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No-go theorem for quantum structural phase transitions

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Abstract. We prove that quantum fluctuations can suppress structural phase transitions. We give a rigorous proof for a one-component ($\mathbb{R}^1$) quantum crystal with local double-well anharmonism under the condition that the masses of the atoms in the lattice sites of $\mathbb{Z}^d$ ($d \geqslant 3$) are light enough.

1. Introduction

Rigorous proofs about the absence of spontaneous symmetry breaking started with the celebrated works of Mermin, Wagner and Hohenberg based on the Bogoliubov inequality [1–3]. Originally the proofs were about continuous symmetry groups, and the theorems work as well for classical as for quantum systems. The type of systems considered showing absence of symmetry breaking were considered to have short-range interactions and low dimensionality. Later, techniques were developed in order to obtain similar results for discrete symmetries, based on energy–entropy inequalities [4, 5]. It was essential in this area that no genuine different physical ideas were implied for either classical or quantum systems or for this type of symmetry.

These methods give immediate results for dimensions $d = 1$ and sometimes for $d = 2$, when thermal fluctuations are strong enough to destroy the order parameter.

In this paper we want to add a new rigorous result to the field based on a new mechanism excluding spontaneous symmetry breaking, which has a typical quantum nature, i.e. it exploits the fact that quantum fluctuations increase when the mass of the particles becomes smaller.

For heavy particles, rigorous results exist for spontaneous breaking of the symmetry in ferroelectrics for classical as well as for quantum systems [6–9]. The question concerns light particles. We prove for a quantum one-site anharmonic crystal model (structural instability or ferroelectric model) that the quantum fluctuations are strong enough to destroy the spontaneous symmetry breaking if the particles are light enough. In the spherical approximation of anharmonic crystals, this fact is well known, see e.g. [10] and [11].

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2. The model

Let $\mathbb{Z}^d$ be a d-dimensional cubic lattice. At each lattice point $l \in \mathbb{Z}^d$ we associate a quantum particle of the mass m with position $Q_l \in \mathbb{R}^1$ and momentum P_l such that $[P_l, Q_l] = \frac{\hbar}{i}$. Let $\mathcal{H} = L^2(\mathbb{R}^1)$, then with each $\Lambda \subset \mathbb{Z}^d$ we associate the Hilbert space $\mathcal{H}_\Lambda = \bigotimes_{l\in\Lambda} \mathcal{H}_l$ (tensor product of copies $\mathcal{H}_l = L^2(\mathbb{R}^1)$).

For each finite volume $V = |\Lambda|$ the model Hamiltonian $H_\Lambda(h)$ is a self-adjoint operator

$$H_\Lambda(h) = T_\Lambda + S_\Lambda - \sum_{l\in\Lambda} h \cdot Q_l \qquad h \in \mathbb{R}^1 \tag{2.1}$$

with the natural domain $D(H_\Lambda) \subset \mathcal{H}_\Lambda$. Here

$$T_\Lambda = \sum_{l\in\Lambda} \frac{P_l^2}{2m} + \frac{1}{4} \sum_{l,l'\in\Lambda} \phi_{ll'}(Q_l - Q_{l'})^2 + \frac{a}{2} \sum_{l\in\Lambda} Q_l^2 \tag{2.2}$$

where (for simplicity) we suppose that the harmonic matrix $\phi_{ll'}$ corresponds to the interaction between nearest-neighbour sites: $\phi_{ll'} = c\delta_{(l',l+\hat{l}_\alpha)}$; $\alpha = 1, 2, \ldots, d$; $c > 0$. The site operator S_Λ is given by

$$S_\Lambda = \sum_{l\in\Lambda} W(Q_l) \tag{2.3}$$

and represents (one-component) local anharmonic potentials in each $l \in \mathbb{Z}^d$, we assume the following conditions on the potential:

$$\begin{aligned} &\text{(a) } W(x) \in C(\mathbb{R}^1)\\ &\text{(b) } W(x) = W(-x)\\ &\text{(c) } \min_{x\geqslant 0}(\tfrac{1}{2}ax^2 + W(x)) = \tfrac{1}{2}ax_0^2 + W(x_0),\ x_0 > 0 \text{ and } x \mapsto \tfrac{1}{2}ax^2 + W(x)\\ &\quad \text{is monotonically increasing for } x \geqslant x_0. \end{aligned} \tag{2.4}$$

For standard examples (see e.g. [12]) one could refer to the case:

$$\tfrac{1}{2}aQ_l^2 + W(Q_l) = \tfrac{1}{2}aQ_l^2 + \tfrac{1}{4}bQ_l^4 \qquad a < 0,\ b > 0 \tag{2.5}$$

or to the case [10]:

$$\tfrac{1}{2}aQ_l^2 + \tfrac{1}{2}b\mathrm{e}^{-\eta Q_l^2} \qquad a > 0,\ b > 0,\ \eta > 0.$$

3. Order parameter

For each $\Lambda \subset \mathbb{Z}^d$ we take local algebra of observables $\mathcal{B}_\Lambda$ generated by the canonical position and moment operators Q_l and P_l, $l \in \Lambda$. The algebra of local observables of the system is then $\mathcal{A} = \bigcup_\Lambda \mathcal{B}_\Lambda$. For temperatures $T > 0$ ($\beta = 1/kT < \infty$), a state $\omega(\cdot)$ on $\mathcal{A}$ is an equilibrium state if it satisfies the energy–entropy balance correlation inequalities:

$$\beta\omega(A^*\delta(A)) \geqslant \omega(A^*A) \ln \frac{\omega(A^*A)}{\omega(AA^*)} \qquad \beta = 1/kT \tag{3.1}$$

for all $A \in \mathcal{A}$ [13]. Here the derivation δ is defined by the weak limit

$$\omega(A\delta(B)) = \lim_\Lambda \omega(A[H_\Lambda, B]) \qquad A, B \in \mathcal{A}. \tag{3.2}$$

In writing this equilibrium condition, we assume implicitly that we are looking at those solutions ω for which these limits exist. The existence of the limiting equilibrium states, $\lim_\Lambda \omega_\Lambda(\cdot) \equiv \omega(\cdot)$ where ω_Λ is the Gibbs state for the finite volume Λ, for quantum anharmonic crystals is considered in [14, 15]. It is a consequence of the stability of the Hamiltonian (2.1).

For any $a \in \mathbb{Z}^d$ we denote by τ_a the lattice translation $*$-automorphism defined on $\mathcal{A}$ by $\tau_a Q_l = Q_{l+a}$, $\tau_a P_l = P_{l+a}$. A state ω is called lattice translation invariant if $\omega \cdot \tau_a = \omega$ for all $a \in \mathbb{Z}^d$.

We are interested in the ergodic equilibrium states, i.e. the extremal lattice translation invariant states ω_h, determined by the Hamiltonian (2.1). If $h = 0$, the Hamiltonian has the $\mathbb{Z}_2$-symmetry with respect to the transformations $Q_l \to -Q_l$ for all l. From (3.1) one obtains easily, the following properties.

Proposition 3.1. Let $\omega_h(\cdot) = \lim_\Lambda \omega_h^\Lambda(\cdot)$ be any limiting equilibrium state of (2.1), i.e. with

$$\omega_h^\Lambda(A) = \frac{\operatorname{tr} \mathrm{e}^{-\beta H_\Lambda(h)} A}{\operatorname{tr} \mathrm{e}^{-\beta H_\Lambda(h)}} \qquad A \in \mathcal{B}_\Lambda$$

then the state $\omega_h(\cdot)$ satisfies (3.1).

If one takes periodic boundary conditions on the boundary $\partial\Lambda$ one has

$$\omega_{h=0}^\Lambda(Q_l) = 0$$

but $\omega_{h>0}^\Lambda(Q_l) > 0$ and

$$\omega_{h>0}(Q_l) \equiv \langle Q \rangle_{h>0} > 0 \qquad l \in \mathbb{Z}^d. \tag{3.3}$$

From the time invariance of the state ω_h one gets

$$\lim_\Lambda \omega_h([P_l, H_\Lambda(h)]) = 0 \qquad \text{for all } l \in \mathbb{Z}^d. \tag{3.4}$$

We define the *order parameter* of the system by

$$\langle Q \rangle_\pm = \lim_{h \to 0^\pm} \langle Q \rangle_h = \pm \langle Q \rangle_+. \tag{3.5}$$

If $\langle Q \rangle_+ \neq 0$, then the system shows spontaneous $\mathbb{Z}_2$-symmetry breaking, which yields a structural phase transition for this system. Hence if one can show that $\langle Q \rangle_+ = 0$, one proves the absence of the structural phase transition in this model.

Using the so-called infrared bounds [16, 17], the Trotter product formula approximation for Gibbs semigroups [18] and the localization bound [19] for a fixed mass m large enough, say for m larger than some M, one can prove (see [8] and [9]) that there exists a critical temperature $T_c(m) > 0$, such that for all $T < T_c(m)$, the $\mathbb{Z}_2$-symmetry of the state $\omega_{h=0}(\cdot)$ is broken. One proves in fact that

$$\sigma^2 \equiv \lim_\Lambda \omega_{h=0}^\Lambda\left(\left(\frac{1}{|\Lambda|}\sum_{l\in\Lambda} Q_l\right)^2\right) > 0 \qquad \text{for } T < T_c(m) \tag{3.6}$$

showing that the limit state $\omega_{h=0}(\cdot)$ is not extremal. However, when the mass is too small, $m < M$, the infrared bound analysis proving (3.6) breaks down.

Our aim is now to prove that for light atomic masses m, say smaller than some critical mass $m_c < M$, but for all temperatures $T \geqslant 0$, the order parameters $\langle Q \rangle_\pm$ vanish, i.e. $\langle Q \rangle_\pm = 0$. According to common wisdom [17], one has that $\langle Q \rangle_\pm \geqslant \sigma$. Therefore $\langle Q \rangle_\pm = 0$ also implies $\sigma = 0$ for $m < m_c$ and all $T \geqslant 0$. We will show that this is a consequence of the large quantum fluctuations, due to the small size of the atomic masses m.

We start the proof of this 'no-go theorem', first, by assuming the following technical condition on the potentials which is in addition to (2.4) but not really a limitation of the generality; we assume

$$\text{(i) } a < 0 \qquad \text{(ii) } W'(x) = xV(x^2) \quad \text{with } V : \mathbb{R}^1_+ \to \mathbb{R}^1_+, \text{ monotonic and } V'' \geqslant 0. \tag{3.7}$$

Conditions (2.4) and (3.7) are satisfied by examples (2.5).

We derive a first result from proposition 3.1.

Proposition 3.2. For any translation invariant equilibrium state we obtain

$$-a\langle Q\rangle_+ = \langle W'(Q)\rangle_+. \tag{3.8}$$

Proof. This follows immediately from formula (3.4) using the explicit form of the Hamiltonian (2.1) and after taking the limit $h \to 0^+$. □

4. Correlation inequalities and main results

For the anharmonic potential W, satisfying conditions (2.4) and (3.7), we get the following crucial inequality, using the Feynman–Kac representation.

Proposition 4.1]. For all finite temperatures, one obtains

$$\langle W'(Q_l)\rangle_+ \geqslant \langle Q_l\rangle_+ \langle V(Q_l^2)\rangle_+. \tag{4.1}$$

Proof. The proof is done via the following steps:

(i) By proposition 3.1, it is clear that for inequality (4.1), it is sufficient to prove the inequality for each finite volume $\Lambda \subset \mathbb{Z}^d$, namely

$$\omega^\Lambda_{h>0}(W'(Q_l)) \geqslant \omega^\Lambda_{h>0}(Q_l)\omega^\Lambda_{h>0}(V(Q_l^2)).$$

(ii) Now we use the explicit form of the Gibbs state ω_h^Λ (proposition 3.1) in its Wiener integral representation [20, 21]. By the Feynman–Kac formula, one gets for any $l \in \Lambda$, that

$$\omega_h^\Lambda(f(Q_l)) = \int_{\mathbb{R}^{|\Lambda|}} \prod_{r\in\Lambda} \mathrm{d}\xi_r(0)\, f(\xi_l(0)) \int_{\Omega^\beta_{x,x=\xi_r(0)}} \mathrm{d}\tilde{\mu}^\beta_{x,x=\xi_r(0)}(\xi_r) \times \exp\frac{c}{2}\int_0^\beta \mathrm{d}\tau \sum_{r',\|r-r'\|=1} \xi_r(\tau)\xi_{r'}(\tau) \tag{4.2}$$

where

$$\Omega^\beta_{x,x=\xi_r(0)} = \{\xi_r(\cdot) \in C([0,\beta]); \xi_r(0) = \xi_r(\beta) = x\}$$

is the space of closed continuous trajectories starting at x, and where

$$\mathrm{d}\tilde{\mu}^\beta_{x,x}(\xi) = Z_\Lambda^{-1}\,\mathrm{d}\mu^\beta_{xx}(\xi)\exp\left\{-\int_0^\beta \mathrm{d}\tau\,(\tilde{W}(\xi(\tau)) - h\xi(\tau))\right\}$$

with $\mathrm{d}\mu^\beta_{x,x}(\xi)$ the Wiener measure on $\Omega^\beta_{x,x}$, and

$$\tilde{W}(\xi) = \left(\frac{a}{2} + cd\right)\xi^2 + W(\xi).$$

(iii) If one takes $f(Q_l) = W'(Q_l)$, then inequality (4.1) is a Griffiths–Kelley–Sherman (GKS) inequality for our ferromagnetic system state (4.2), see e.g. [21].

In order to check this we follow the line of reasoning inspired by [21, ch IV]. First we use the Trotter product formula for the Gibbs semigroup $\exp\{-\beta H_\Lambda(h)\}$, and obtain

$$\omega_h^\Lambda(A) = \frac{\operatorname{tr} A \lim_{n\to\infty}(\exp(-\frac{\beta}{n}T_\Lambda)\exp[-\frac{\beta}{n}(S_\Lambda - h\sum_l Q_l)])^n}{\operatorname{tr}\lim_{n\to\infty}(\exp(-\frac{\beta}{n}T_\Lambda)\exp[-\frac{\beta}{n}(S_\Lambda - h\sum_l Q_l)])^n}.$$

Using the result of [16], one obtains

$$\begin{aligned}\omega_h^\Lambda(A) &= \lim_{n\to\infty}\frac{\operatorname{tr} A(\exp(-\frac{\beta}{n}T_\Lambda)\exp[-\frac{\beta}{n}(S_\Lambda - h\sum_{l\in\Lambda} Q_l)])^n}{\operatorname{tr}(\exp(-\frac{\beta}{n}T_\Lambda)\exp[-\frac{\beta}{n}(S_\Lambda - h\sum_{l\in\Lambda} Q_l)])^n}\\ &\equiv \lim_{n\to\infty}\omega_{h,n}^\Lambda(A).\end{aligned}$$

Now one checks easily (see e.g. [21, ch IV]) that the lattice approximation $\omega_{h,n}^\Lambda(\cdot)$ of the state (4.2) in the direction $[0,\beta]$ yields a ferromagnetic state on the lattice $\Lambda\times[0,\frac{\beta}{n},\frac{2\beta}{n},\ldots,\beta]$. Therefore we have the GKS inequality

$$\omega_{h>0,n}^\Lambda(W'(Q_l)) \geqslant \omega_{h>0,n}^\Lambda(Q_l)\,\omega_{h>0,n}^\Lambda(V(Q_l^2)).$$

The proposition follows, by taking the limits, first $n\to\infty$, then $\Lambda\to\mathbb{Z}^d$ and $h\to 0^+$. □

Combining the results of proposition 3.2, formula (3.8), and proposition 4.1, formula (4.1), one obtains for all temperatures T:

$$-a\langle Q\rangle_+ \geqslant \langle Q\rangle_+\langle V(Q^2)\rangle_+. \tag{4.3}$$

Now we start the final argument. Suppose there exists for some temperature T, a state with a non-zero order parameter $\langle Q\rangle_\pm \neq 0$. Take $\langle Q\rangle_+ > 0$, then it follows from (4.3) that

$$-a \geqslant \langle V(Q^2)\rangle_+. \tag{4.4}$$

We will work towards a contradiction of (4.4), by proving that (4.4) is violated for all temperatures if the mass m is small enough. To this end note first that using the ferromagnetic character of the system (see (4.2)) again and the inequality (4.1), and the convexity of the function V (3.7), one obtains

Proposition 4.2.

$$\langle V(Q_l^2)\rangle_+(T) \geqslant V(\langle Q_l^2\rangle_+(T)) \geqslant V(\langle Q_l^2\rangle(T=0)) \tag{4.5}$$

where $\langle\cdot\rangle_+(T)$ is the state $\langle\cdot\rangle_+$ at the temperature T.

Furthermore, in the Hamiltonian (2.1), the interaction term is given by

$$-\frac{c}{2}\sum_{\langle ll'\rangle} Q_l Q_{l'} \tag{4.6}$$

and because c is taken to be positive, the system is of ferromagnetic type. Considering the derivative of the expectation value $\omega_{h\geqslant 0}^\Lambda(Q_l^2)$ only with respect to this coupling constant (i.e. not a derivative with respect to the constant c, which also appears in the self-energy $\tilde{W}$), one obtains (see [21] again), on the basis of the GKS inequality,

Proposition 4.3.

$$\omega_{h\geqslant 0}^\Lambda(Q_l^2) \geqslant \omega_{h\geqslant 0}^\Lambda(Q_l^2)_0 \tag{4.7}$$

where the right-hand side means the expectation value of Q_l^2 for the non-interacting system with $c=0$ in the term (4.6), i.e. for the quantum lattice system of independent sites.

Collecting together the results (4.5) and (4.7) one gets, from (3.7),

$$\langle V(Q_l^2)\rangle_+(T) \geqslant V(\langle Q_l^2\rangle_{+,0}(T=0)) \tag{4.8}$$

where the right-hand side expectation is taken for the quantum lattice system of independent sites, given by

$$H_{0,\Lambda} = \sum_{l\in\Lambda} H_{0,l}$$
$$H_{0,l} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial Q_l^2} + \tilde{W}(Q_l) \tag{4.9}$$

with $\tilde{W}(x) = (\frac{1}{2}a + cd)x^2 + W(x)$, (see proof of proposition 4.1). This means that

$$\langle Q_l^2\rangle_{+,0}(T=0) = (\psi_0, Q^2\psi_0) \tag{4.10}$$

where $\psi_0 \in L^2(\mathbb{R}^1)$, is the ground-state wavefunction for the Schrödinger operator (4.9).

In the following, we study the behaviour of the ground-state fluctuation $(\psi_0, Q^2\psi_0)$ of the position operator Q if the mass m of the particle is small. We prove that this fluctuation diverges in the limit of small masses.

Proposition 4.4. Suppose that the asymptotics of the one-site potential $\tilde{W}$ behaves as $\tilde{W}(x) \sim |x|^\gamma$, $\gamma > 0$ for large values of $|x|$. Denote $\lambda = m^{-1/(2+\gamma)}$ and $\varepsilon_0(m)$, the ground-state energy for the Hamiltonian (4.9). Then for m small one has

(i) $\varepsilon_0(m) \sim \lambda^\gamma$

(ii) $(\psi_0, Q^2\psi_0) \sim \lambda^2$.

Proof. From the assumption of the asymptotic behaviour of the potential one can write

$$\tilde{W}(x) = A|x|^\gamma + v(x) \qquad |v(x)| \leqslant C|x|^\eta \qquad \eta < \gamma$$

with $A > 0$. After rescaling $x \to \lambda^{-1}x = z$ one gets, for the Schrödinger equation,

$$\left(-\frac{\hbar^2}{2}\partial_z^2 + A|z|^\gamma\left(1 + \frac{v(\lambda z)}{\lambda^\gamma|z|^\gamma}\right)\right)\psi_0^\lambda(z) = \lambda^{-\gamma}\varepsilon_0(m)\psi_0^\lambda(z)$$

here $\psi_0^\lambda(z) = \lambda^{1/2}\psi_0(\lambda z)$.

Considering the limit $m \to 0$ ($\lambda \to \infty$), one can conclude immediately the result (i). Otherwise, (ii) follows from

$$(\psi_0, x^2\psi_0) = \lambda^2\int_{\mathbb{R}^l} \mathrm{d}z\, z^2|\psi_0^\lambda(z)|^2.$$

□

We have now derived sufficient results with which to formulate our main statement.

Theorem 4.5. For m small enough, system (2.1) does not show $\mathbb{Z}_2$-symmetry breaking for all temperatures $T \geqslant 0$, i.e. $\langle Q\rangle_\pm(T) = 0$.

Proof. Suppose that there exists a state such that $\langle Q\rangle_+ > 0$, then from (4.4)

$$-a \geqslant \langle V(Q^2)\rangle_+.$$

However, using the monotonicity of V (see (3.7)) and (4.8), one obtains

$$-a \geqslant V(\langle Q^2\rangle_{+,0}).$$

However, from proposition 4.4, it follows that there is a m_c such that

$$\langle V(\langle Q^2\rangle_{+,0}) > |a|$$

for $m < m_c$, which is a contradicition. Hence $\langle Q\rangle_+ = 0$. □

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