic folklore in quantum field theory.
5. For finite systems adiabatic invariance does not characterize the canonical density matrix. Any function of H has this property.

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