UWThPh-1992-29

Stability of Pure Thermodynamic Phases in Quantum Statistics

Heide Narnhofer
Institut für Theoretische Physik
Universität Wien

Abstract

We discuss how measurements can distinguish between pure and mixed thermodynamical phases and look for arguments in favour of pure thermodynamical phases.

1 Introduction

It is a well accepted fact that in quantum mechanics the equilibrium states are described by the KMS condition [1,2]. States satisfying the KMS condition form a simplex so there exists a unique decomposition into extremal KMS states that coincide with the factorial decomposition. Furthermore, extremal KMS states cluster for every asymptotic abelian automorphism, so especially for space translations and therefore in extremal KMS states global densities carry no dispersion.

In classical theory we are accustomed with this fact, but already before we have taken the thermodynamic limit. A superposition of pure thermodynamic phases corresponds to our incomplete knowledge of the system. But also the pure thermodynamic phases are defined by probability arguments. The pure state corresponds to a point in configuration space, and refinement of the measurements can improve our knowledge which point it is.

Quantum mechanics produces dispersions as a consequence of noncommutativity and we have first to discuss how superpositions of states for large systems influences the theory of measurement in quantum mechanics.

2 Theory of Measurement for KMS States

Let A be an observable in quantum mechanics of a single particle with nondegenerate pure point spectrum corresponding to eigenvalues a_i and eigenvectors φ_i. If the system is in a state corresponding to the vector ψ then a measurement of A has an outcome a_i with probability $|\langle\psi|\varphi_i\rangle|^2$ so that in the average $E(A) = \langle\psi|A|\psi\rangle$. If we repeat the measurement immediately then with security we will measure a_i, which means that by the measurement of A ψ has turned into the state φ_i [3,4].

Now we assume ω to be a superposition of states. For instance, $A = \sigma_z$ and ω corresponding to the density matrix $\begin{pmatrix} 1/2 & \\ & 1/2 \end{pmatrix}$. Either we can consider the state as superposition of states corresponding to $\left| \begin{matrix} 1 \\ 0 \end{matrix} \right\rangle$ and $\left| \begin{matrix} 0 \\ 1 \end{matrix} \right\rangle$ with probability 1/2, but also as superposition of $\left| \begin{matrix} 1 \\ 0 \end{matrix} \right\rangle$ and

$\left| \begin{array}{c} 1/2 \\ \sqrt{3}/2 \end{array} \right\rangle$ and $\left| \begin{array}{c} 1/2 \\ -\sqrt{3}/2 \end{array} \right\rangle$ with probability 1/3. In all cases the outcome of the measurement of σ_z will be 1 with probability

$$\sum \alpha_i \left| \langle \psi_i \left| \begin{array}{c} 1 \\ 0 \end{array} \right\rangle \right|^2 = \mathrm{Tr} \left| \begin{array}{c} 1 \\ 0 \end{array} \right\rangle \left\langle \begin{array}{c} 1 \\ 0 \end{array} \right| \rho \frac{1}{2}, \tag{2.1}$$

therefore independent of the chosen decomposition.

Now take A to have degenerate pure point spectrum, e.g.,

$$A = \frac{1}{2}|\varphi_1 + \varphi_2\rangle \langle \varphi_1 + \varphi_2| + \frac{1}{2}|\varphi_1 - \varphi_2\rangle \langle \varphi_1 - \varphi_2| = |\varphi_1\rangle \langle \varphi_1| + |\varphi_2\rangle \langle \varphi_2|.$$

If a measurement of A gives the value $\mathbf{1}$ the corresponding projection is $P = \sum_i |\varphi_i\rangle\langle\varphi_i|$ and the original state corresponding to a vector ψ changes to a state corresponding to the vector $A\psi$, given by the density matrix

$$\sum_{i,j} |\varphi_i\rangle \langle \varphi_j|\langle \psi|\varphi_j\rangle \langle \varphi_i|\psi\rangle = |P\psi\rangle\langle P\psi| \tag{2.2}$$

so independent of the basis taken in the space of degeneracy.

In the thermodynamic limit observables are local and therefore have a highly degenerate spectrum. On the other hand, the decomposition of a state into pure ones is not only nonunique but also less meaningful, since in contradistinction to the classical situation a pure state of the quasilocal algebra

$$\mathcal{A} = \overline{\bigcup_\Lambda \mathcal{A}_\Lambda}$$

is in general not pure for a local subalgebra which contains the real observables. Avoiding to refer to pure states the outcome of a measurement can be described in the following way:

Let ω be the state of an algebra. Take $A = \sum_{i=1}^n a_i P_i$ as observable, so with discrete finite spectrum. Define

$$\omega_i(B) = \frac{\omega(P_i B P_i)}{\omega(P_i)}. \tag{2.3}$$

After the measurement of A the system will be in the state ω_i with probability $\omega(P_i) = \lambda_i$ and will give the result $\omega_i(A) = a_i$, such that the average expectation of $A = \sum \lambda_i \omega_i(A) = \omega(A)$. This is in agreement with the previous example. Among the states that are linear superpositions of states with $\xi_i(A^2)=\xi_i(A)^2$ the state $\sum\lambda_i\omega_i$ minimizes the free energy $S(\sum\mu_i\xi_i|\omega)$ and is in this sense optimal.

In fact, fix $\{\xi_i\}$ corresponding to density matrices $\sigma_i=P_i\sigma_iP_i$ and optimize $\{\mu_i\}$. This gives

$$\frac{\partial}{\partial\mu_j}(\text{Tr }(\rho\log\rho-\rho\log\sum\mu_i\sigma_i)-\sum\alpha\mu_i)=-\frac{\partial}{\partial\mu_j}\sum_i(\text{Tr }P_i\rho P_i\log\mu_i\sigma_i+\alpha\mu_i)=0,$$

$$\text{Tr }P_i\rho P_i=\alpha\mu_i,\qquad\sum\alpha\mu_i=1\qquad\text{or}\qquad\mu_i=\omega(P_i).$$

Next we optimize σ_i to

$$\inf S(\omega|\sigma_i)=\inf(\text{Tr }\rho\log\rho-\text{Tr }P_i\rho P_i\log P_i\sigma_iP_i)=\text{Tr }\rho\log\rho-\text{Tr }P_i\rho P_i\log P_i\rho P_i.$$

Repeating the measurement immediately gives the same result. If, however, we let time pass and if we assume that in the thermodynamic limit the time evolution is asymptotic abelian, if, in addition, we assume that ω is extremal time invariant, so a pure thermodynamic phase, then ω_i, which belongs to the same folium as ω, satisfies $\lim_{t\to\infty}\omega_i\circ\alpha_t=\omega$. Thus repeating the same measurement in long enough intervals we can find by experiment the probability distribution $\{\lambda_i\}$ corresponding to ω (and therefore $\omega(A)=\sum_i\lambda_ia_i$). Here we do not need an ensemble to determine ω, where insecurity in preparing the probe can give a probability character to ω, but we keep observing the same system.

Now consider ω to be a superposition of, let us say, two extremal invariant states, $\omega=\alpha_1\omega_1+\alpha_2\omega_2$. If we now measure A, and find a_i, then according to our rule the state ω is changed into the state

$$\varphi_i(B)=\frac{\alpha_1\omega_1(P_iBP_i)+\alpha_2\omega_2(P_iBP_i)}{\alpha_1\omega_1(P_i)+\alpha_2\omega_2(P_i)}\tag{2.4}$$

with probability $\alpha_1\omega_1(P_i)+\alpha_2\omega_2(P_i)$. In the course of time this state evolves to

$$\omega_{i1}=\frac{\alpha_1\omega_1(P_i)\omega_1+\alpha_2\omega_2(P_i)\omega_2}{\alpha_1\omega_1(P_i)+\alpha_2\omega_2(P_i)}$$

which by a new measurement of A which gives, say a_j, and after waiting long enough turns into

$$\omega_{ij}=\mathcal{N}(\alpha_1\omega_1(P_i)\omega_1(P_j)\omega_1+\alpha_2\omega_2(P_i)\omega_2(P_j)\omega_2).\tag{2.5}$$

Therefore we can observe a different probability distribution for the outcome of measurements. Repeating the measurement for n times,

$$\prod\omega_1(P_j)^{\ell_j}\qquad\text{or}\qquad\prod\omega_2(P_j)^{\ell_j}$$

with $\sum \ell_j = n$ will for a given $\{\ell_j/n\}$ dominate so that we press by infinitely many measurements the system into the pure thermodynamic phase ω_k with probability α_k. Therefore apart from fluctuations at the beginning we cannot observe by measurement of the same system whether we have started with a mixed phase. To determine the probabilities α_k we have to make copies of the sample and the mixed state can be interpreted as the ensemble of pure phases with the probability distribution α_k.

We can conclude that in quantum mechanics it seems meaningful to assign to a pure phase more reality than a probabilistic one. In the following we will concentrate which arguments might support pure thermodynamic phases.

3 Decomposition into Pure Thermodynamic Phases and the Algebra at Infinity

We consider as observable algebra the quasilocal algebra

$$\mathcal{A} = \overline{\bigcup \mathcal{A}_\Lambda}, \qquad \mathcal{A}_\Lambda \subset \mathcal{A}_{\bar{\Lambda}} \text{ if } \Lambda \subset \bar{\Lambda}. \tag{3.1}$$

Every state $\omega(A)$ corresponds to a GNS representation

$$\omega(A) = \langle \Omega | \pi(A) | \Omega \rangle. \tag{3.2}$$

In this representation we can define the algebra at infinity [5],

$$\mathcal{A}_\infty = \bigcap_\Lambda \left(\bigcup_{\bar{\Lambda} \subset \Lambda^c} \pi(\mathcal{A}_{\bar{\Lambda}}) \right)''. \tag{3.3}$$

If $\mathcal{A}$ is simple – what we can assume – then $\mathcal{A}_\infty$ corresponds to the center $\mathcal{Z} = \pi(\mathcal{A})'' \cap \pi(\mathcal{A})'$. Now we assume that the time evolution is given by an automorphism group α_τ. The equilibrium states are those that satisfy the KMS condition

$$\omega(AB) = \omega(B \tau_{i\beta} A). \tag{3.4}$$

If $\bar{\omega} < \omega$ also satisfies the KMS condition, then it can be written as

$$\bar{\omega}(A) = \langle \Omega | z \pi(A) | \Omega \rangle \quad \text{with} \quad z \in \mathcal{Z}$$

and equivalently every such z defines a KMS state ω_z.

Therefore the decomposition of a KMS state into extremal KMS states is unique, coincides with the central decomposition and physically can be interpreted as the roughest decomposition into states with trivial algebra at infinity.

4 Pure KMS States are Stable under Perturbation

By a local operator P time evolution can be perturbed to

$$\tau_t^P(A) = \tau_t(A) + \sum_{n\geq 1} i^n \int_{0\leq s_1\ldots\leq s_n} ds_1 \ldots ds_n[\tau_{s_1}(P), \ldots, [\tau_{s_n}(P), \tau_t A]] \tag{4.1}$$

such that in a time covariant representation with

$$\pi(\tau_t A) = e^{iHt}\ \pi(A)\ e^{-iHt} \tag{4.2}$$

we have

$$\pi(\tau_t^P A) = e^{i(H+\pi(P))t}\ A\ e^{-i(H+\pi(P))t}. \tag{4.3}$$

Then analyticity in the KMS states allows to define a perturbed state ω^P KMS with respect to τ_t^P by

$$\omega^P(A) = \frac{\langle\Omega|\pi(A)\ e^{-(H+\pi(P))}|\Omega\rangle}{\langle\Omega|e^{-H-\pi(P)}|\Omega\rangle}. \tag{4.4}$$

This idea was used in Ref. 6 to favour pure KMS states:

Consider a sequence $\{P_\alpha\}$ such that

$$\lim_{\alpha\to\infty} \|\tau_t^{P_\alpha} A - \tau_t A\| = 0. \tag{4.5}$$

Arrange P_α such that it converges to $z \in \mathcal{Z} = \mathcal{A}_\infty$. Then

$$\lim_{\alpha\to\infty} \omega^{P_\alpha}(A) = \frac{\langle\Omega|\pi(A)\ e^{-z}|\Omega\rangle}{\langle\Omega|e^{-z}|\Omega\rangle} \neq \omega(A), \tag{4.6}$$

if $z \neq \lambda\mathbf{1}$, which is possible in mixed KMS states, but not in pure ones. Therefore pure KMS states seem to be more stable under small changes of the dynamics. But we will argue in the next section that the perturbation theory offered here is not the really relevant one.

5 Dynamical Stability as Criterium for Equilibrium

In Ref. 7 it is proposed to characterize equilibrium by stability under perturbations of the dynamics and it is shown that this stability under appropriate additional assumptions demands that the equilibrium state satisfies the KMS condition.

Again we consider the perturbed dynamics τ_t^P. But we do not start with a KMS state but just assume that we have an invariant state $\omega = \omega \circ \tau_t$ and can do some kind of perturbation theory so that there exist states $\omega^P = \omega^P \circ \tau_t^P$ with

$$\text{n-}\lim_{P \to 0} \omega^P = \omega. \tag{5.1}$$

In addition we assume that τ_t is strongly asymptotically abelian and that ω is a factor state. Then we expand $\omega^{\lambda P} = \omega^{\lambda P} \circ \tau_t^{\lambda P}$ in λ. Asymptotically abelianness together with norm convergence implies

$$\lim_{t \to \infty} \left. \frac{d\omega^\lambda(\tau_t A)}{d\lambda} \right|_{\lambda=0} = 0. \tag{5.2}$$

The other term in the expansion to order λ gives

$$\lim_{T \to \infty} \int_{-\infty}^{+\infty} \omega([P, \tau_t A]) dt = 0. \tag{5.3}$$

Using once more that ω is a factor state and therefore clustering in t it is shown in Ref. 7 that ω has to satisfy the KMS condition for some temperature β^{-1}.

If we examine the assumptions we notice that ω to be a factor is only of technical importance. Otherwise we could have a superposition of two KMS states with two different temperatures without violating dynamic stability. Conversely, we notice that following the construction in Sect. 4 every pure KMS state is dynamically stable and so is every superposition of KMS states.

It remains to check if an enlargement of the permitted perturbations to nonlocal ones can favour pure thermodynamic phases, for sure such perturbations will lead to states that are not normal with respect to the unperturbed one, and we have to clarify whether norm convergence of the states can be relaxed.

6 Adiabatic Stability

Dynamic stability can be interpreted in the following way: We note that we do not know the time evolution to all accuracy, and we can only rely on those observations that are only mildly affected by our ignorance. Adiabatic stability now accepts that time evolution itself undergoes small fluctuations due to the surroundings and equilibrium states are those where these fluctuations do not add to a global effect. So especially if we switch on and off a local perturbation slowly, the we should return to the initial state. In this way the probabilistic argument for dynamic stability can be turned to a dynamic one.

In Ref. 8 again it was assumed that the time evolution is asymptotic abelian in the sense that a scattering transformation between locally perturbed and unperturbed automorphisms exists, i. e.,

$$\text{n-}\lim_{t\to\pm\infty} \tau_t^P \tau_{-t} a = \gamma_\pm^P a. \tag{6.1}$$

Now adiabatic switching on and off allows the system to react completely on the perturbed dynamics so that the effect of switching and the invariance of the state ω under this operation can be expressed as

$$\omega \circ (\gamma_-^P)^\dagger \gamma_+^P(a) = \omega(a) \tag{6.2}$$

or

$$\omega \circ \gamma_+^P = \omega \circ \gamma_-^P \tag{6.3}$$

which again implies to first order in P

$$\lim \int_{-T}^{+T} \omega([P, \tau_t a])dt = 0 \tag{6.4}$$

so that we are back to dynamic stability. The difference is that there we assumed a perturbation of the state – $\omega \circ \gamma^P$ demanding normality. Here we obtain the perturbed state as time limit and require independence of the time direction.

In this context we also notice that (4.4) is not really the relevant perturbation. Of course, it is mathematically perfectly well defined, but the perturbation of a mixed KMS state that reflects the dynamic reaction of the system on a perturbation is given by

$$\omega(a) = \int d\mu(z)\omega_z(a) = \int d\mu(z)\langle\Omega_z|\pi_z(a)|\Omega_z\rangle \longrightarrow$$

$$\longrightarrow \bar{\omega}^P(a) = \int d\mu(z) \frac{\langle \Omega_z | \pi_z(a) e^{-H_z - \pi_z(P)} | \Omega_z \rangle}{\langle \Omega_z | e^{-H_z - \pi_z(P)} | \Omega_z \rangle} \tag{6.5}$$

and here $\lim_\alpha \bar{\omega}^{P_\alpha} = \omega$, iff $\lim \tau_t^{P_\alpha} = \tau_t$ and there is no condition on the purity of ω.

7 Global Perturbation

Local perturbation of the dynamics can be expressed on the level of the C^* algebra, so linear superposition of states cannot find its reflection in less stability. On the other hand, at least on the lattice we know how to treat global perturbations and know their effect on the KMS states. In Ref. 2 we find the following characterization of KMS states for lattice systems:

We introduce the Banach space of translationally invariant interactions, which has a norm dense intersection with the strictly local operators of the quasilocal C^* algebra. On this Banach space we define the free energy density functional which is convex and continuous. Its tangent functionals that at every point form a simplex define states on $\mathcal{A}$, that satisfy the KMS condition, and even more, all translationally invariant KMS states (which satisfy the Gibbs condition and maximize the S-H_ϕ functional on ω, whose maximum coincide with the free energy density) can be obtained in this way. Furthermore, theory of convex functionals tells us that every extremal tangent functional can be obtained as limit of tangent functionals that are unique. For a convex function $R \to R$ also the converse is true: only the extremal tangent functionals can be obtained in this way (right and left derivatives). In higher dimensions mixed phases can be limits of pure phases only if they correspond to phase transition points.

If we translate these observations into response to time dependent perturbation, we obtain the following:

Let P be a local operator, let $P_n = \sum_{x \in \Lambda_n} \sigma_x P$ and $\Lambda_n \nearrow Z^d$. Let ω be a τ_t-KMS state, τ_t asymptotic abelian. Define

$$\omega^0(A) = \lim_{\lambda \to 0} \lim_{n \to \infty} \lim_{t \to \infty} \omega(\tau_t^{\lambda P_n} A). \tag{7.1}$$

Then ω^0 is almost surely an extremal τ_t-KMS state.

Proof: $\lim_{t \to \infty} \omega(\tau_t^{\lambda P_n} A)$ is a $\tau_t^{\lambda P_n}$-KMS state in the same folium as discussed in Sects. 5 and 6.

Further, $\lim_{n\to\infty} \|\tau_t^{\lambda P_n} A - \tau_t^{\lambda \bar{P}} A\| = 0$, where $\tau_t^{\lambda\bar{P}}$ is a globally disturbed time evolution. This guarantees that the weak limit points $\omega^{\lambda\bar{P}}$ of $\omega^{\lambda P_n}$ are $\tau_t^{\lambda\bar{P}}$ KMS. Now almost surely $\omega^{\lambda\bar{P}}$ is unique. Again for local A

$$\lim_{\lambda\to 0} \|\tau_t^{\lambda\bar{P}} A - \tau_t A\| = 0$$

so $\lim_{\lambda\to 0} \omega^{\lambda\bar{P}}$ is an extremal KMS state almost surely by the properties of a convex functional.

Of course, one would prefer to exchange $\lim_{n\to\infty} \lim_{t\to\infty}$ or even more treat adiabatic switching of global perturbations. To do this we would need additional assumption on space-time correlations. The Møller automorphisms $\gamma_\pm$ do for sure not exist and would only hinder to favour pure states.

We have concentrated here on quantum statistics. Since the algebra at infinity has its counterpart also in classical statistical mechanics, equivalent results can be obtained also in this context as is discussed in Ref. 9 in chapter 7, Corollary 7.30, though not expressed in terms of time evolution.

8 Surface Perturbation

The shortcoming in the above argument lies in the fact that our result is restricted to translation invariant KMS states. Therefore we miss crystals – to restrict the previous arguments on a sublattice seems artificial, because we would have to know the lattice size a priori – and also local coexistence of e.g. water and vapor in separated regions.

Global perturbation can be expressed on the local level in the following way:

We start with $\omega^{\lambda\bar{P}}$ and restrict it to $\mathcal{A}_\Lambda$. There it is a KMS state – Ω is cyclic and separating – with respect to some Hamiltonian

$$H_\Lambda + \lambda \sum_{x\in\Lambda} \sigma_x P + W_\Lambda. \tag{8.1}$$

We know that

$$\lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \omega^{\lambda P}(W_\Lambda(\lambda)) = 0 \tag{8.2}$$

and in this sense is a surface term. Whether it is really concentrated on the surface is harder to estimate due to noncommutativity effects.

$$H_\Lambda + \lim_{\lambda \to 0} W_\Lambda(\lambda) = H_\Lambda + W_\Lambda \tag{8.3}$$

determines ω^0 restricted to $\mathcal{A}_\Lambda$. In this sense our last result means that almost all W_Λ which lead to translationally invariant states lead to pure phases. This should be generalized to arbitrary W_Λ where of course one has to specify what is meant with almost all. So far W_Λ has to be small with respect to the volume, but we would prefer finite with respect to the surface. Also we should find some insight how weak decay of local correlations – as it happens, if a continuous symmetry is broken – influences the stability of pure thermodynamic phases. So far results mainly exist for the Ising model where we have enough mathematical tools to ask more detailed questions. Compare e.g. R. Dobrushin [10] in this volume where a global change in the boundary conditions of a pure phase of length n can only influence an area of depth $\sqrt{n}$ and thus cannot produce a mixed phase.

Acknowledgements

I want to thank the auditorium for the encouraging discussion, especially Joel Lebowitz for insisting to clarify the theory of measurement for thermal states. Also I thank Walter Thirring for critical remarks on the manuscript.

References

[1] R. Haag, N.M. Hugenholtz, M. Winnink, *Commun. Math. Phys.* **5** (1967) 215.

[2] O. Bratteli and D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics I and II* (Springer, New York, 1981).

[3] J. von Neumann, *Mathematische Grundlagen der Quantenmechanik* (Berlin, 1932).

[4] J.S. Bell, *Speakable and Unspeakable in Quantum Mechanics* (Cambridge University Press, 1987).

[5] D. Ruelle, in *Cargèse Lectures in Physics* (Gordon and Breach, New York, 1970).

[6] H. Narnhofer and D.W. Robinson, *Commun. Math. Phys.* **41** (1975) 89.

[7] R. Haag, D. Kastler, E.B. Trych-Pohlmeyer, *Commun. Math. Phys.* **38** (1974) 173.

[8] H. Narnhofer and W. Thirring, *Phys. Rev.* **A26** (1982) 3646.

[9] H.O. Georgii, *Gibbs Measures and Phase Transitions* (Walter de Gruyter, Berlin, 1988).

[10] R. Dobrushin, this volume.