Long-Range Order in Classical Lattice Linear Oscillator Systems and Peierls Argument

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Existence of the ferromagnetic long-range order is proven for Gibbs classical lattice systems of linear oscillators with a strong polynomial pair nearest neighbor ferromagnetic potential.

1 Introduction

Mathematical theory of phase transitions began its quick development half a century ago by describing critical properties of the Ising-type finite valued spin systems in terms of a contour technique [1]. This technique gave rise to Pirogov–Sinai (PS) theory, based on a knowledge of ground states, which allows to calculate a phase diagram at low temperatures, and can be successfully applied not only to classical spin systems with finite number of ground states but also to quantum ones. Generalization of the PS theory to Gibbs lattice systems with discrete or continuous set of ground states, such as systems of rotators and oscillators, characterized by continuous variables associated to lattice sites of the hypercubic lattice $\mathbb{Z}^d$, demands a profound combinatorial and probabilistic technique. Such a technique was proposed in [2] for linear lattice oscillator systems with nearest neighbor interaction. In this important paper the intuitive idea that the number of phases is determined by the number of global minima of the polynomial external field was justified. The technique of this paper was used also in proving of existence of an order parameter (the ground state expectation value of the squared absolute value of the Higgs field) in the $SU(n)$ lattice Higgs gauge field model [3]. In the infinite gauge interaction limit the Euclidean action, i.e. the potential energy of the Gibbs system, is reduced to the potential energy of oscillator system from the previous paper.

If one deals with classical systems of oscillators interacting with spins or fermions having simple self-interaction then, integrating out the variables corresponding to the spins and fermions in the partition function, one obtains an effective lattice oscillator system. Such an effective oscillator system is derived in the stationary quantum Holstein model.

To describe a phase diagram of a Gibbs system with a continuous set of ground states one has at first to look at decrease of correlations and then find long-range order (lro) and the associated order parameter. For different nearest neighbor lattice anisotropic systems with nearest neighbor (n-n) interaction, including linear oscillator systems, occurrence of lro was established with the help of the generalized Peierls argument in [4]. Lro means that there is no decrease of correlations. For high temperatures or weak coupling there is always a decrease of correlations for usual interactions. The order parameter always has a jump at critical values of the temperature or a coupling constant, i.e. it is a discontinuous function of these parameters. This fact can often be attributed to a breakdown of a discrete symmetry, for instance, Z_2 symmetry associated to a change of signs of all (infinite) spin variables when potential energy is an even function.

Since general oscillator systems are quite important there emerged a necessity to generalize the Peierls argument to non-nearest neighbor interactions. This argument has been already generalized for the linear oscillator system appeared in the stationary Holstein model in [5] but the technique of this paper gave no hint how to do this in a general case.

2 Peierls argument and lro

The Peierls argument is based on the contour bound for the Gibbs average on a compact connected set Λ (hypercube)

$$\langle \prod_{\langle x,y\rangle \in \Gamma} \chi_x^+ \chi_y^- \rangle_\Lambda \leq e^{-|\Gamma| E},$$

where the contour energy $E > 0$ is independent of Λ and Γ, Γ is the set of nearest neighbors with left and right sides in Γ belonging to different sides of a contour γ that is a completely connected (without holes) set of faces of completely connected union of unit cubes, centered at lattice sites, i.e. Γ is a set of nearest neighbors associated to γ, $|\Gamma| = 2|\gamma|$ is the number of lattice sites in Γ or twice the hyper-area of the contour γ, γ is closed if the faces adjacent to the boundary of Λ are added,

$$\chi_x^+(q_\Lambda) = \chi_{(0,\infty)}(q_x), \qquad \chi_x^-(q_\Lambda) = \chi_{(-\infty,0)}(q_x), \qquad q_x \in \mathbb{R},$$

$\chi_{(a,b)}$ is the characteristic function of the open interval (a, b). q_x may be one of the component of a many-component oscillator or rotator.

For classical linear oscillator systems with the potential energy U and the inverse temperature β the Gibbs average is given by

$$\langle F_X \rangle_\Lambda = Z_\Lambda^{-1} \int F_X(q_X) e^{-\beta U(q_\Lambda)} dq_\Lambda = \int F_X(q_X) \rho^\Lambda(q_X) dq_X, \qquad q_X = (q_x, x \in X),$$

$$\rho^\Lambda(q_X) = Z_\Lambda^{-1} \int e^{-\beta U(q_\Lambda)} dq_{\Lambda\setminus X}, \qquad Z_\Lambda = \int e^{-\beta U(q_\Lambda)} dq_\Lambda.$$

Here the integrations are performed over $R^{|\Lambda|}$, $R^{|X|}$, $R^{|\Lambda\setminus X|}$ and ρ^Λ are the correlation functions, where $|X|$ is the cardinality (number of sites) of X.

When E diverges at zero temperature or infinite strength of nearest neighbor ferromagnetic interaction (coupling constant) then the Peierls argument yields inequality [4,6] for sufficiently low temperature or large coupling constant

$$\langle \chi_x^+ \chi_y^- \rangle_\Lambda \leq a e^{-2dE}. \tag{1}$$

where a is a positive constant independent of Λ. This leads immediately to ferromagnetic lro for unit spins s_x, where a' is independent of Λ, inequality $\langle m_\Lambda^2 \rangle_\Lambda \geq a'$ and non-triviality of the order parameter

$$m_\Lambda = |\Lambda|^{-1} \sum_{x \in \Lambda} s_x.$$

in the thermodynamic limit, i.e. $\Lambda \to \mathbb{Z}^d$. This order parameter is an analog of the Ising magnetization.

Indeed, from $\chi_x^{+(-)} = \frac{1}{2}[1 \pm s_x]$ one obtains

$$4\langle \chi_x^+ \chi_y^- \rangle_\Lambda = 1 + \langle s_x \rangle_\Lambda - \langle s_y \rangle_\Lambda - \langle s_x s_y \rangle_\Lambda.$$

For systems invariant under the transformation of changing signs of the oscillator variables the third and the second terms in the right-hand side of latter equality are equal to zero and

$$\langle s_x s_y \rangle_\Lambda = 1 - 4\langle \chi_x^+ \chi_y^- \rangle_\Lambda.$$

The average in the right-hand side of this equality is arbitrarily small due to (1) and the unit spin lro occurs.

To derive (1) one has to insert

$$1=\prod_{l\in\Lambda}(\chi_l^+ + \chi_l^-) = \sum_{s_\Lambda, s_x=\pm 1}\prod_{l\in\Lambda}\chi_l^{s_l}$$

into the left-hand side of the contour bound. The sum over spin configurations is equivalent to a sum over contours $\gamma_{x,y}$ separating x, y which may end on the boundary of Λ and be non-closed (the resummation over spin configurations outside of the set of nearest neighbors Γ built on the contour γ should be performed). That is, the left-hand side of (1) is bounded by

$$\sum_{\gamma_{x,y}\in\Lambda}\langle\chi_x^+\chi_y^- \prod_{x',x''\in\Gamma(\gamma_{x,y})}\chi_x^+\chi_{x'}^-\rangle_\Lambda \le \sum_{\gamma_{x,y}\in\Lambda}\langle\prod_{x',x''\in\Gamma(\gamma_{x,y})}\chi_{x'}^+\chi_{x''}^-\rangle_\Lambda \le \sum_\gamma\langle\prod_{x',x''\in\Gamma(\gamma)}\chi_{x'}^+\chi_{x''}^-\rangle_\Lambda,$$

where γ is a closed contour. The sum over the closed contours is bounded by the right-hand side of (1) [7, Lemmas 5.3.5–6].

From the Frohlich–Lieb argument [4] one derives the following inequality for oscillator systems an arbitrary positive r

$$\langle\sigma_x\sigma_y\rangle_\Lambda \ge r^2\langle s_x s_y\rangle_\Lambda - \langle\sigma_x^2\sigma_y^2\rangle_\Lambda^{\frac{1}{2}} - 4, \qquad \sigma_x(q_\Lambda)=q_x\in\mathbb{R}.$$

For systems with potential energy satisfying super-stability and regularity conditions [7, 12] the second term in the right-hand side of the inequality is uniformly bounded in Λ and unit spin lro implies occurrence of the ferromagnetic oscillator lro

$$\langle\sigma_x\sigma_y\rangle_\Lambda \ge a'' > 0,$$

where a'' does not depend on Λ. This, of course, means non-triviality of the oscillator order parameter

$$M_\Lambda = |\Lambda|^{-1}\sum_{x\in\Lambda}\sigma_x.$$

The subtle point is that the contour bound has to hold for systems with non-zero nearest-neighbor ferromagnetic interaction.

3 Results

Let us consider the linear oscillator system with the potential energy (an even function)

$$U(q_\Lambda)=\sum_{x\in\Lambda}u(q_x)+\sum_{\langle x,y\rangle\in\Lambda}\phi(q_x,q_y)+U'(q_\Lambda), \qquad q_x\in\mathbb{R},$$

where u is the external field which is a bounded below even polynomial of $2n$-th degree ($2\le n\in\mathbb{Z}$)

$$\phi(q_x,q_y)=-g(q_x^k q_y^l + q_x^l q_y^k), \qquad ptk+l=2n_0,$$

u does not depend on g, U' is expressed as a finite sum of products $q_{x_j}^{l_j}$ with negative coefficients and U satisfies the super-stability and regularity conditions which almost guaranteed existence of the thermodynamic limit. g is the strength of the ferromagnetic nearest-neighbor interaction. There is an remarkably simple derivation of the contour bound, proposed in [8] for the case $n_0=1$, which is based on the fact that the Gibbs average satisfies GKS inequality (generalized Griffiths inequality) [9] and the bound

$$\chi_x^+\chi_y^- \le e^{-\frac{g\beta}{2}(\sigma_x^k\sigma_y^l+\sigma_x^l\sigma_y^k)}. \tag{2}$$

This bound follows from

$$\chi_x^+\chi_y^- = e^{-\frac{g\beta}{2}(\sigma_x^k\sigma_y^l+\sigma_x^l\sigma_y^k)}e^{\frac{g\beta}{2}(\sigma_x^k\sigma_y^l+\sigma_x^l\sigma_y^k)}\chi_x^+\chi_y^- \le e^{-\frac{g\beta}{2}(\sigma_x^k\sigma_y^l+\sigma_x^l\sigma_y^k)}\chi_x^+\chi_y^- \le e^{-\frac{g\beta}{2}(\sigma_x^k\sigma_y^l+\sigma_x^l\sigma_y^k)}.$$

Here one takes into account that $\sigma_x \ge 0$, $\sigma_y \le 0$. The latter inequality is employed for the proof of the contour bound as follows

$$\langle \prod_{\langle x,y\rangle\in\Gamma} \chi_x^+\chi_y^-\rangle_\Lambda \le \langle e^{-\frac{g\beta}{2}\sum_{\langle x,y\rangle\in\Gamma}(\sigma_x^k\sigma_y^l+\sigma_x^l\sigma_y^k)}\rangle_\Lambda$$
$$= \left(\langle e^{\frac{g\beta}{2}\sum_{\langle x,y\rangle\in\Gamma}(\sigma_x^k\sigma_y^l+\sigma_x^l\sigma_y^k)}\rangle_{\Lambda[\Gamma]}\right)^{-1} \le e^{-\frac{g\beta}{2}\sum_{\langle x,y\rangle\in\Gamma}\langle(\sigma_x^k\sigma_y^l+\sigma_y^k\sigma_y^l)\rangle_{\Lambda[\Gamma]}} = e^{E_\Gamma}.$$

where $\langle\cdot,\cdot\rangle_{\Lambda[\Gamma]}$ is the average corresponding to the potential energy

$$U_\Gamma(q_\Lambda) = U(q_\Lambda) + \frac{g}{2}\sum_{x,y\in\Gamma}(q_x^kq_y^l + q_x^lq_y^k).$$

In latter line we applied the Jensen inequality. Taking into account that the Gibbs average is a monotone increasing function in interaction (a consequence of the GKS inequality) we obtain

$$E_\Gamma \ge E|\Gamma|, \qquad E = \beta g\langle\sigma^k\sigma'^l + \sigma^l\sigma'^k\rangle,$$

where

$$\langle\sigma^k\sigma'^l + \sigma^l\sigma'^k\rangle = Z^{-1}(2)\int(q_1^kq_2^l + q_1^lq_2^k)e^{-\beta u(q_1,q_2)}dq_1dq_2,$$
$$Z(2) = \int e^{-\beta u(q_1,q_2)}dq_1dq_2, \qquad u(q_1,q_2) = u_0(q_1) + u_0(q_2) - g\big(q_1^kq_2^l + q_1^lq_2^k\big),$$

k, l are positive integers, $k = 2s-1$, $l = 2(n_0-s)-1$, i.e. $k+l = 2n_0$ and β is the inverse temperature. This expression for E is the generalized BF contour bound.

We show [10] that E diverges at infinity in g and that means that the unit spin and oscillator lro occur in the system at sufficiently large g. We establish that

$$q_x^kq_y^l + q_x^lq_y^k = q_x^{2n_0} + q_y^{2n_0} - (q_x-q_y)^2Q(q_x,q_y),$$

where Q is a homogeneous positive polynomial. This means that the effective external potential $u(q) - gq^{2n_0}$ has minima whose depth depends on g. This representation implies that ground states are ferromagnetic.

More interesting systems are described by finite-range U' which has non-ferromagnetic terms. In this case the above arguments are not useful. Let us consider the case

$$\phi(q_x,q_y) = g_0(q_x-q_y)^{2n_1}Q'(q_x,q_y), \qquad g_0 = g^{\frac{\xi}{2(n-n_0)}} = z^{-\xi}, \qquad u(q) = u_0(q) - gq^{2n_0},$$

where u_0 is a bounded below even polynomial with $2n$ degree, Q' is the positive symmetric even homogeneous polynomial with the degree $2n_2$, $n_2 < n - n_1$ and $Q(1,1) = 1$. The case of non-positive translation invariant U' small for large g and $Q' = 1$, $n_1 = 1$, $n_0 = 1$, $g_0 = g$, $u_0 = \eta q^{2n}$ was considered in [6, 10–11].

A derivation of the contour bound was based on the superstability bound for the rescaled correlation function (the variables are rescaled by $g^{-\frac{1}{2}}$) translated by the minimum e_0 of the rescaled external field u_g and the analog of (2)

$$\chi^+(q_x)\chi^-(q_y) \le \exp\{\beta[Q_g(q_x,q_y) - e_0]\}, \tag{3}$$

where

$$Q_g(q_x, q_y) = e_0^{-1}\left[(q_x - q_y)^2 + \frac{4}{3}\left(|q_x^2 - e_0^2| + |q_y^2 - e_0^2|\right)\right].$$

It is derived easily from two inequalities ($R = e_0$, $c = \beta e_0^{-1}$)

$$\chi^+(q_x)\chi^-(q_y) \le e^{-c[R^2-(q_x-q_y)^2]}, \qquad |q_x|, |q_y| \ge 2^{-1}R,$$
$$\chi^+(q_x)\chi^-(q_y) \le e^{-c\left[R^2-\frac{4}{3}(|q_x^2-R^2|+|q_y^2-R^2|)\right]}, \qquad |q_x|, |q_y| \le 2^{-1}R.$$

For $|q_x| \le \frac{R}{2}$, $|q_y| \ge \frac{R}{2}$ the second term in the expression for Q is not less than cR^2.

More precisely, we demand that the following super-stability and regularity conditions hold

$$U(q_\Lambda) \ge \sum_{x\in\Lambda} u^-(q_x), \qquad u^-(q) = u(q) - \zeta v^0(zq) - \zeta_0, \qquad z = g^{-\frac{1}{2(n-1)}},$$

$$|W'(q_X; q_Y)| \le \sum_{x\in X,\, y\in Y} \Psi'(|x-y|)\left(v^0(z^{1-n}q_x) + v^0(z^{1-n}q_y)\right), \qquad v^0(q) = \sum_{j=1}^{n-1} q^{2j},$$

where ζ, ζ_0 are positive constants, $\Psi' \in L^1(\mathbb{Z}^d)$ and

$$W'(q_X; q_Y) = U'(q_\Lambda) - U'(q_Y) - U'(q_X), \qquad \Lambda = X \cup Y.$$

The second term in the expression for u^- guarantees that the contribution of the non-positive part of U' is small for large g.

Let $\rho_*^\Lambda(q_X)$, U_*, u_*, u_*^- denote, respectively, the rescaled and translated by e_0, correlation functions, potential energy, potentials u and u^- and put. From the translation invariant character of the Lebesque measure it follows that ρ_*^Λ is expressed in terms of U_*. In our method we have to rely on the following important theorem [6].

Theorem 1. *For the correlation functions ρ_*^Λ the following superstability bound is valid*

$$\rho_*^\Lambda(q_X) \le \exp\left\{|X|e_*(g) - \beta\left[U_*^+(q_X) + \sum_{x\in X} u_*^+(q_x)\right]\right\},$$

where

$$u_*^+ = u_*^- - 3\epsilon v^0, \qquad \epsilon = z^{2n(n-1)},$$

$e_*(g)$ depends neither on oscillator variables nor Λ, U_*^+ is the positive part of U_* generated by a pair potential and for arbitrary $\delta > 0$ and sufficiently large g

$$\delta e_0 \ge e_*(g).$$

From (3) and the superstability bound it follows that for $e_0 > 1$ the contour bound holds with

$$E = \beta e_0 - e_*(g) + 2\ln I_*\big(g, Q^0\big),$$

where

$$I_*(g, Q^0) = \int e^{-\beta[u_*^+(q) - e_0^{-1}Q^0(q;e_0)]}dq, \qquad Q^0(q; e_0) = \frac{4}{3}|q(q+2e_0)|.$$

The term with U_*^+ in the super-stability bound plays an important role: it cancels the term generated by the first term in the expression for Q_g. It is not difficult to see that $\ln I_*(g, Q^0)$ diverges at infinity in g as δe_0, where $\delta > 0$ is arbitrary small. That is, E diverges in g at infinity as e_0, which is proportional to $g^{\frac{n}{2(n-1)}}$, and this proves occurrence of lro. If one uses the usual Ruelle superstability [12, 13] bound without the term U_*^+ in its right-hand side then the first term in Q_g yields an additional term $\beta e_0^{-1} q^2$ under the sign of the exponent in the expression for I_* and the method fails.

By the similar arguments we prove occurrence of lro for the above pair potential ϕ and non-translation invariant U' satisfying the superstability and regularity conditions guaranteeing that non-ferromagnetic part of U' is small at large g [14]. We also establish how g_0 has to depend on g in order to preserve lro. g_0 should not be very small to permit U_*^+ to cancel the contribution of the first term in the expression for Q_g in and it cannot be very large because it has to permit the rescaled and translated by e_0 ferromagnetic n-n interaction to satisfy the uniform in g regularity condition.

Resume. Our results show that the ferromagnetic lro in lattice linear oscillator systems occurs only if a depth of the effective potential and the strength of the polynomial ferromagnetic n-n interaction are large and correlated and the non-ferromagnetic part of the potential energy is sufficiently small.

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