ON THE DYNAMICS OF THE HOLSTEIN MODEL FROM THE ANTICONTINUOUS LIMIT

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Abstract. We consider the Holstein model describing an electron interacting with a lattice of identical oscillators. We remark that the on site system (i.e. the system in which the interaction between the different sites of the lattice vanishes) is integrable and anisocronous. This allows to apply some recent Nekhoroshev type results to show that corresponding the majority of initial data in which the electron probability is concentrate on a finite number of sites, the electron probability distribution is approximatively constant for times growing exponentially with the inverse of the coupling parameter. Moreover, for the same times, the total energy of the oscillator system is approximatively constant.

1. Introduction

In this paper we consider the adiabatic Holstein model describing one electron in interaction with an infinite lattice of identical oscillators. It will be studied as a classical (infinite dimensional) nonlinear dynamical system. Scaling suitably time and the oscillator's variables, the equations of the system can be written in the form

$$\begin{aligned} -i\dot{\psi}_i &= -q_i\psi_i - \epsilon[(\psi_i - \psi_{i-1}) + (\psi_i - \psi_{i+1})] \\ \ddot{q}_i &= -\omega^2 q_i + |\psi_i|^2 \end{aligned} \quad , \qquad i \in \mathbf{Z} \tag{1.1}$$

where q_i are the oscillator's variables, and $|\psi_i|^2$ is the probability of finding the electron at site i; ϵ is the coupling between the different sites, and ω the frequency of the oscillators.

The present work was stimulated by a paper by Hennig [1] where the dynamics of the Holstein model in the case $\omega \gg 1$ was studies. Hennig applied the Nekhoroshev type techniques of [2] to show that if ω is large enogh, then there is no exchange of energy between the oscillator's system and the electron system for times growing exponentially with ω. He also presented some numerical simulations showing that if ϵ is small enough also each of the probability amplitudes $|\psi_i|^2$ remain constant. Finally he gave an heuristic explaination of such a phenomenon.

In the present paper we prove rigorously, at least in some quite general situation, and for long times, the constancy of the electron probability distribution, i.e. of the quantities $|\psi_i|^2$. More precisely, we will consider the class of initial data in which the electron probability distribution $|\psi_i|^2$ is essentially localized at a finite number of sites. We will prove that, provided ϵ is below some threshold (which could be explicitly computed), then corresponding to the majority of such initial data the quantities $|\psi_i|^2$ are approximatively constant, and moreover the total harmonic energy of the oscillators is approximatively constant for very long times, namely for times of order $\exp(C\epsilon^{-a})$ with positive C and a.

The result is obtained in two steps. First we consider the anticontinuous limit $\epsilon = 0$ in which the system is decoupled into infinitely many identical systems with two degrees of freedom (on site system). Our starting point is the remark that the on site system is an integrable Hamiltonian system. So, first of all we introduce its action angle variables. In this way it becomes clear that the on site system is anysocronous, i.e. the frequencies of its motion depend on the initial data. We come to the second step; to explain in a simple way the key idea consider initial data in which the electron probability is concentrated at one single site of the lattice, say the site $\bar{i}$. It turns out that, in the on site system, the phase of the electron's probability $\psi_{\bar{i}}$ rotates with a frequency which depends on the initial datum and therefore, in general, is nonresonant with ω. Moreover, the phases related to ψ_i $i \neq \bar{i}$ do not move at all. Then one can hope to use perturbation theory to show that also when $\epsilon \neq 0$ the total energy of the oscillator's system and the electron probabilities $|\psi_i|^2$ are essentially constant. The situation is similar when the electron probability is concentrated at a finite number of sites.

To show that this is actually what happens we use a Nekhoroshev type result which was recently proved by the author [3] (for an improved version applicable to PDE's see [4]). In [3] a perturbation of an infinite dimensional system with $n < \infty$ frequencies was considered, and it was proved that there exist n functions which remain approximatively constant when the system is subjected to a smooth perturbation. In the present case such functions are $n-1$ electron probabilities and the total harmonic energy of the oscillator system. Exploiting also the conservation of the total probability of finding an electron in the lattice we are able to conclude that the whole probability distribution of the electron is approximatively constant for teh considered times.

Finally we recall that Holstein model was already studied from the anticontinuous limit by Aubry [5] who proved that, provided ϵ is small enough, the Holstein model has quasiperiodic breathers, i.e. quasiperiodic localized solutions. Such solutions physically correspond to the situation in which one of the oscillator performs large amplitude oscillations while the other are approximatively at rest; the electron probability distribution is constant, but the phases rotate uniformly.

The paper is organized as follows: in sect. 2 we discuss the on site dynamics; in sect. 3 we recall the main abstract theorem of [3], state and prove the main result of the present paper (freezing of the electron's probabilities, and of the oscillator's energy). Finally in sect. 4 we discuss some possible extensions of these results.

2. The on site dynamics

Consider the adiabatic Holstein model (1.1), define x_i, and y_i as the real and imaginary parts of ψ_i; then it is easy to verify that (1.1) are the Hamilton's equations of

$$H := \sum_i H_{os}(p_i, q_i, x_i, y_i) + \frac{1}{2}\epsilon \sum_i \left[(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2\right] , \tag{2.1}$$

where

$$H_{os}(p_i, q_i, x_i, y_i) := \frac{p_i^2 + \omega^2 q_i^2}{2} + q_i \frac{x_i^2 + y_i^2}{2} \tag{2.2}$$

and (p_k, q_k), (x_i, y_i) are canonically conjugated variables.

Remark 2.1. *The quantity $\sum_i (x_i^2 + y_i^2)/2$ is a constant of motions for the dynamics of the Holstein model. It represents the probability of finding an electron in the lattice, so it should be subjected to the normalization condition*

$$\sum_i \frac{x_i^2 + y_i^2}{2} = 1 .$$

For simplicity in the following we will drop this condition.

We begin by studying the on site dynamics described by the Hamiltonian (2.2). It is immediate to realize that the system (2.2) is integrable. Indeed the action $(x_i^2 + y_i^2)/2$, is a constant of motion, and the Hamiltonian itself is the second constant.

Fix i, then one can explicitly construct action angle variables for H_{os} in two steps. First define the variables (J_i, ϕ_i) by

$$x_i = \sqrt{J_i} \cos\phi_i , \quad y_i = \sqrt{J_i} \sin\phi_i ;$$

the Hamiltonian of the on site system takes the form

$$H_{os} = \frac{p_i^2 + \omega^2 q_i^2}{2} + q_i J_i . \tag{2.3}$$

Then the canonical transformation

$$Q_i = q_i + \frac{J_i}{\omega^2} , \quad P_i = p_i , \quad J_i' = J_i, \quad \phi_i' = \phi_i + \frac{P_i}{\omega^2}$$

(with generating function $P_i(q_i + \frac{J_i'}{\omega^2}) + J_i'\phi_i$) reduces the Hamiltonian (2.3) to the form

$$\frac{P_i^2 + \omega^2 Q_i^2}{2} - \frac{1}{2\omega^2} J_i^2 \tag{2.4}$$

where we omitted the prime from J. The main feature of this Hamiltonian is that it clearly shows that it is integrable and that the frequency of the electron's system is J_i/ω^2, which depends on the electron density at the considered site.

Remark 2.2. *The quantity*

$$J_i = \frac{x_i^2 + y_i^2}{2}$$

is the probability of finding an electron at the site i of the lattice.

The integration of this system is immediate and gives

$$\begin{aligned} P_i(t) &= P_{i,0}\cos(\omega t) - \omega Q_{i,0}\sin(\omega t) \\ Q_i(t) &= Q_{i,0}\cos(\omega t) + \frac{P_{i,0}}{\omega}\sin(\omega t) \\ J_i(t) &= J_{i,0} \\ \phi_i'(t) &= \frac{J_i}{\omega^2}t + \phi_{i,0}' \end{aligned}$$

So, along the solutions the electron density J_i is a constant of motion, the corresponding phase ϕ' rotates uniformly, and the variables P_i, Q_i oscillate with frequency ω around zero. In terms of the original variables the solution appears as follows: the phase of the electron rotates and moreover performs an oscillation with frequency ω, while the oscillator still oscillates with frequency ω, but around the shifted equilibrium position $q_i = -J_i/\omega^2$.

3. The complete system

We use now perturbation theory to study the dynamics of the complete system. We will concentrate on the situation in which the electron's probability is concentrated at a finite number of sites of the lattice. Moreover, in order to avoid the singularity introduced by the action angle coordinates we prefer to give the main statement in terms of the original variables p, q, x, y. So, in the statement of the forthcoming theorem J_i must be interpreted as a short notation for $(x_i^2 + y_i^2)/2$; moreover we will denote by

$$h_0 := \sum_i \frac{1}{2}\left(p_i^2 + \omega^2\left(q_i + \frac{J_i}{\omega^2}\right)^2\right)$$

the total harmonic energy of the oscillators.

We fix a subset $\mathcal{L} \subset \mathbf{Z}$ with cardinality $n < \infty$ and an n-dimensional vector $\nu = \{\nu_i\}_{i\in\mathcal{L}}$ which fulfills the following diophantine condition

$$|\nu\cdot k + \omega l| \geq \frac{\gamma}{|(k,l)|^\tau}\ , \quad \forall (k,l) \in \mathbf{Z}^{n+1}\setminus\{0\}\ , \tag{3.1}$$

where $|(k,l)| := |l| + \sum |k_i|$, and γ and τ are strictly positive constants.

We will prove the following

Theorem 3.1. *There exists a positive ϵ_*, and positive constants $C_1, ..., C_4$ with the following properties: assume $\epsilon < \epsilon_*$, and consider an initial datum satisfying*

$$\left|J_i(0) - \nu_i\omega^2\right| \le C_1\epsilon \ , \quad \forall i \in \mathcal{L} \ ; \qquad \sum_{i \notin \mathcal{L}} J_i(0) \le C_1\epsilon \ , \qquad h_0(0) < \infty \ ; \tag{3.2}$$

then, along the corresponding solution one has

$$\begin{aligned} |J_i(t) - J_i(0)| &\le C_2\epsilon^{1/2(\tau+1)}\epsilon \ , \quad \forall i \in \mathcal{L} \\ \sum_{i \notin \mathcal{L}} J_i(t) &\le C_2\epsilon \\ |h_0(t) - h_0(0)| &\le C_2\epsilon^{1/2(\tau+1)}h_0(0) \end{aligned} \tag{3.3}$$

for exponentially long times, namely for the times t fulfilling

$$|t| \le C_3 \exp\left(\frac{C_4}{\epsilon}\right)^{1/2(\tau+1)} \tag{3.4}$$

The proof will be obtained by applying the normal form theorem of [3]. Before going to the details we recall the result of [3] that will be applied here. We simplify slightly its statement since for the present application we need only to deal with a strongly symplectic space.

Consider a strongly symplectic Banach space $\mathcal{P}$, i.e. a Banach space endowed by a skew symmetric nondegenerate form Ω. Then one can define the application $\mathcal{P} \ni X \mapsto \Omega(X, .) \in \mathcal{P}^*$, which is injective. We recall that Ω is said to be strongly nondegenerate if such a map is also surjective. In this case the Poisson tensor J which is the inverse of this map is a linear *bounded* operator. It follows that the Hamiltonian vector field X_f of a C^∞ function f (which is defined by $X_f := Jdf$) is also of class C^∞. Consider the complexification $\mathcal{P}^{\mathbf{C}}$ of $\mathcal{P}$; we will denote by $B_R(z) \subset \mathcal{P}^{\mathbf{C}}$ the ball of radius R with center at z. Moreover, given a set $\mathcal{G} \subset \mathcal{P}$ we will denote

$$\mathcal{G}_R := \bigcup_{z \in \mathcal{G}} B_R(z)$$

On a set $\mathcal{G}$ consider a Hamiltonian function

$$H = h_\omega + f \tag{3.5}$$

Fix a positive R; we will assume that both h_ω and f extend to complex analytic functions on $\mathcal{G}_R$. The main abstract result of [3] ensures that, if h_ω generates a quasiperiodic flow which leaves invariant $\mathcal{G}_R$, and f is small, the system has a certain number of approximate constant of motion, for times growing exponentially with a power of the inverse of the size of f.

To give a precise statement we write more explicitly the assumptions. We will denote by Φ_t the flow generated by the Hamiltonian vector field of h_ω. We assume

1 $\Phi_t(\mathcal{G}_r) \subset \mathcal{G}_r$, for any $r \leq R$;
2 Φ_t is quasiperiodic, namely there exists a group action $\Psi : \mathbf{T}^n \times \mathcal{G}_R \to \mathcal{G}_R$ and an n dimensional real vector ω such that

$$\Phi_t(z) = \Psi_{\omega_1 t, \omega_2 t, \ldots, \omega_n t}(z) \ , \quad \forall z \in \mathcal{G}_R \ .$$

Moreover, there exist functions $I_1, ..., I_n$ analytic in $\mathcal{G}_R$ whose Hamiltonian vector fields generate the flows $\Psi_{\phi_1,0,0\ldots,0}\ldots \ \Psi_{0,0,\ldots,0,\phi_n}$.
3 The frequency vector is diophantine, namely there exist positive γ and τ such that

$$|\omega \cdot k| \geq \frac{\gamma}{|k|^\tau} \ , \quad \forall k \in \mathbf{Z}^n \setminus \{0\} \ .$$

4 Denote by $\mathbf{T}^n + i\sigma$ the set of the $\phi's$ belonging to the complexified torus such that $|\mathrm{Im}\, \phi_i| \leq \sigma$. There exist positive σ and $r_* > R/2$ such that Ψ extends to an analytic map $\Psi : \mathbf{T}^n + i\sigma \times \mathcal{G}_{r_*} \to \mathcal{G}_R$.
5 Finally we assume that there exists a finite constant ϵ_f such that

$$\frac{1}{R} \sup_{z \in \mathcal{G}_R} \|X_f(z)\| \leq \epsilon_f \ . \tag{3.6}$$

Then Corollary 4.2 of [3] states that

Theorem 3.2. *Under the above assumptions there exist constants C_5, C_6, C_7, independent of R, such that, provided $\epsilon_f \leq \epsilon_*$, then along the solutions of the Cauchy problem for (3.5), with initial data in $\mathcal{G}_{R/4}$, one has*

$$|I_i(z(t)) - I_i(z(0))| \leq C_5 \epsilon_f^{1/(\tau+1)} \sup_{z \in \mathcal{G}_R} |I_i(z)| \ , \quad i = 1, .., n$$

for all times $t \leq \min\{T_0, T_*\}$, where T_0 is the escape time of the solution from the domain $\mathcal{G}_{3R/8}$, and

$$T_* := \frac{C_7}{\epsilon_f} \exp\left[\frac{C_6}{\epsilon_f}\right]^{1/(\tau+1)}$$

Proof of theorem 3.1 We will apply the above theorem 3.2, and then we will show that the escape time T_0 is larger than T_*. We prepare the system by introducing "action angle" variables $(J_i, \phi_i), (P_i, Q_i)$ for the on site system at the sites $i \in \mathcal{L}$; making a translation of the action J_i, namely introducing the variables

$$I_i := J_i - \nu_i \omega^2 \ ,$$

the Holstein model assumes the form

$$H = h_\omega + f_1 + f_2 + f_3 \ ,$$

where

$$h_\omega := h_0 - \sum_i \nu_i I_i$$

$$f_1 := \epsilon H_{int} \ , \quad f_2 := -\sum_{i\in\mathcal{L}} \frac{I_i^2}{2\omega^2} \ , \quad f_3 := -\sum_{i\notin\mathcal{L}} \frac{J_i^2}{2\omega^2}$$

where,

$$H_{int} = \frac{1}{2}\sum_i \left[(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2\right]$$

and, for $i \in \mathcal{L}$, x_i and y_i must be intended as functions of the action angle variables, while, for $i \notin \mathcal{L}$, the symbols P_i, Q_i and J_i must be intended as short notations for their complete expression. We fix a parameter R and define the norm of a sequence

$$z = \Big(\{P_i, Q_i, I_i, \phi_i\}_{i\in\mathcal{L}} \, , \{p_i, q_i, x_i, y_i\}_{i\notin\mathcal{L}}\Big)$$

by

$$\|z\|^2 :=$$
$$\sum_{i\in\mathcal{L}} \frac{|P_i|^2 + \omega^2|Q_i|^2}{2} + \sum_{i\notin\mathcal{L}} \frac{|p_i|^2 + \omega^2|q_i|^2}{2} + \max_{i\in\mathcal{L}} |I_i|^2 + \max_{i\in\mathcal{L}} R^2|\phi_i|^2 + R\sum_{i\notin\mathcal{L}} \frac{|x_i|^2 + |y_i|^2}{2}$$

and define $\mathcal{P}$ as the completion of set of sequences with compact support in this norm. We choose the domain $\mathcal{G} \subset \mathcal{P}$ to be the set

$$\left\{ z \in \mathcal{P} \ : \ h_0(z) \le 2E \ , \ I_i = 0 \ , \ \forall i \in \mathcal{L} \ , \quad J_i = \frac{x_i^2 + y_i^2}{2} = 0 \ , \ \forall i \notin \mathcal{L} \right\} \ .$$

And we extend it to the complex using again the parameter R.

It is now easy to compute ϵ_f. To this end remark that H_{int} is a bounded polynomial of the variables x, y, so it is analytic as a function of these variables. Since the change of variables involving action angle variables is also analytic, H_{int} is analytic also as a function of these variables. Moreover H_{int} is independent of the p, q variables. It follows that there exists a constant independent of ϵ and R which bounds the norm of the Hamiltonian vector field of f_1. Concerning the vector field of f_2, it has only ϕ components. It is linear in J, and therefore it is bounded by a constant times R^2. Finally consider f_3: the corresponding vector field is a cubic polynomial in x, y and therefore the square of its norm is bounded by a constant times R times R^3. It follows that we have

$$\frac{1}{R}\|X_f\| \le C\left(\frac{\epsilon}{R} + \epsilon + R\right)$$

with a suitable constant C. Choosing $R = \sqrt{\epsilon}$ we have

$$\epsilon_f = C'\sqrt{\epsilon} \ . \tag{3.7}$$

We define now the group action Ψ. We denote by ψ_1, ψ_2 the angels on the torus. Then $(P, Q, J, \phi, p, q, x, y) := \Psi_{\psi_1,\psi_2,...,\psi_{n+1}}(P_0, Q_0, J_0, \phi_0, p_0, q_0, x_0, y_0)$ is defined by

$$
\begin{aligned}
I_i &= I_{i,0} \ , \quad i \in \mathcal{L} \\
\phi_i(\psi_{j_i}) &= \phi_{0,i} + \psi_{j_i} \ , \quad i \in \mathcal{L} \\
P_i(\psi_1) &= P_{0,i} \cos\psi_1 - \omega Q_{0,i} \sin\psi_1 \ , \quad i \in \mathcal{L} \\
Q_i(\psi_1) &= Q_{0,i} \cos\psi_1 + \frac{P_{0,i}}{\omega} \sin\psi_1 \ , \quad i \in \mathcal{L} \\
q_i(\psi_1) &= \left(q_{0,i} + \frac{J_i^2}{\omega^2} \right) \cos\psi_1 + \frac{p_{0,i}}{\omega} \sin\psi_1 - \frac{J_i}{\omega^2} \ , \quad i \notin \mathcal{L} \\
p_i(\psi_1) &= -\omega \left(q_{0,i} + \frac{J_i}{\omega^2} \right) \sin\psi_1 + \frac{p_{0,i}}{\omega} \cos\psi_1 \ , \quad i \notin \mathcal{L} \\
x_i(\psi_1) &= x_{0,i} \cos\left(\frac{p_i(\psi_1) - p_{i,0}}{\omega^2} \right) + y_{0,i} \sin\left(\frac{p_i(\psi_1) - p_{i,0}}{\omega^2} \right) \ , \quad i \notin \mathcal{L} \\
y_i(\psi_1) &= x_{0,i} \sin\left(\frac{p_i(\psi_1) - p_{i,0}}{\omega^2} \right) + y_{0,i} \cos\left(\frac{p_i(\psi_1) - p_{i,0}}{\omega^2} \right) \ , \quad i \notin \mathcal{L}
\end{aligned}
$$

where j_i is defined by $j_i \in [2, ..., n+1]$, $i < i'$ implies $j_i < j_{i'}$.

So it is possible to apply theorem 3.2 obtaining the estimates (3.3) for times which are the minimum between the escape time from $\mathcal{G}_{3R/8}$ and the times (3.4). To bound the escape time remark that the function h_0 can be used as a Lyapunov functions to show that the variables P, Q cannot leave their domains for the times we are interested in. The same is obviously true for the variables I_i. To bound also the escape time for the variables $\{x_i, y_i\}_{i \notin \mathcal{L}}$ just use the information that $\sum_i \frac{x_i^2+y_i^2}{2}$ is a constant of motion. This allows to conclude that

$$
\sum_{i \notin \mathcal{L}} \frac{x_i(t)^2 + y_i(t)^2}{2} \leq \sum_{i \notin \mathcal{L}} \frac{x_i(0)^2 + y_i(0)^2}{2} + \sum_{i \in \mathcal{L}} |I_i(t) - I_i(0)|
$$

but the latter quantity is estimated by (3.3), and therefore also the variables x_i, y_i cannot escape from their domain. So the theorem is proved. □

4. Discussion

So, we have proved that, provided ϵ is small enough, and corresponding to the majority of initially localized electron probability distributions, the electron probabilities $|\psi_i|^2$ and the total energy of the oscillators are essentially constant for very long times. One can ask what happens corresponding to the other initial data.

We expect that the electron probability distribution should be essentially constant corresponding to *any* initial datum with $|\psi_i|^2$ concentrated at a finite number of sites. Namely we expect that there is no need of the diophantine condition (3.1). The reason is that the Holstein model appears as a perturbation of the Hamiltonian

$$h_0 - \sum_i \frac{J_i^2}{2\omega^2} ,$$

which is quasiconvex as a function of J_i and h_0. For quasiconvex systems with finitely many degrees of freedom Nekhoroshev theory ensures that the actions are approximatively constant under perturbation, and for exponentially long times. This of course requires the development of the geometric part of Nekhoroshev theorem. The Holstein model however is infinite dimensional; we recall that the extension of the geometric part of Nekhoroshev's theorem to some infinite dimensional systems has been carried out (following the finite dimensional proof by Lochak [6]) in [2] and [7]. We expect the techniques of [7] to be applicable to the present case. However, since there is not a general theorem which is directly applicable to Holstein model, one should repeat the whole argument of [7]. For this reason we limited ourselves to deal with the much simpler nonresonant case.

For what concerns probability distributions which are not concentrated, we have not a precise idea, but we expect that (in general) there should not be an analogue of theorem 3.1.

In the present paper we limited ourselves to the one electron Holstein model. However it is easy to see that also the on site dynamics of the M electron Holstein model is integrable, and that its Hamiltonian, in terms of action angle variables has exactly the form (2.4). So, one can expect theorem 3.1 (and its possible extensions) to hold also in the M electron case. However, its proof is much more difficult in the case of M electrons. This is due to the sigularities that appear introducing action angle variables. which are much harder in the M electron case. We expect that it should be possible to overcome such difficulties using the techniques developed by Niedermann [8] which avoid completely the introduction of action angle variables (see also [9]).

Finally we remark that the case where the linear restoring force for the oscillators is substituted by a nonlinear force (as in [5]) can also be dealt with by the same techniques developed here. Indeed also in this case the on site system is integrable. However, since the explicit introduction of action angle variables cannot (in general) be done, the prove of theorem 3.1 would turn out to be slightly more difficult. On the contrary the case of a nonlinear interaction between different sites can be treated without additional difficulties.

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