J. Phys. A: Math. Gen. 21 (1988) L37–L41. Printed in the UK

LETTER TO THE EDITOR

Low-temperature phase diagram for models with small quasiperiodic interactions

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Received 13 October 1987, in final form 29 October 1987

Abstract. We extend the Pirogov–Sinai theory to some class of quasiperiodic interactions and we describe the phase diagram at low temperatures.

Although there is no obvious relation between the ground states of the Hamiltonian and the phase diagram at low temperature for classical spin systems it is intuitively appealing that such a relation exists. The Pirogov–Sinai theory [1] makes rigorous this intuition; it allows under some general conditions the description of the phase diagram at low temperature as a small perturbation of the diagram at zero temperature. Moreover, it shows that the corresponding Gibbs states arise as small perturbations of ground states of the Hamiltonian. In recent years it has proved that this theory provides a powerful tool for the study of a general class of models [2–7] in the case of absence of any symmetry in the Hamiltonian. (See [2,4,7,8] for more detailed references.)

All the developments of the Pirogov–Sinai theory up to now have considered the case of translation-invariant (or periodic) Hamiltonians. At a first glance, the translation invariance seems to be very important in many steps of the theory. However, if one analyses what is really needed one realises that it is sufficient to have only a translation invariance 'in the mean' with fluctuations in the volume having a magnitude smaller than a 'surface term' of this volume. This condition is fulfilled in many interesting models.

The aim of this letter is to present some development of the Pirogov–Sinai theory for the case of quasiperiodic interactions (at least for a special class of models with a small quasiperiodic perturbation). Roughly speaking, we show that for a small quasiperiodic perturbation of the translation-invariant Hamiltonian, the phase diagram of the model is only a small perturbation of the original phase diagram. In the following, we only sketch the main lines of the theory and its extension to the case of quasiperiodic interactions. For a more detailed exposition, see [8].

The study of this problem is not of purely academic interest. In the last few years many new materials have been discovered exhibiting a quasiperiodic structure; it therefore seems interesting to understand the statistical physics of these objects. As a first step in this direction we study simplified models where the spins live on a regular lattice but they interact via quasiperiodic interactions. Such models could even describe quite precisely thin epitaxial layers of two different species of adatoms on a quasiperiodic substratum. In this case the adatoms arrange themselves on a regular

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lattice but the choice of the adatom species (A or B say) is modulated by the underlying quasiperiodicity of the bulk. Such models precisely fall into the class of interactions we study here.

We consider a spin, living on a lattice $\mathbb{Z}^\nu$ (with $\nu \geq 2$) and taking values in a discrete finite set S. A configuration, x, is an element of $S^{\mathbb{Z}^\nu}$. The Hamiltonian is written as usual in terms of the interaction potentials Φ_A

$$H(x) = \sum \Phi_A(x). \tag{1}$$

We assume that the interactions have a finite interaction range r, i.e. $\Phi_A \equiv 0$ if diam $A > r$. In our case some of the potentials are quasiperiodic. As a concrete example of a quasiperiodic model, consider an Ising model with a quasiperiodic external field described, for instance, by the Hamiltonian

$$H_\Lambda(\sigma) = \sum_{\langle ij \rangle} \tfrac{1}{2}(1 - \sigma_i \sigma_j) + \sum h_i \sigma_i \tag{2}$$

with $h_i = \alpha \sin(2\pi\omega_1 i_1 + \ldots + 2\pi\omega_\nu i_\nu)$, where $\{\omega_l, 1\} l = 1, \ldots, \nu$ are rationally independent having some special Diophantine properties that are explained later, and α is small. The following setting is, however, much more general and not necessarily attached to this particular model.

We express the Hamiltonian (1) in terms of contours as usual in the Pirogov–Sinai theory, i.e. we first choose some constant reference states $\{x^q, q \in Q\}$ indexed by an index set $Q \subset S$. These reference states may be considered as the ground states of the Hamiltonian without quasiperiodic interactions (unperturbed Hamiltonian). The generalisation to non-constant reference states, for instance quasiperiodic ones, seems feasible. Work in this direction is in progress.

The important notion of the contour is introduced as follows [9]. One first defines a q-correct point for the configuration x as a site $i \in \mathbb{Z}^\nu$ in the r-neighbourhood of which the configuration x is equal to x^q. Consequently, an incorrect point is a site $i \in \mathbb{Z}^\nu$ for which there is no q such that i is a q-correct point. The contours Γ of x are defined as the restriction of the configuration x to the connected components of the set of incorrect points. These connected components are denoted by supp Γ and the interior (int Γ) and exterior (ext Γ) are defined in an obvious way. We say that Γ is a q-contour Γ^q if the configuration on ext Γ is equal to x^q. Defining the local energy density $e_q(t)$ for the q-reference state by

$$e_q(t) = \sum_{A \ni t} \frac{\Phi_A(x^q)}{|A|} \qquad t \in \mathbb{Z}^\nu \tag{3}$$

and the contour weight $\Phi(\Gamma^q)$ by

$$\Phi(\Gamma^q) = \sum_{A \subset \mathbb{Z}^\nu} \Phi_A(x) \frac{|A \cap \operatorname{supp} \Gamma^q|}{|A|} - \sum_{t \in \operatorname{supp} \Gamma} e_q(t)$$

the Hamiltonian (1) can be written in the volume Λ as

$$H(x_\Lambda) = \sum_{q' \in Q} \sum_i \Phi(\Gamma_i^{q'}) + \sum_{q' \in Q} \sum_{t \in \Lambda_{q'} \cup_i \operatorname{supp} \Gamma_i^{q'}} e_{q'}(t)$$

provided that all contours $\Gamma_i^{q'}$ satisfy the condition supp $\Gamma_i^{q'} \subset \Lambda$. ($\Lambda_q$ denotes the set of points $i \in \Lambda$ where the configuration x is equal to the q-reference state; i.e. $x_i = x_i^q$). The contour weights are required to fulfil the so-called Peierls condition

$$\Phi(\Gamma) \geq \tau |\operatorname{supp} \Gamma|$$

for some $\tau = \tau(\beta)$ which becomes big at low temperature. (Typically, τ is proportional to β.)

The 'diluted' partition function with q-boundary condition, $Z^q(\Lambda)$, is defined as usual and the mean free energy of the model as

$$h_q = \lim_{\Lambda\uparrow Z^\nu} \frac{1}{|\Lambda|} Z^q(\Lambda).$$

Let W be some finite subset of $\mathbb{Z}^\nu$. A W-local function f_W of the spin configuration x is a function depending on the values the configuration x takes on W, i.e. if $(t_1, \ldots, t_{|W|})$ denote the points of W taken in some order (e.g., lexicographic), $f_W = f_W(x_{t_1}, \ldots, x_{t_{|W|}})$. We call this the extrinsic dependence of f_W on W. For example, the interaction potentials Φ_A are A-local functions. The W-local functions are introduced to formulate the properties of the interaction potentials in an abstract manner. One must remember that we wish to deal with a situation where some of the interactions are not translation invariant (in fact they are quasiperiodic). Hence, the dependence of the W-local functions on the values of the configuration x on W *does not exhaust* all its functional dependence on W as should be the case if all the interactions were translation invariant. What will play an important role in the following is the intrinsic dependence of W-local functions on W. Let W_s be the parallel transport of W by $s \in \mathbb{Z}^\nu$ and $(t'_1, \ldots, t'_{|W_s|})$ be the points of W_s taken in the lexicographic order. To grasp the intrinsic dependence of f_W on W we introduce $f_{W_s}(x_{t'_1-s}, \ldots, x_{t'_{|W_s|}-s})$. For any two vectors $a, b \in \mathbb{R}^\nu$ we define $ab \in \mathbb{R}^\nu$ to be the vector obtained by componentwise multiplication. Now, assume that there exist M vectors $\omega^{(i)} \in \mathbb{R}^\nu$, $i = 1, \ldots, M$, and a function g_W of $2M$ vector variables ($g_W: \mathbb{R}^{2M\nu} \to \mathbb{R}$), periodic in each of the last M vector variables with periods $P^{(i)} \in \mathbb{R}^\nu$, $i = 1, \ldots, M$, and $(P^{(i)}_\alpha, \omega^{(i)}_\alpha)$, $i = 1, \ldots, M$; $\alpha = 1, \ldots, \nu$ being rationally independent, and such that we can write $f_{W_s}(x_{t'_1-s}, \ldots, x_{t'_{|W_s|}-s}) = g_W(\omega^{(1)}, \ldots, \omega^{(M)}; \omega^{(1)}s, \ldots, \omega^{(M)}s)$; then f_{W_s} is called a quasiperiodic W-local function. Strictly speaking, g_W depends also on the values of the configuration x on the set W (before its translation by s) but this dependence is not explicitly stated. In the example given at the beginning of this letter, the one-particle potential $\Phi_{\{i\}}(\sigma_i) = \alpha \sin 2\pi(\omega, i)\sigma_i$ provides a particularly simple illustration of a quasiperiodic $\{i\}$-local function since $\Phi_{\{i+s\}}(\sigma_{i+s-s}) = [\alpha \sin 2\pi(\omega, i)\sigma_i] \cos 2\pi(\omega, s) + [\alpha \cos 2\pi(\omega, i)\sigma_i] \sin 2\pi(\omega, s)$. The set $L_f = \{m_1\omega^{(1)} + \ldots + m_M\omega^{(M)} | m_1, \ldots, m_M \in \mathbb{Z}^\nu\}$ is called the frequency module of f generated by $\omega^{(i)}$. For simplicity we consider, in the following, quasiperiodic functions with frequency module generated by a unique vector ω. Generalisations to more complicated frequency modules introduce solely notational difficulties. Since some interactions are quasiperiodic, all the subsequently defined functions of geometrical objects (e.g. $\Phi(\Gamma)$, $e_q(t)$, etc) will be quasiperiodic, even if it is not explicitly mentioned.

Suppose that the original Hamiltonian admits $m+1$ degenerate states. Then the mean energy densities

$$e_q = \lim_{\Lambda\uparrow Z^\nu} \frac{1}{|\Lambda|} \sum_{t\in\Lambda} e_q(t)$$

will be the same for $q_1, \ldots, q_{m+1}$. Hence, at zero temperature we have the coexistence of $m+1$ states. To construct the phase diagram at zero temperature it is sufficient to introduce a set of m external fields removing the degeneracy of the ground states, i.e. to introduce a suitable vector parameter $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_m)$ in the Hamiltonian. The mean energy densities become functions of $\boldsymbol{\xi}$, $e_q = e_q(\boldsymbol{\xi})$ and the degeneracy $e_{q_1}(\mathbf{0}) = \ldots = e_{q_{m+1}}(\mathbf{0})$ should be removed in the sense explained below (see the theorem).

Knowing the phase diagram at zero temperature means that a map z is given on the space of parameters ξ of the form

$$z:\mathbb{R}^m \to \mathbb{R}^m \qquad z(\xi)=(e_{q_2}-e_{q_1},\ldots,e_{q_{m+1}}-e_{q_1}).$$

Equivalently, the phase diagram at low temperature is described by a map l of the form

$$l:\mathbb{R}^m \to \mathbb{R}^m \qquad l(\xi)=(h_{q_2}-h_{q_1},\ldots,h_{q_{m+1}}-h_{q_1}).$$

Intuitively one expects that the phase diagram at low temperature looks very similar to (i.e. it has the same number of phases, the same number of coexistence lines, etc, as) the phase diagram at zero temperature. The Pirogov-Sinai theory makes this intuition rigorous establishing that under certain conditions the map $l^{-1}\circ z:\mathbb{R}^m\to\mathbb{R}^m$ exists and it is a homeomorphism near the identity or, stated differently, the map l is a homeomorphic deformation of z. However, this property for $l^{-1}\circ z$ cannot be proved for every quasiperiodic interaction. The generator ω of the frequency module must verify the Diophantine property $\|n\omega/\pi\|\geqslant 1/K_1n^2$ for every $n\in\mathbb{Z}^\nu\backslash\{0\}$($\|\cdot\|$ means the distance to the nearest integer), and the interaction must be smooth enough such that we have the following bound for the derivatives of the contour weight

$$\left|\frac{\mathrm{d}^k}{\mathrm{d}(\omega t)^k}\exp(-\Phi(\Gamma_t))\right|\leqslant \varepsilon^{|\mathrm{supp}\,\Gamma|}$$

(t being the lexicographically first point of supp Γ) and the very mild bound

$$\left|\frac{\mathrm{d}^k}{\mathrm{d}(\omega t)^k}e_q(t)\right|\leqslant K \qquad k=1,2,3,4.$$

Under these conditions we can prove the following theorem.

Theorem. Let $|Q|=m+1$ and ξ be a vector parameter written in the form $(\xi_1,\ldots,\xi_m)$. Let $e_q(\xi)$ be all the same for $\xi=0$ and the matrix

$$M=\left(\frac{\partial(e_{q_i}-e_{q_1})}{\partial\xi_j}\right)$$

with $i=2,\ldots,m+1$ and $j=1,\ldots,m$ be invertible. Then, if $\tau=\tau(\beta,\|M^{-1}\|)$ is sufficiently large, and the previous conditions on ω and the derivatives of $\exp(-\Phi)$ and $e_q(t)$ are fulfilled, the mapping

$$l(\xi)=(h_{q_2}-h_{q_1},\ldots,h_{q_{m+1}}-h_{q_1})$$

is invertible and one-to-one between some neighbourhood of $\mathbf{0}$ in $\mathbb{R}^m$ and an open $\nu\ni 0$ in $\mathbb{R}^m$. The map $l^{-1}\circ z$ where z is given by $z(\xi)=(e_{q_2}-e_{q_1},\ldots,e_{q_{m+1}}-e_{q_1})$ is moreover smooth.

We do not give any proof here; it uses some standard tools from analysis like the inverse map theorem. All the technical steps can be found in [8].

It is easy to generalise our results to take into account much larger sets of irrational ω. However, the less restricting the conditions are on ω, the more restricting the requirements should be on the derivability, i.e. if $\|n\omega/\pi\|\geqslant 1/K_1n^{1+\alpha}$ holds for some integer α, then to prove the theorem we need a control on the derivatives $\mathrm{d}^k/\mathrm{d}(\omega t)^k$ up to the order $3+\alpha$. We conjecture that the phase diagram at low temperature is different from the one at zero temperature if the control on derivatives stops to some order less than required by the Diophantine properties of ω.

The authors wish to thank the referee for pointing out an obscure statement in the original formulation of quasiperiodicity. This work was partially supported by the Swiss National Science Foundation.

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