Freezing of the optical–branch energy in a diatomic FPU chain

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Abstract

We study the exchange of energy between the modes of the optical branch and those of the acoustic one in a diatomic chain of particles, with masses $m_1$ and $m_2$. We prove that, at small temperature and provided $m_1 \gg m_2$, for the majority of the initial data the energy of each branch is approximately constant for times of order $\beta S^2$, where $S = \lfloor \sqrt{m_1/m_2}/2 \rfloor$ and $\beta$ is the inverse temperature. The result is uniform in the thermodynamic limit.

1 Introduction

In the present paper we study a variant of the Fermi–Pasta–Ulam (FPU) chain, namely the Born and von Kármán lattice which consists of a chain of particles with nearest neighbour interaction, having alternating heavy and light masses $m_1$ and $m_2$. In this model the spectrum of the normal modes splits into two separated branches called the acoustic and the optical branch. The dynamics was studied numerically in and a quite clear behaviour was observed: the energy of the optical branch seems to be essentially an integral of motion, possibly also in the thermodynamic limit. This could have a relevant consequence for the thermodynamic behaviour of this model, so that a theoretical confirmation of this phenomenon seems to be in order.

In the present paper we actually prove that, uniformly in the thermodynamic limit and for the majority of initial data, the energy of the optical branch remains substantially constant over times which increase as $\beta S^2$, where $S = \lfloor \sqrt{m_1/m_2}/2 \rfloor$, with $m_1 \gg m_2$, and where $\beta$ is the inverse temperature. A detailed comparison of our result with numerical observations will be provided at the end of Section.
Our method of proof is a development of the ideas introduced in [3] and [4, 5, 6]. Such tools allow one to implement perturbation theory for the majority of initial data, in a regime of interest for statistical mechanics. In particular, in the paper [6] the original FPU model was studied, showing that essentially any packet of harmonic modes does not change significantly its energy for times of order $\beta$. The obstruction to go to longer times was due to the existence of small denominators. As already remarked in [2, 7], the problem of small denominators does not show up in studying the freezing of the optical energy in the diatomic chain, so that the techniques developed in [6] can be adapted to it. Here, however, the main difficulty is that the form of the normal modes is more complicated and the estimates of the variances of the relevant functions (see Lemma 3 below) have to be rewritten from scratch. Indeed, one has to work here on the Bravais lattice, whose points are pairs of particles, and, moreover, one has to introduce combinatorial techniques based on the construction of suitable graphs and trees.

The problem we study is closely related that of equipartition of energy in the original FPU model, in which all masses are equal, see [8]. Relevant contributions were given by several authors, among which [9, 10, 11, 12, 13]; for a recent review see [14]. Further dynamical properties, concerning the existence of localized solutions were investigated both for the original FPU model (see [15, 16, 17, 18, 19, 20]) and the diatomic model considered here (see [21]).

For the present model, the first analytic results on the freezing of the optical energy were obtained in [2], applying the main theorem of [22] to this model. In [2] the authors provided a Nekhoroshev type result, valid however for total energy $E$ smaller than some inverse power of the number $N$ of degrees of freedom. In the subsequent paper [7] the authors introduced a suitable functional framework which enabled them to prove energy freezing for any $N$, but still for a finite total energy $E$, i.e., in a regime not relevant for statistical mechanics. Instead, the result of the present paper is uniform in the thermodynamic limit, in which $E/N$ remains constant as $N$ goes to infinity.

The description of the model and a precise statement of the result is given in Section [2] where the result on the conservation of the energy of the optical (and also of the acoustic) branch is given in Corollary [1] which is deduced in a few lines from the corresponding Theorem [1] expressed in terms of time correlations. In turn, Theorem [1] is a simple consequence of the related Theorem [2] which concerns the conservation of an auxiliary
quantity. The latter Theorem, which contains the main technical part of the work, is proved in Section 3 whereas in Section 4 the deduction of Theorem 1 and Corollary 1 is given. A short discussion of the physical consequences of the result is provided in the concluding Section 5. A detailed analysis of the normal modes of the system is given in Appendix A, while the remaining appendices contain some technical Lemmas which have been isolated in order to clarify the exposition of the proofs.

2 Description of the model and main results

We consider a one-dimensional diatomic chain, constituted by two species of masses $m_1$ and $m_2$ (with $m_1 > m_2$). The Hamiltonian of the system is

$$H = \sum_{j=1}^N \left( \frac{p_{j,1}^2}{2m_1} + \frac{p_{j,2}^2}{2m_2} \right) + \sum_{j=1}^N \left( V(x_{j,2} - x_{j,1}) + V(x_{j+1,1} - x_{j,2}) \right), \quad N \gg 1,$$

in the canonically conjugated coordinates $p = \{ p_{j,i} \}$, $x = \{ x_{j,i} \}$ in the phase space $\mathcal{M} = \mathbb{R}^{4N}$, where $j = 1, \ldots, N$, $i = 1, 2$. The potential $V$ corresponds to a nearest neighbour interaction, which we assume of the form

$$V(r) = \frac{K}{2} r^2 \left( 1 + Ar + Br^2 \right).$$

As in the original work of Born and von Kármán [1], we impose periodic boundary conditions, i.e., $x_{N+j} = x_j$ and $p_{N+j} = p_j$, where we denote $x_j \overset{\text{def}}{=} (x_{j,1}, x_{j,2})$ and $p_j \overset{\text{def}}{=} (p_{j,1}, p_{j,2})$. Introducing the normal modes of the system (see Appendix A), the quadratic part of the Hamiltonian takes the form

$$H_0 = \frac{1}{2} \sum_k \sum_{l=\pm} \left( |\hat{p}_k^l|^2 + \omega_{\pm}^l |\hat{q}_k^l|^2 \right),$$

where $\hat{p}_k^\pm$, $\hat{q}_k^\pm$, for $k = [-N/2] + 1, \ldots, [N/2]$, are complex canonically conjugated variables. This is a Hamiltonian of $2N$ harmonic oscillators with frequencies

$$\omega_{\pm}^k = \left( K \frac{m_1 + m_2}{m_1 m_2} \pm \sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \cos(2\pi k/N)} \right)^{1/2}. \quad (1)$$
The index \( l = \pm \) splits the frequencies into two branches, which, using a common terminology of solid state physics, will be called optical branch (for \( l = + \)) and acoustic branch (for \( l = - \)). Notice that the frequencies of the acoustic branch range from 0 to \( \sqrt{2K/m_1} \), while those of the optical branch range from a minimum value \( \sqrt{2K/m_2 \cdot 1 + m_1/m_2} \) to \( \sqrt{2K/m_2} \). Thus, a gap exists between the maximum value of the branch \( \omega^+_k \) and the minimum value of the branch \( \omega^-_k \), and the gap increases with the ratio \( m_1/m_2 \). Consider the total energy \( E^+ \) of the normal modes in the optical branch, and that of the acoustic branch, \( E^- \), namely

\[
E^+ \overset{\text{def}}{=} \frac{1}{2} \sum_k \left( |\hat{p}_k|^2 + \omega^+_k |\hat{q}_k|^2 \right), \quad E^- \overset{\text{def}}{=} \frac{1}{2} \sum_k \left( |\hat{p}_k|^2 + \omega^-_k |\hat{q}_k|^2 \right).
\]

In order to formulate precisely this statement (see Theorem 1), we introduce the Gibbs measure in phase space \( \mathcal{M} = \mathbb{R}^{2N} \times \mathbb{R}^{2N} \), namely,

\[
\mu(dp \, dx) \overset{\text{def}}{=} \frac{\exp(-\beta H(p, x))}{Z(\beta)} \, dp \, dx,
\]

where \( dp \, dx \) denotes the Lebesgue measure \( \prod_j dp_{j,1} dp_{j,2} dx_{j,1} dx_{j,2} \), while \( \beta > 0 \) is the inverse temperature and \( Z(\beta) \overset{\text{def}}{=} \int_{\mathcal{M}} \exp(-\beta H(p, x)) \, dp \, dx \) the partition function. It is well known that \( \mu \) is invariant for the flow. For any dynamical variable \( F \), the mean \( \langle F \rangle \) and the variance \( \sigma^2_F \) are thus defined by

\[
\langle F \rangle \overset{\text{def}}{=} \int_{\mathcal{M}} F \, d\mu, \quad \sigma^2_F \overset{\text{def}}{=} \langle (F - \langle F \rangle)^2 \rangle.
\]

The time autocorrelation \( C_F(t) \) of \( F \) is defined by

\[
C_F(t) \overset{\text{def}}{=} \langle F_t F \rangle - \langle F \rangle^2,
\]

in which \( F_t = F \circ g^t \) and \( g^t \) is the flow generated by \( H \).

In the spirit of the statistical approach pursued here, the result on the conservation of the energies \( E^+ \) and \( E^- \) of the optical and the acoustic branch is naturally stated in terms of their correlations

**Theorem 1** There exist constants \( \beta^* > 0, N^* > 0, M > 2 \) and \( K_1, K_2 > 0 \) such that, for any \( \beta > \beta^* \), \( N > N^* \) and for any value of \( m_1/m_2 > M \), the following bounds hold

\[
|C_{E^\pm}(t) - C_{E^\pm}(0)| \leq K_2 \left( \frac{1}{\sqrt{\beta}} + \frac{m_2}{m_1} \right) \sigma^2_{E^\pm}, \quad \text{for } t \leq K_1 \beta^{S/2}, \quad (2)
\]

where \( S = [\sqrt{m_1/m_2}/2] \).
Corollary 1  There exist a measurable set $J$ and $C > 0$ such that $\mu(J^c) < C\beta^{-S/2}$ and

$$\left| \frac{E^\pm(g^t x) - E^\pm(x)}{\sigma_{E^\pm}} \right| \leq C \left( \frac{1}{\sqrt{\beta}} + \frac{m_2}{m_1} \right), \quad \text{for } |t| \leq C\beta^{S/2},$$

if $x \in J$.

It is interesting to compare our result with the numerical observations of [2]. In that paper the authors measured some average of $\frac{d}{dt} E^+$ bounding this quantity by

$$A(N) \frac{m_2}{m_1} \exp \left( -B \frac{m_1}{m_2} \right),$$

with a constant $A(N)$ which diverges less than logarithmically as $N$ increases and $B$ independent of $N$. We remark that the small parameter of [2] is $m_2/m_1$. Furthermore the initial data considered in [2] did not have small specific energy: only the specific energy present in the optical branch was assumed to be small. Our result is somehow stronger than the one observed in [2] since it is completely uniform with $N$. On the other hand our small parameter is the temperature, so that we are studying a more particular regime.

3 Proof of Theorem 1: main technical part

The proof is performed by formally constructing a constant of motion $\Phi$ through a formal series expansion starting from

$$\Phi_0 = \sum_k \frac{1}{2\omega_k^+} \left( |\hat{p}_k^+|^2 + \omega_k^+ |\hat{q}_k^+|^2 \right),$$

which is the sum of the actions of the modes in the optical branch. The series is then truncated at a given order $S$, and it is shown that $S$ can be so chosen that the time autocorrelation of the truncated quantity $\Phi(S)$ has small variation over long times. Indeed, the main technical part of the present work can be summarized in the following

Theorem 2 There exist a polynomial $\Phi(S)$ of degree $S = \lfloor \sqrt{m_1/m_2}/2 \rfloor$ and constants $\beta^* > 0$, $N^* > 0$, $M > 2$ and $K_1, K_2 > 0$ such that, for any $\beta > \beta^*$, $N > N^*$ and for any value of $m_1/m_2 > M$,

$$\sigma_{\Phi(S)} \leq \frac{K_1}{\beta^{S/2}} \sigma_{\Phi(S)}$$

$$\sigma_{\Phi(S) - \Phi_0} \leq \frac{K_2}{\sqrt{\beta}} \sigma_{\Phi_0}.$$  

(3)
The proof of Theorem 1 easily follows, through standard arguments, as shown in the following Section 4.

The rest of the present section is devoted to the proof of Theorem 2. We briefly illustrate first the formal construction scheme for the integral of motion in section 3.1. In order to give quantitative estimates, in section 3.2 we define the classes of functions with which we have to deal, which are actually suitable polynomials, and construct a sequence of Banach spaces \( P_s \) of homogeneous polynomials of degree \( s \), with a suitable norm. This is basically an adaptation of the techniques of [23] to our class of polynomials, with the adoption of some tools from [24]. The relation between the norms \( P_s \) and the variances with respect to the Gibbs measure, which are the ones we are interested in, is displayed in the following section 3.3. Here (and in the related Appendix [1]) is contained the main technical novelty of the work, namely, a complete reformulation and extension of the techniques introduced in [6] to control the relation between the norms, based on a careful counting of the terms entering the variances, through the introduction of suitable graphs and trees. In section 3.4 the final estimates are summed up and the proof of Theorem 2 is completed.

### 3.1 The formal construction scheme for the constant of motion

We construct a formal integral of motion \( \Phi \) by using the algebraic algorithm involving Lie transforms which was presented in [23]. First, given a generating sequence \( \chi = \{ \chi_s \}_{s \geq 1} \), consider the formal linear operator \( T_\chi \), acting on formal polynomials, defined by

\[
T_\chi = \sum_{s \geq 0} E_s, \quad \text{where } E_0 = 1, \quad E_s = \sum_{j=1}^{s} \frac{j}{s} L_{\chi_j} E_{s-j},
\]

in which \( L_{\chi_j} \cdot = \{ \chi_j, \cdot \} \) and \( \{ \cdot, \cdot \} \) denotes Poisson brackets.

The sequence \( \chi_j \), in turn, is determined in the following way. Expand the Hamiltonian in homogeneous polynomials, \( H = \sum_{s \geq 0} H_s \), with \( H_s \) homogeneous polynomials of degree \( s + 2 \) in the canonical coordinates. The functions \( \chi_s \) are then determined recursively by solving an equation of the form

\[
L_0 \chi_s = Z_s - \Psi_s, \quad (4)
\]
where $L_0 = L_{H_0}$, $\Psi_s$ is given and $Z_s$ is a normal form, that must commute with $\Phi_0$, or, equivalently, with the resonant part of the Hamiltonian

$$H_\Omega = \Omega \sum_k \frac{|p_k|^2 + \omega_k^2}{2\omega_k^+} |q_k|^2 = \Omega \Phi_0,$$

with $\Omega$ maximum optical frequency, i.e.,

$$\Omega = \omega_0^+ = \sqrt{ \frac{2K(m_1 + m_2)}{m_1 m_2} }.$$

One of the main points is the construction of $Z_s$ and $\chi_s$ solving (4). Recall first that any polynomial $\Psi_s$ can be decomposed into a kernel and a range component of the operator $L_\Omega = L_{H_0}$. Denote by $\Pi_N$ and $\Pi_R$ the corresponding projections. We define $Z_s = \Pi_N \Psi_s$ and then solve through Neumann formula (see [25, 24])

$$L_0 \chi_s = (L_\Omega + L_{H_0 - H_0}) \chi_s = \Pi_R \Psi_s.$$

The quantity $\Psi_s$ is recursively defined by the formula

$$\Psi_1 = H_1,$$

$$\Psi_s = H_s + \sum_{l=1}^{s-1} \frac{l}{s} L_{\chi_l} H_{s-l} + \sum_{l=1}^{s-1} \frac{l}{s} E_{s-l} Z_l , s \geq 2,$$

and $\chi_s, Z_s$ are the solutions of the homological equation (5). Then, by considering

$$\Phi = T\chi \Phi_0 = \sum_{j \geq 0} \Phi_j \quad \text{and} \quad \Phi^{(S)} \overset{\text{def}}{=} \sum_{j=0}^{S} \Phi_j ,$$

the theory of [23] ensures that

$$\Phi^{(S)} \overset{\text{def}}{=} \{ \Phi_S, H_1 + H_2 \} + \{ \Phi_{S-1}, H_2 \} ,$$

which is the formula to be used for the quantitative estimates.
3.2 Definition of the class of polynomials and quantitative estimates

We start with a further (standard) change of variables that makes the operator $L_0$ diagonal:

$$
\xi_k^\pm = \hat{p}_k^\pm + i \omega_k^\pm \hat{q}_k^\pm / \sqrt{2}, \quad \eta_k^\pm = \hat{p}_{-k}^\pm - i \omega_k^\pm \hat{q}_k^\pm / \sqrt{2}.
$$

(6)

This transformation brings to the Poisson brackets

$$
\{\xi^l_{k,l}, \eta^l_{k',l'}\} = i \omega_k^\pm \delta_{k,k'} \delta_{l,l'}
$$

and gives the quadratic Hamiltonian the form $H_0 = \sum_k \sum_{\pm} \xi_k^\pm \eta_k^\pm$.

In order to define the class of polynomials we will meet, we start by introducing the monomials

$$
\Xi_{\sigma,k,l}^{\pm} \overset{\text{def}}{=} \xi_{l_1}^{(1+\sigma_1)/2} \eta_{k_1}^{(1-\sigma_1)/2} \cdots \xi_{l_s}^{(1+\sigma_s)/2} \eta_{k_s}^{(1-\sigma_s)/2}, \quad s \geq 3,
$$

(7)

which have degree $s$, where

$$
\sigma = (\sigma_1, \ldots, \sigma_s), \quad \sigma_j = \pm 1,
$$

$$
k = (k_1, \ldots, k_s), \quad k_j = \lfloor -N/2 \rfloor + 1, \ldots, \lfloor N/2 \rfloor,
$$

$$
l = (l_1, \ldots, l_s), \quad l_j = \pm 1,
$$

(7)

and observe that a fundamental property of all monomials is that the indices $k$ have a relation of the form

$$
\tilde{\tau} \cdot k = nN,
$$

(8)

for some

$$
\tilde{\tau} = (\tilde{\tau}_1, \ldots, \tilde{\tau}_s), \quad \tilde{\tau}_l = \pm 1 \quad n = \lfloor -(s-1)/2 \rfloor, \ldots, \lfloor (s-1)/2 \rfloor.
$$

(9)

In the following we will denote by $I_s$ the set of indices $(\sigma, \tilde{\tau}, k, l, n)$ of the form (7), (9).

**Definition 1** We say that $f \in \mathcal{P}_s$ if it can be written as

$$
f = \frac{1}{N^{(s-2)/2}} \sum_{(\sigma, \tilde{\tau}, k, l, n) \in I_s} f_{\sigma,\tilde{\tau},l,n} \left( \frac{k_1}{N}, \ldots, \frac{k_s}{N} \right) \Xi_{\sigma,k,l}^{\pm} \delta_{\tilde{\tau},k}^{\pm},
$$

(10)

where $f_{\sigma,\tilde{\tau},l,n} : [0,1]^s \to \mathbb{C}$ are continuous functions and $\delta_j^n$ is a shortcut for the Kronecker delta $\delta_{j,nN}$. 

8
In $\mathcal{P}_s$ we define the norm
\[
\|f\|_+ \overset{\text{def}}{=} \max_{(\sigma, \tilde{\tau}, k, l, n) \in I_s} \left| f_{\sigma, \tilde{\tau}, n} \left( \frac{k_1}{N}, \ldots, \frac{k_s}{N} \right) \right| \delta_{\tilde{\tau}, k}. \tag{11}
\]

One has the lemma (proved in Appendix B)

**Lemma 1** If $f \in \mathcal{P}_s$, $g \in \mathcal{P}_r$, then $\{f, g\} \in \mathcal{P}_{r+s-2}$. Moreover, one has
\[
\|\{f, g\}\|_+ \leq 2^4 \Omega^{r+s} \min(r, s) \|f\|_+ \|g\|_+. \tag{11}
\]

We now have all the tools needed in order to construct the solutions for the homological equation (4): we intend to show, in a way completely analogous to [24], to which the reader will be referred for some proofs, that in our case eq. (4) can be solved for $s \leq S = S(m_1/m_2)$, with $\chi_s, Z_s$ and $\Psi_s$ belonging to the Banach spaces $\mathcal{P}_{s+2}$.

First, we point out that the monomials $\Xi_{\sigma, k, l}^s$ are eigenfunctions for the operators $L_0$ and $L_\Omega$, with eigenvalues given by
\[
L_0 \Xi_{\sigma, k, l}^s = i \left( \sum_{j=1}^{s} \sigma_j \omega_{k_j}^l \right) \Xi_{\sigma, k, l}^s, \quad L_\Omega \Xi_{\sigma, k, l}^s = i \Omega \left( \sum_{j=1}^{s} \sigma_j \delta_{l_j, +} \right) \Xi_{\sigma, k, l}^s. \tag{12}
\]

For this reason, both $L_0$ and $L_\Omega$ map $\mathcal{P}_s$ in itself and, in particular, $\mathcal{P}_s$ is the direct sum of $\mathcal{N}_s$ and $\mathcal{R}_s$, the kernel and the range of $L_\Omega$, respectively. Since $L_0 = L_\Omega + L_{\Theta_0}$, where
\[
\Theta_0 = \sum_k \left( \left( 1 - \frac{\Omega}{\omega_k^+} \right) \frac{\left| \hat{p}_k^+ \right|^2 + \omega_k^+ \left| q_k^+ \right|^2}{2} + \frac{\left| \hat{p}_k^- \right|^2 + \omega_k^- \left| q_k^- \right|^2}{2} \right),
\]
we note then that
\[
L_0^{-1} = (I + K)^{-1} L_\Omega^{-1}, \quad \text{with } K \overset{\text{def}}{=} L_\Omega^{-1} L_{\Theta_0}
\]
and that $K : \mathcal{R}_s \mapsto \mathcal{R}_s$, because $L_{\Theta_0} f \in \mathcal{R}_s$, if $f \in \mathcal{R}_s$, as it can be shown in virtue of the Jacobi identity and of the fact that $\{\Theta_0, H_\Omega\} = 0$ (cfr. Lemma 4.1 in [24]). The operator $L_0$ can be then inverted on $\mathcal{R}_s$, by using Neumann formula, which holds provided $\|K\| < 1$ on $\mathcal{R}_s$.

This ensures that a solution for the homological equation (4) up to a given order can be constructed, as is expressed by the following lemma, whose proof is deferred to Appendix C.
Lemma 2 Let \( S = \lfloor \sqrt{m_1/m_2}/2 \rfloor \). Then for \( s \leq S \) we have that \( \Psi_s \in \mathcal{P}_{s+2} \) and \( K : \mathcal{R}_s \to \mathcal{R}_s \), with \( \| K \| \leq 1/2 \) on \( \mathcal{R}_s \). Moreover, for \( s \leq S \) there exist \( Z_s, \chi_s \in \mathcal{P}_{s+2} \) such that:

1. they are solutions for \( (4) \);
2. \( Z_s \) is in involution with \( H_{\Omega} \), i.e., \( Z_s \in \mathcal{N}_{s+2} \);
3. If \( \| H_s \|_+ \leq B^s s! \) there exists \( C > 0 \) such that, for \( 1 \leq s \leq S \),

\[
\| Z_s \|_+ \leq \| \Psi_s \|_+ \leq B^s C^{s-1} s! ,
\]

(13)

4. for \( f_l \in \mathcal{P}_{l+2} \) and \( 1 \leq s \leq S \), one has \( E_s f_l \in \mathcal{P}_{s+l+2} \), with

\[
\| E_s f_l \|_+ \leq \frac{1}{4} B^s C^s (s + l)! \left( \frac{1}{s!} + \frac{1}{l+1} \right) \| f_l \|_+ , \quad \text{for } l \geq 1 ,
\]

\[
\| E_s f_l \|_+ \leq \frac{1}{4} B^s C^s (s + 1)! \| f_l \|_+ , \quad \text{for } l = 0 .
\]

(14)

3.3 Estimate for the variances

The main result of this section is that, for any \( f \in \mathcal{P}_s \), its variance can be bounded from above by the following

Lemma 3 There exist \( N_0 > 0 \) and \( C > 0 \) such that, for any \( 2 \leq s \leq S \), for any \( N > N_0 \) and any \( f \in \mathcal{P}_s \), one has

\[
\sigma^2_f \leq N \frac{C^{2s}}{\beta^s} (2s!)^{3/2} \| f \|_+^2 .
\]

Proof. By the definition of variance and that of the class \( \mathcal{P}_s \) one has

\[
\sigma^2_f = \frac{1}{N_{s-2}} \sum_{\sigma,\tilde{s},k,l,n \in \mathcal{I}_s} \sum_{(\sigma',\tilde{s}',k',l',n') \in \mathcal{I}_s} f_{\sigma,\tilde{s},l,n} f_{\sigma',\tilde{s}',l',n'} \delta_{\sigma,k}^{\sigma',k'}
\]

\[
\times \left( \langle \Xi^s_{\sigma,k,l} \Xi^s_{\sigma',k',l'} \rangle - \langle \Xi^s_{\sigma,k,l} \rangle \langle \Xi^s_{\sigma',k',l'} \rangle \right)
\]

\[
\leq \frac{1}{N_{s-2}} \| f \|_+^2 \left( \sum_{(\sigma,\tilde{s},k,l,n) \in \mathcal{I}_s} \sum_{(\sigma',\tilde{s}',k',l',n') \in \mathcal{I}_s} \delta_{\sigma,k}^{\sigma',k'} \left| \langle \Xi^s_{\sigma,k,l} \Xi^s_{\sigma',k',l'} \rangle - \langle \Xi^s_{\sigma,k,l} \rangle \langle \Xi^s_{\sigma',k',l'} \rangle \right| \right) .
\]

(15)
The main part of the proof is then to show that the sum in the last line can be bounded from above by \( N^{s-1}C^{2s}(2s)!^{3/2}/\beta^s \). This seems quite difficult, and in particular the dependence on \( N \) seems to pose a big problem: note, in fact, that the sum over \( k \) and \( k' \), taking into account the constraint imposed by the Kronecker deltas, contains a number of terms of order \( N^{2s-2} \). A huge number of terms in the sum must thus vanish, in order to reduce the size, precisely as many as would vanish if \( \Xi_{s,k,l}^{\sigma} \) and \( \Xi_{s',k',l'}^{\sigma'} \) were uncorrelated for \( k \neq k' \). This is not the case, but it can be proved that the correlation between the two monomials is always zero, unless the components \( k \) and \( k' \) satisfy some linear relations, which will be expressed by the introduction of some suitable Kronecker deltas, as we detail now.

Fix a positive integer \( R \), and consider the vectors \( \tau = (\tau_1, \ldots, \tau_R) \), with the \( j \)-th component \( \tau_j = 0, \pm 1 \). Denote by \( \mathbb{Z}_R^R \) the set of such vectors and by \( \text{supp}(\tau) \) the set of indices \( j \) such that \( \tau_j \neq 0 \).

**Definition 2** A collection \( \tau^{(1)}, \ldots, \tau^{(S_1)} \) of vectors \( \tau^{(i)} \in \mathbb{Z}_R^R \) will be said \( R \)-admissible, or simply admissible, if \( S_1 \leq R \), the supports \( \text{supp}(\tau^{(i)}) \) constitute a partition of the set \( \{1, \ldots, R\} \) in disjoint subsets and if

\[
\min(\text{supp}(\tau^{(i)})) < \min(\text{supp}(\tau^{(j)})) \iff i < j.
\]

We will denote by \( \mathcal{T}_R \) the set of \( R \)-admissible vectors; the introduction of this class enables us to state the following lemma, which comes from the fact that \( (p_j, r_j) \), with \( r_j \overset{\text{def}}{=} (x_{j,2} - x_{j,1}, x_{j,1} - x_{j-1,2}) \), are exchangeable variables (see Appendix \( \square \)), where the proof of this Lemma is reported:

**Lemma 4** For any \( S_1 < s + s' \) there exist constants \( c_n^{(\tau^{(1)}, \ldots, \tau^{(S_1)})} > 0 \), independent of \( k, k' \) and \( N \), such that

\[
\left| \left( \Xi_{\sigma,k,l}^{s} \Xi_{\sigma',k',l'}^{s'} - \langle \Xi_{\sigma,k,l}^{s} \rangle \langle \Xi_{\sigma',k',l'}^{s'} \rangle \right) \right| \leq \sum_{S_1 = 1}^{s+s'} N^{S_1-(s+s')/2} \sum_{(\tau^{(1)}, \ldots, \tau^{(S_1)}) \in \mathcal{T}_{s+s'}^{n_1, \ldots, n_{S_1}}} \delta_{\tau^{(1)}}^{n_1} \cdots \delta_{\tau^{(S_1)}}^{n_{S_1}} c_{n_1, \ldots, n_{S_1}}^{(\tau^{(1)}, \ldots, \tau^{(S_1)})},
\]

(16)
in which \( K = (k_1, \ldots, k_s, k'_1, \ldots, k'_{s'}) \).

**Remark:** In each sum over \( n_i \) the terms \( \delta_{\tau^{(i)}}^{n_i} \) can be different from zero only for \( n_i \) ranging from \( [-n_i/2] + 1 \) to \( [n_i/2] \), where \( n_i \) is the cardinality of \( \text{supp} \tau^{(i)} \). This because \( \tau^{(i)} \cdot K \) ranges from \( n_i([-N/2] + 1) \) to \( n_i[N/2] \).
We come back to the estimate of the variance and insert (16) into (15), observing that
\[ \sigma^2 \leq \|f\|^2 + \sum_{n,n'} \delta^n_k \delta^{n'}_{k'} \sum_{S_1=1}^{2S_1+2-2s} \sum_{(\tau^{(1)},\ldots,\tau^{(S_1)}) \in T_{S_1}} \delta^n_{\tau^{(1)}-K} \cdots \delta^{n_{S_1}}_{\tau^{(S_1)}-K} \cdot n_{S_1} \cdot \prod_{i=1}^{S_1} n_i. \]

The Kronecker deltas \( \delta^n_{\tau^{(i)}-K} \) represent some linear relations that the vector \( K = (k,k') \) has to satisfy, relations which are all independent, because the supports of \( \tau^{(i)} \) are disjoint. Thus, in the sum over \( (k,k') \) only \( 2s - S_1 \) independent terms are left. In the general case, it cannot be proved that the further constraints imposed by \( \delta^n_k \) and \( \delta^{n'}_{k'} \) entail another independent linear restriction on the sum, but this certainly happens outside a set of indices \( (\tau^{(1)},\ldots,\tau^{(S_1)}) \) which we now specify. Consider the collection \( \bar{T} \subset T_{2s} \) of \( (\tau^{(1)},\ldots,\tau^{(S_1)}) \) such that, for any \( \tau^{(i)} \), either \( \text{supp} \tau^{(i)} \subset \{1,\ldots,s\} \), or \( \text{supp} \tau^{(i)} \subset \{s+1,\ldots,2s\} \), and denote by \( \bar{T}^c \) its complement in \( T_{2s} \). Then it can be shown that (as is proved in Lemma 9 of [6]), for \( (\tau^{(1)},\ldots,\tau^{(S_1)}) \in \bar{T}^c \), at least one among \( \delta^n_k \) and \( \delta^{n'}_{k'} \) implies a constraint on the sum over \( (k,k') \) which is independent of those imposed by \( \delta^n_k \).

Coming to formulas, this means that, since
\[ \sum_{i \in \text{supp}(\tau^{(i)})} \sum_{n_i} \delta^n_{\tau^{(i)}-K} \leq n_{\text{supp}(\tau^{(i)})} N^{n_{\text{supp}(\tau^{(i)})}-1}, \]
if \( N > s \), one has
\[ \sum_{k,k'} \sum_{n,n'} \delta^n_k \delta^{n'}_{k'} \sum_{n_1,\ldots,n_{S_1}} \delta^n_{\tau^{(1)}-K} \cdots \delta^{n_{S_1}}_{\tau^{(S_1)}-K} \leq \prod_{i=1}^{S_1} n_i N^{n_{\text{supp}(\tau^{(i)})}-1} = N^{2s-S_1} \prod_{i=1}^{S_1} n_i. \]

If, moreover, \( (\tau^{(1)},\ldots,\tau^{(S_1)}) \in \bar{T}^c \), on account of Lemma 9 of [6] the estimate can be refined with
\[ \sum_{k,k'} \sum_{n,n'} \delta^n_k \delta^{n'}_{k'} \sum_{n_1,\ldots,n_{S_1}} \delta^n_{\tau^{(1)}-K} \cdots \delta^{n_{S_1}}_{\tau^{(S_1)}-K} \leq N^{2s-S_1-1} \sum_{i=1}^{S_1} n_i. \]
We can then write
\[
\sigma_2^2 \leq N \|f\|^2_+ \sum_{S_1=1}^{2s} \left( \sum_{(\tau(1),\ldots,\tau(S_1)) \in \mathcal{T}^c} n_1 \cdots n_{S_1} c_{s,s}(\tau(1),\ldots,\tau(S_1)) \right) + N \sum_{(\tau(1),\ldots,\tau(S_1)) \in \mathcal{T}} n_1 \cdots n_{S_1} c_{s,s}(\tau(1),\ldots,\tau(S_1)) \right).
\]

This is enough for our aims, since in our case (see Appendix D) a precise estimate of the constants \(c\) entering the previous formula is available:

**Lemma 5** There exists \(C > 0\) such that
\[
\sum_{S_1=1}^{2s} \sum_{(\tau(1),\ldots,\tau(S_1)) \in \mathcal{T}^c} n_1 \cdots n_{S_1} c_{s,s}(\tau(1),\ldots,\tau(S_1)) \leq C \frac{(2s)!^{3/2}}{\beta s}. \]
\[
\sum_{S_1=1}^{2s} \sum_{(\tau(1),\ldots,\tau(S_1)) \in \mathcal{T}} n_1 \cdots n_{S_1} c_{s,s}(\tau(1),\ldots,\tau(S_1)) \leq \frac{1}{N} C \frac{(2s)!^{3/2}}{\beta s}.
\]

The thesis of lemma 3 follows then easily by applying this estimate.

### 3.4 Conclusion of the proof of Theorem 2

In virtue of Lemma 2, we can construct approximants of the first integral \(\Phi\) as \(\Phi^{(r)} = \sum_{s=0}^{r} \Phi_s\), with \(\Phi_s = E_s \Phi_0 \in \mathcal{P}_{s+2}\) and \(\|\Phi_s\|_+ \leq s! C^s\). This can be done for any \(r \leq S = \lfloor \sqrt{m_1/m_2/2} \rfloor\).

Since the variables \(p_j\) are independent of the variables \(x_j\), it is easy to show that
\[
\sigma_{\Phi_0} \geq \sigma_{\sum_k |p_k|^2/2\omega_k^2} \geq \frac{\sqrt{NC_1}}{\beta}, \quad (18)
\]
while
\[
\sigma_{\Phi^{(s)} - \Phi_0} \leq \sum_{s=1}^{S} \sigma_{\Phi_s} \leq \sqrt{N} \sum_{s=1}^{S} \frac{C_2^s}{\beta^{(s+2)/2}} (s!)^{5/2}, \quad (19)
\]
because of Lemma 3. Hence follows
\[
\sigma_{\Phi^{(s)}} \geq \sigma_{\Phi_0} - \sigma_{\Phi^{(s)} - \Phi_0} \geq \frac{\sqrt{NC_3}}{\beta} \left(1 - \sum_{s=1}^{S} \frac{C_3^s}{\beta^{s/2}} (s!)^{5/2}\right), \quad (20)
\]
and, for \( \beta \) large enough, that

\[ \sigma_{\Phi(S) - \Phi_0} \leq \frac{K_2}{\sqrt{\beta}} \sigma_{\Phi_0}, \]

i.e., the second statement of (3).

In order to estimate the derivative with respect to the flow of \( \Phi(S) \), as already remarked we point out that (see [23]) this is equal to

\[ \dot{\Phi}^{(S)} = \sum_{s=0}^{S} \{ \Phi_s, \sum_{s' \geq S-1} H_s' \}. \]

In our case, in which \( H_s = 0 \) for \( s \geq 3 \), we have to estimate

\[ \Upsilon_S = \{ \Phi_S, H_1 \} + \{ \Phi_{S-1}, H_2 \}, \quad \Upsilon_{S+1} = \{ \Phi_S, H_2 \}, \]

with \( \Upsilon_r \in \mathcal{P}_{r+3} \). Therefore, again by Lemmas 2, 3, we get

\[ \sigma_{\Phi(S)} \leq \sigma_{\Upsilon_S} + \sigma_{\Upsilon_{S+1}} \leq \sqrt{N} C_4^S (S!)^{5/2} \beta^{-3(S+3)/2} (1 + \beta^{-1/2}) \].

For \( \beta \) large enough, this estimate and relation (20) give the first statement in (3) and conclude the proof.

4 Proof of Theorem 1 and Corollary 1

The proof of Theorem 1 for \( E^+ \) lays on an application of Theorem 1 of [27] to the difference

\[ E^+ - \Omega \Phi_0 = \frac{1}{2} \sum_k \left( 1 - \frac{\Omega}{\omega_k^+} \right) \left( |\rho_k^+|^2 + \omega_k^+ |\eta_k^+|^2 \right) = \frac{1}{2} \sum_k \left( 1 - \frac{\Omega}{\omega_k^+} \right) \xi_k^+ \eta_k^+. \]

Indeed, if \( m_1/m_2 > 2 \),

\[ \| E^+ - \Omega \Phi_0 \|_+ = \sup_k \left( 1 - \frac{\Omega}{\omega_k^+} \right) \leq \frac{1}{\sqrt{2}} \frac{m_2}{m_1}, \]

so that, on account of Lemma 3 there exists \( C_1 > 0 \) such that

\[ \sigma_{E^+ - \Omega \Phi_0} \leq \sqrt{N} \frac{m_2}{m_1} \beta \quad \Rightarrow \]

\[ \sigma_{E^+ - \Omega \Phi(S)} \leq \sigma_{E^+ - \Omega \Phi_0} + \Omega \sigma_{\Phi(S) - \Phi_0} \leq \sqrt{N} \frac{C_1}{\beta} \left( \frac{m_2}{m_1} + \frac{1}{\sqrt{\beta}} \right), \]
where, in the second line, use is made of (3). In a way identical to (18) it is then shown that there exists \( C_2 > 0 \) such that
\[
\sigma_{E^+} \geq \sqrt{N \frac{C_2}{\beta}} ,
\]
and thus, by using Theorem 1 in [27], there exists \( K_2 > 0 \) such that
\[
|C_{E^+}(t) - C_{\Omega \Phi(s)}(t)| \leq K_2 \left( \frac{m_2}{m_1} + \frac{1}{\sqrt{\beta}} \right) \sigma_{E^+}^2 .
\]
From Theorem 2 then Theorem 1 for \( E^+ \) is immediately deduced.

Coming to the statement for \( E^- \), we observe that
\[
E^- = H - E^+ - H_{nl} ,
\]
where we have defined \( H_{nl} = H - H_0 \). Since \( H \) is a constant of motion,
\[
\langle H_t \cdot F \rangle = \langle HF_t \rangle = \langle HF \rangle ,
\]
for any dynamical variable \( F \), thus showing that
\[
C_{E^-}(t) - C_{E^-}(0) = C_{E^+}(t) - C_{E^+}(0) + C_{H_{nl}}(t) - C_{H_{nl}}(0)
- \langle (E^+_t - E^+) (H_{nl} - \langle H_{nl} \rangle) \rangle
- \langle (H_{nl})_t - H_{nl} \rangle (E^+ - \langle E^+ \rangle) .
\]  
We notice that, because of Lemma 3, the following inequalities hold:
\[
\sigma_{H_0 - H} \leq C_1 \frac{\sqrt{N}}{\beta^{3/2}} , \quad \sigma_{E^+} \leq C_2 \frac{\sqrt{N}}{\beta},
\]
for suitable \( C_1, C_2 > 0 \). This, together with the fact that
\[
C_{H_{nl}}(t) \leq \sigma_{H_{nl}}^2 ,
\]
\[
\langle (E^+_t - E^+) (H_{nl} - \langle H_{nl} \rangle) \rangle \leq \sqrt{2} \sigma_{E^+} \sigma_{H_{nl}} ,
\]
\[
\langle ((H_{nl})_t - H_{nl}) (E^+ - \langle E^+ \rangle) \rangle \leq \sqrt{2} \sigma_{E^+} \sigma_{H_{nl}} ,
\]
enable us to infer from (21) that
\[
|C_{E^-}(t) - \sigma_{E^-}^2 | \leq |C_{E^+}(t) - C_{E^+}(0)| + 2C_1^2 \frac{N}{\beta^3} + 2C_1C_2 \frac{N}{\beta^{5/2}} .
\]
Hence, since \( \sigma_{E^-} \geq C_3 \sqrt{N} / \beta \) for a suitable \( C_3 > 0 \) and by the already proved statement for \( E^+ \), the thesis of Theorem 1 follows.

Corollary 1 is then easily deduced, by applying Cebyshev inequality to the quantity
\[
\langle (E^\pm(t) - E^\pm)^2 \rangle = \frac{1}{2} |C_{E^\pm}(t) - C_{E^\pm}(0)| .
\]
5 Concluding remarks: discussion of the heat capacity of the system

We have proved that both the energy of the optical branch and the energy of the acoustic branch are approximately conserved variables, i.e., their time autocorrelations stay close to the initial value for long times. This seems to be in contrast with the idea of thermalization and shows that the system is not mixing on the considered time scales. But does such a lack of ergodicity entail some consequences for the thermodynamic observables? This is not obvious at all, but in this particular case we can imagine, in a completely heuristic way, a mechanism for which this slow decay of correlations might show up in the measurement of an actual physical quantity, the heat capacity $C$ of the chain. Recall, indeed, that the expression of the heat capacity $C$ of a system put in contact with a thermostat, in the linear response theory approximation (see, for instance, [28]), is the following

$$C(t) = C_H(0) - C_H(t),$$

where $t$ denotes the duration of the measurement process, while the averages are taken with respect to an invariant measure and the flow is the one given by the full system (i.e., system of interest with Hamiltonian $H$, plus thermostat and the interaction terms between the two). By writing $H = H_0 + H_{nl}$ and $H_0 = E^+ + E^−$, such an expression becomes

$$C(t) = (C_{E^−}(0) - C_{E^−}(t)) + (C_{E^+}(0) - C_{E^+}(t))$$
$$+ \langle (E^+_i - E^+) (E^-_i - E^-) \rangle$$
$$+ (C_{E^+}(0) - C_{E^+}(t)) + 2\langle (H_0)_t - H_0 \rangle ((H_{nl})_t - H_{nl}), \quad (23)$$

where the terms in the third line can be neglected for small temperatures (see formulas (22) above and the subsequent remarks).

One can imagine a thermostat which exchanges energy mainly with one of the two branches, as it happens if we model the thermostat as a gas of particles, each interacting with the leftmost particle of the FPU chain through a short–range smooth potential (see [29]). In absence of a mechanism of energy exchange between the branches, this would imply that, at low temperatures and for times $t$ of order $\beta^{S/2}$, one has

$$\langle (E^+_i - E^+) \rangle^2 = 2 (C_{E^+}(0) - C_{E^+}(t)) \ll \sigma^2_{E^+},$$
for the complete system, too. Since the second line of (23) can be bounded from above by
\[
\langle (E_t^+ - E^+)(E_t^- - E^-) \rangle \leq \sigma E^+ \sqrt{2 \langle (E_t^+ - E^+)^2 \rangle},
\]
this implies that, for not too long times,
\[
C(t) \approx C_{E^+}(0) - C_{E^-}(t).
\]
As \(C_{E^-}(t)\) is expected to decay quickly to zero, this means that the measured heat capacity would stabilize around the value \(\sigma^2\), which is significantly smaller than the equilibrium value \(\sigma_H^2\).

This is, of course, just the rough cast of an idea, but a result of this kind would be of extreme interest, and we plan to work in the near future to establish, following the example of [22], whether a result of this kind can be proved as a theorem, by suitably choosing the properties of the thermostat.

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### A Normal modes of oscillation

We are looking for a change of variables to the normal modes of oscillation of the form
\[
x_j = \sum_k \sum_{l=\pm} u_k^l q_k^l e^{i\kappa j},
\]
i.e., for solutions of the linearized dynamics as \(x_j = u e^{i(\kappa j - \omega t)}\), with \(\kappa = 2\pi k/N\), and \(k = [-N/2] + 1, \ldots, [N/2]\).

Corresponding to the frequencies
\[
(\omega_k^\pm)^2 = K \frac{m_1 + m_2 \pm \sqrt{\Delta_k}}{m_1 m_2},
\]
in which \(\Delta_k = m_1^2 + m_2^2 + 2m_1 m_2 \cos \frac{2\pi k}{N}\),
a solution for \(u_k^\pm\) is
\[
u_k^\pm = c_k^\pm \left(\begin{array}{c}
\cos \frac{k}{2} \\
(m_2 - m_1 \mp \sqrt{\Delta_k})e^{i\kappa j/2} / 2m_2
\end{array}\right), \quad \text{for } k \neq N/2,
\]
\[
u_{N/2}^+ = \frac{1}{\sqrt{N}} \left(\begin{array}{c}
0 \\
1/\sqrt{m_2}
\end{array}\right), \quad \nu_{N/2}^- = \frac{1}{\sqrt{N}} \left(\begin{array}{c}
1/\sqrt{m_1} \\
0
\end{array}\right),
\]
where the second line is needed only if \( N \) is even and we have introduced a normalization factor

\[
c_k^\pm = \left( \frac{N \sqrt{\Delta_k}}{2m_2} \left( \sqrt{\Delta_k} \mp (m_2 - m_1) \right) \right)^{-1/2}.
\]

Such a normalization is so chosen that, for the Hermitian product in \( \mathbb{C}^2 \), denoted by \( \langle \cdot, \cdot \rangle \), it holds

\[
\langle u_k^l, M u_{k'}^{l'} \rangle = \frac{1}{N} \delta_{k,k'} \delta_{l,l'} , \quad \text{with } M = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} .
\] (25)

Notice that, since \( x_j \) are real, while \( u_k^\pm = \bar{u}_{-k}^\pm \), the complex coordinates (coordinates of the normal modes) \( \hat{q}_k^\pm \) satisfy the relations \( \hat{q}_{-k}^\pm = \hat{q}_k^\pm \), for \( k \neq 0, N/2 \), whereas they are real for \( k = 0, N/2 \).

In order to invert (24) we start from relation

\[
u_k^+ \hat{q}_k^+ + u_k^- \hat{q}_k^- = \sum_j x_j e^{-i\kappa j} ,
\] (26)

and take the Hermitian product, respectively, with \( M u_k^+ \) and \( M u_k^- \). We thus get

\[
\hat{q}_k^\pm = \sum_j \langle x_j, M u_k^\pm \rangle e^{-i\kappa j} = \sum_j \left( m_1 x_{j,1} \text{Re} u_{k,1}^\pm + m_2 x_{j,2} \text{Re} u_{k,2}^\pm \right) e^{-i\kappa j} .
\] (27)

For the conjugate moments \( \hat{p}_k^\pm \), the condition of canonicity imposes then

\[
\hat{p}_k^\pm = \sum_j \left( \frac{p_{j,1}}{\sqrt{m_1}} \text{Re} \sqrt{m_1} u_{k,1}^\pm + \frac{p_{j,2}}{\sqrt{m_2}} \text{Re} \sqrt{m_2} u_{k,2}^\pm \right) e^{i\kappa j} .
\] (28)

Remark that, on account of (25), \( | \text{Re} \sqrt{m_i} u_{k,i} | \leq 1/\sqrt{N} \).

A.1 The transformation to the difference coordinates

In order to express the Hamiltonian as a function of the normal modes coordinates, it will be useful to write explicitly the relation between them and the difference coordinates \( r_j \) defined as

\[
r_j = (x_{j,2} - x_{j,1}, x_{j,1} - x_{j-1,2}) , \quad \text{i.e.,}
\]

\[
r_j = \sum_k \left( w_k^+ \hat{q}_k^+ + w_k^- \hat{q}_k^- \right) e^{i\kappa j} , \quad \text{with } w_k^\pm = \begin{pmatrix} u_{k,2}^\pm - u_{k,1}^\pm \\ u_{k,1}^\pm - u_{k,2}^\pm e^{-i\kappa} \end{pmatrix}
\] (29)
Here, an explicit calculation shows that
\[
\begin{align*}
\mathbf{w}_k^\pm = c_k \left( -\frac{m_1 \omega_k^\pm \cos \frac{k}{2}}{K} + i \frac{m_2 - m_1 \mp \sqrt{\Delta k}}{2m_2} \sin \frac{k}{2} \right) = \frac{\omega_k^\pm}{\sqrt{2NK}} \begin{pmatrix} e^{i\alpha_k^+} \\ -e^{-i\alpha_k^+} \end{pmatrix},
\end{align*}
\]
with the complex phase \(\alpha_k\) determined by
\[
e^{2i\alpha_k^\pm} = \pm \frac{m_2 + m_1 e^{i\kappa}}{\sqrt{\Delta_k}}.
\]

From here, it can be immediately shown that, for any \(m\),
\[
\sum_{j=1}^N r_{j,m}^3 = \sum_{k_1,\ldots,k_s,l_1,\ldots,l_s = \pm} (w_{k_1,m}^l q_{k_1}^l \cdots w_{k_s,m}^l q_{k_s}^l) \sum_{j=1}^N e^{i(\kappa_1 + \cdots + \kappa_s)j} = \sum_{k_1,\ldots,k_s,l_1,\ldots,l_s = \pm} (w_{k_1,m}^l q_{k_1}^l \cdots w_{k_s,m}^l q_{k_s}^l) \sum_n \delta_n^{k_1 + \cdots + k_s},
\]
where we made use of
\[
\sum_{j=1}^N e^{i2\pi kj/N} = N \sum_{n \in \mathbb{Z}} \delta_k^n, \quad \text{with} \quad \delta_k^n = \delta_{k,nN},
\]
which is valid for any integer \(k\). This is particularly relevant, because the perturbing parts of the Hamiltonian can be written as
\[
H_1 = \frac{KA}{2} \sum_j (r_{j,1}^3 + r_{j,2}^3), \quad H_2 = \frac{KB}{2} \sum_j (r_{j,1}^4 + r_{j,2}^4),
\]
so that it is immediately seen that they belong to \(P_3\) and \(P_4\), respectively.

Relation (29) can then be easily inverted, by using Fourier series properties, which give
\[
\mathbf{w}_k^+ \hat{q}_k^+ + \mathbf{w}_k^- \hat{q}_k^- = \frac{1}{N} \sum_{j=1}^N r_j e^{-i\kappa_jj}.
\]
We are however interested in equations which rely separately \(\hat{q}_k^+\) and \(\hat{q}_k^-\) to \(r_j\). Since \(\mathbf{w}_k^+\) and \(\mathbf{w}_k^-\) are orthogonal with respect to the Hermitian product
in $\mathbb{C}^2$ and $\langle w_k^+, w_k^- \rangle = \omega_k^+, \omega_k^−/(NK)$, we multiply both sides of (31) by $w_k^+$ and $w_k^-$, and get

$$\frac{\omega_k^+ \cdot q_k^-}{NK} = \frac{1}{N} \sum_j (r_j, w_k^+) e^{-i\kappa j} = \frac{\omega_k^-}{N\sqrt{2NK}} \sum_j \left( r_{j,1} \cos \alpha_k^+ - r_{j,2} \cos \alpha_k^- \right) e^{-i\kappa j}.$$ 

From here, the crucial equality follows

$$\omega_k^+ q_k^- = \sqrt{\frac{K}{2N}} \sum_j \left( r_{j,1} \cos \alpha_k^+ - r_{j,2} \cos \alpha_k^- \right) e^{-i\kappa j}. \quad (32)$$

**B Proof of Lemma**

We can write explicitly the Poisson brackets as

$$\{f, g\} = \frac{i}{N(r+s-4)/2} \sum_{(\sigma, \tilde{\sigma}, k, l, n) \in \mathcal{I}_\sigma} \sum_{(\sigma', \tilde{\sigma}', k', l', n') \in \mathcal{I}_{\sigma'}} f_{\sigma, \tilde{\sigma}, l, n} g_{\sigma', \tilde{\sigma}', l', n'} \sum_{j=1}^s \sum_{m=1}^r \frac{\omega_{k_j} l_{j} \xi_{\tilde{k_j}} l'_{j}}{\omega_{k_j} l_{j} \xi_{\tilde{k_j}} l'_{j}} \delta_{\sigma_j, -\sigma_m} \delta_{k_j, k'_m} \delta_{l_j, l'_m} \frac{\omega_{\tilde{k_j}} l_{j}}{\omega_{\tilde{k_j}} l_{j}} \delta_{\tilde{l_j}, \tilde{l}'_m} \delta_{\tilde{k_j}, k'_m}.$$ 

We exchange the order of the sums over $j$ and $m$ with those over $(\sigma, \tilde{\sigma}, k, l, n)$ and $(\sigma', \tilde{\sigma}', k', l', n)$, by summing first over $(\sigma_j, k_j, l_j, \tilde{\sigma}, n)$ and $(\sigma'_m, k'_m, l'_m, \tilde{\sigma}', n')$: this gives

$$\{f, g\} = \frac{i}{N(r+s-4)/2} \sum_{j=1}^s \sum_{m=1}^r \sum_{i, i'} \Xi_i^{s-1} \Xi_{i'}^{r-1} \sum_{\sigma_j, k_j, l_j, \tilde{\sigma}, n} \sum_{\sigma'_m, k'_m, l'_m, \tilde{\sigma}', n'} f_{\sigma, \tilde{\sigma}, l, n} g_{\sigma', \tilde{\sigma}', l', n'} \sigma_j \omega_{k_j} l_{j} \delta_{\sigma_j, -\sigma_m} \delta_{k_j, k'_m} \delta_{l_j, l'_m} \omega_{\tilde{k_j}} l_{j} \delta_{\tilde{l_j}, \tilde{l}'_m} \delta_{\tilde{k_j}, k'_m}$$

where

$$i = \{\{\sigma_i\}_{i \neq j}, \{k_i\}_{i \neq j}, \{l_i\}_{i \neq j}\}, \quad i' = \{\{\sigma'_i\}_{i \neq m}, \{k'_i\}_{i \neq m}, \{l'_i\}_{i \neq m}\}.$$ 

We note that

$$\Xi_i^{s-1} \Xi_{i'}^{r-1} = \Xi_{\sigma'' k'' l''}^{s-r+s-2}, \quad \text{with } \sigma'' = \{\{\sigma_i\}_{i \neq j} \cup \{\sigma'_i\}_{i \neq m}, \ldots \}.$$
is a monomial of degree $r+s-2$. We can therefore write $\{f,g\} = h \in P_{r+s-2}$, with
\[
h = \frac{1}{N(r+s-4)/2} \sum_{(\sigma''', \tilde{\sigma}'', k'', l'')} \sum_{(\sigma, \tilde{\sigma}, k, l)} h_{\sigma''', \tilde{\sigma}'', k'', l''} z_{\sigma''', \tilde{\sigma}'', k'', l''} \delta_{\tilde{\sigma}', k', l'}.
\]
Here
\[
h_{\sigma''', \tilde{\sigma}'', k'', l''} = \sum_{j=1}^{s} \sum_{m=1}^{r} \sum_{\sigma_j, k_j, l_j, \tilde{\sigma}_j, n} \sigma_j \omega_{k_j} \delta_{\tilde{\sigma}, k, l} \delta_{\tilde{\sigma}', k', l'} \delta_{\tilde{\sigma}'', k'', l''} \delta_{\tilde{\sigma}', k', l'} \delta_{\tilde{\sigma}'', k'', l''} \delta_{\tilde{\sigma}'', k'', l''}.
\]

where $(\sigma, \tilde{\sigma}, k, l)$ and $(\sigma', \tilde{\sigma}', k', l')$ are determined in terms of $(\sigma'', \tilde{\sigma}'', k'', l'')$, $\sigma_j, k_j, l_j, \tilde{\sigma}_j, \sigma', k', l', \tilde{\sigma}'$. Indeed, one has
\[
\tilde{\sigma} = \{\tilde{\sigma}_j\}_{i<\sigma} \cup \{\tilde{\sigma}_j\}_{j<\sigma},
\]
\[
\tilde{\sigma}' = \{-\tilde{\sigma}_j\}_{i<\sigma} \cup \{\tilde{\sigma}_j\}_{j<\sigma},
\]
\[
\sigma = \{\sigma_i\}_{i<\sigma} \cup \{\sigma_j\}_{j<\sigma},
\]
and similar relations for $k, k', l, l'$. Due to the appearance of Kronecker deltas, $\sigma'_i = -\sigma_j, l'_m = l_j$ and $k'_m = k_j$, whereas $\delta_{\tilde{\sigma}', k}$ imposes $k_j = \tilde{\sigma}_j n = \sum_i \tilde{\sigma}_j \tilde{\sigma}_i$, and $\delta_{\tilde{\sigma}', n-n''}$ fixes $n' = \tilde{\sigma}_m \tilde{\sigma}_n - \tilde{\sigma}_m n''$. Such remarks enable us to estimate the norm of $h$ by summing only on the free indices as
\[
\|h\|_+ \leq \Omega \|f\|_+ \|g\|_+ \sum_{j=1}^{s} \sum_{m=1}^{r} \sum_{\sigma_j, k_j, \tilde{\sigma}_j, n} \sum_{\sigma'_i, k'_i, l'_i, \tilde{\sigma}'_i} \frac{1}{2^{(s-1)/2}}.
\]
By possibly exchanging the role of $n$ with that of $n'$, the thesis is got.

## C Proof of Lemma 2

For what concerns the operator norm of $K$, we note that, if $g \in R_s$, $\|L_\Omega g\|_+ \geq \Omega \|g\|_+$. Since on $P_s$
\[
\|L_{\theta_0}\| \leq s \max\{\max \omega_k^+, \min \omega_k^+, \max \omega_k^-\} = \sqrt{\frac{2K}{m_1}} s \leq s \Omega \sqrt{\frac{m_2}{m_1}},
\]

21
the norm of $K$ on $\mathcal{R}_s$ is smaller than $1/2$ for $s \leq S$. Thus, for any $g \in \mathcal{R}_s$ it holds $\|L_0^{-1}f\|_+ \leq 2\|f\|_+ / \Omega$, by Neumann inversion formula.

Coming to the solutions of the homological equation (which are nontrivial only for $S \geq 3$), we observe first of all that $\Psi_1 = H_1 \in \mathcal{P}_3$, so that $Z_1$ can be chosen as the projection over $\mathcal{N}_1$ of $\Psi_1$. This implies that $Z_1 - \Psi_1 \in \mathcal{R}_3$, and eq. (1) can be accordingly solved, with $\chi_1 \in \mathcal{P}_3$, and $\|\chi_1\|_+ \leq 2\|\Psi_1\|_+ / \Omega$. The estimate $\|Z_1\|_+ \leq \|\Psi_1\|_+ = \|H_1\|_+ \leq B$ is then valid, in agreement with (13) for $s = 1$. For $\Psi_2$, in a similar way, it can be seen that it belongs to $\mathcal{P}_4$, so as $Z_2$ and $\chi_2$, while its norm, due to Lemma 1, is bounded from above by

$$\|\Psi_2\|_+ \leq \|H_2\|_+ + \frac{1}{2}(\|L\chi_1H_1\|_+ + \|L\chi_1Z_1\|_+) \leq B^2(2 + 2^5 \cdot 3^3),$$

which satisfies (13) if $C \geq 2^63^3$.

For all other orders we proceed by induction, observing that, for $s \leq S$, $\Psi_s \in \mathcal{P}_{s+2}$ on account of Lemma 1 and, as a consequence $Z_s$ and $\chi_s$ belong to $\mathcal{P}_{s+2}$, too. This entails, as previously observed, that $\|\chi_s\|_+ \leq 2\|\Psi_s\|_+ / \Omega$, for $s \leq r - 1$. Since the expression for $\Psi_r$ involves $E_sZ_l$, for $1 \leq s \leq r - 1$, and $1 \leq l \leq r - 1$, let us suppose that hypothesis (13) is true for $s \leq r - 1$ and prove first formula (14) by induction on $s$, for $1 \leq s \leq r - 1$ and $l \geq 1$ fixed. For $s = 1$ this is trivially done by using the fact that $n + 1 \leq 2n$ if $n \geq 1$, as

$$\|E_1f_l\|_+ = \|L\chi_1f_l\|_+ \leq 2^53^2B(l + 2)\|f_l\|_+ \leq \frac{1}{4}BC\frac{(l + 1)!}{l!}\|f_l\|_+, \quad \text{if } C \geq 2^83^2.$$

For $s = 2$, instead, we write

$$\|E_2f_l\|_+ = \|L\chi_2f_l\|_+ + \frac{1}{2}\|L^2\chi_1f_l\|_+ \leq 2^6B^2\|f_l\|_+ (2C(l + 2) + 3^4(l + 2)(l + 3)) \leq (BC)^2\|f_l\|_+ \left(\frac{2^{10}(l + 2)!}{C(l + 1)!} + \frac{2^93^4(l + 2)!}{C^2l!}\right).$$

This is in agreement with (14) if $C \geq 2^{12}$. For what concerns the terms with $3 \leq s \leq r - 1$, we repeatedly use the elementary inequality

$$n!m! \leq k!(n + m - k)!, \quad \text{if } n, m \geq k, \quad (33)$$

22
in the following chain of inequalities

$$
\|E_s f_i\|_+ \leq \|L_{\chi_s} f_i\|_+ + \|L_{\chi_{s-1}} L_{\chi_1} f_i\|_+ + \frac{1}{s} \|L_{\chi_1} E_{s-1} f_i\|_+ \\
+ \frac{2}{s} \|L_{\chi_2} E_{s-2} f_i\|_+ + \sum_{j=3}^{s-2} \frac{j}{s} \|L_{\chi_j} E_{s-j} f_i\|_+ \\
\leq B^s C^{s-1} \left(2^6 + \frac{2 \cdot 13^2}{C}\right) (s + 1)! \left(\frac{(l + 3)!}{(l + 1)!}\right) \|f_i\|_+ \\
+ 2^{6^2} B^s \frac{s + l}{s} \|E_{s-1} f_i\|_+ + 2^{12} B^2 C^s \frac{s - l - 1}{s} \|E_{s-2} f_i\|_+ \\
+ \frac{2^5 s - 2}{s} \sum_{j=3}^{s-2} B^3 C^{j-1} (j + 2)! (s - j + 2)^2 \|E_{s-j} f_i\|_+ \\
\leq 2^{6^3} B^s C^{s-1} \frac{(s + l)!}{l!} \|f_i\|_+ \left(\frac{2^3 + 2 \cdot 3^2}{C}\right) \frac{1}{l + 1} \\
+ \frac{3}{4} \left(\frac{1}{s!} + \frac{1}{s(l + 1)}\right) + \frac{2^4}{l + 1} + \frac{2}{l + 1}\right),
$$

which satisfies (14) if $C \geq 2^{13}$.

We come then to the other inductive hypothesis, i.e., (13), noticing that, by the very definition of $\Psi$, one has

$$
\|\Psi_r\|_+ \leq \|H_r\|_+ + \sum_{j=1}^{r-1} \frac{1}{r} \left(j \|L_{\chi_j} H_{r-j}\|_+ + j \|E_{r-j} Z_j\|_+\right).
$$

We treat separately the single terms, making use of inequalities (33). The first addendum is trivially bound from above by hypothesis, while the first term in brackets is bounded from above, due to Lemma [1] via

$$
\frac{3}{4} \left(\frac{1}{s!} + \frac{1}{s(l + 1)}\right) + \frac{2^4}{l + 1} + \frac{2}{l + 1}\right).
$$

The other term in brackets, by inductive hypotheses (13, 14) at the previous
orders, is bounded from above by
\[
\sum_{j=1}^{r-1} \frac{j}{r} \|E_{r-j}Z_j\|_+ \leq B^r C^{r-1} \frac{r!}{4} \sum_{j=1}^{r-1} \left( \frac{1}{(r-j)!} + \frac{j}{r(r+1)} \right) \leq B^r C^{r-1} \frac{r!}{4}(c+1).
\]

Taking the sum over \(j\), this gives
\[
\|\Psi_r\|_+ \leq B^r r! \left( 1 + 2^9 3 C^{r-3} + 2^6 3^2 C^{r-2} + \frac{e + 1}{4} C^{r-1} \right),
\]
from which (13) follows, for \(C \geq 2^{10} 3^2\).

Only the proof of (14) for \(l = 0\) is left, as it was not needed above. This is trivially true for \(s = 1\), while for \(2 \leq s \leq S\), by induction one has
\[
\|E_{s,fi}\|_+ \leq\|L_{\chi_{s-1}}L_{\chi_1}fi\|_+ + \frac{1}{s} \|L_{\chi_1}E_{s-1}fi\|_+ + \sum_{j=2}^{s-2} \frac{1}{s} \|L_{\chi_j}E_{s-j}fi\|_+
\]
\[
\leq 2^{5} B^s C^{s-1} \|fi\|_+ \left( \left( 2^3 + \frac{2^8 3^2}{C} + 2 \cdot 3 \right) (s+1)! \right)
\]
\[
+ \frac{1}{4s} \sum_{j=2}^{s-2} (j+2)!(s-j+3)!
\]
\[
\leq \left( 2^{10} + \frac{2^{13} 3^3}{C} \right) B^s C^{s-1} \|fi\|_+ (s+1)!,
\]
whence (14) for \(C \geq 2^{12}\).

\section{D Proof of Lemmas 4 and 5}

The proof of both Lemmas is performed by expressing the monomials \(\Xi_{\sigma,k,l}^s\) in the coordinates \((p_j, r_j)\), in which the Gibbs measure is easier to control. In fact, it possesses several remarkable properties:

- the variables \(p_j\) and \(r_j\) are mutually independent;
- the variables \(r_{j,i}\) are exchangeable (see [26] for the concept of exchangeability);
- the variables \(p_{j,i}\) are pairwise independent (and so, in particular, they are exchangeable).
In addition, we have an estimate of the mean values of the monomials in such variables, which is expressed in subsequent Lemma 6. There, we denote by
\[ y_j = \left( \frac{p_{j,1}}{\sqrt{m_1}}, \frac{p_{j,2}}{\sqrt{m_2}}, \sqrt{Kr_{j,1}}, \sqrt{Kr_{j,2}} \right), \]
and by
\[ y_{j,\alpha} = y_{j,\alpha_1} \cdots y_{j,\alpha_s}, \quad \text{for } j = (j_1, \ldots, j_s), \]
\[ \alpha = (\alpha_1, \ldots, \alpha_s), \quad \alpha_i = 1, \ldots, 4, \]
while \( J \) denotes the vector \( J = (j, j') \), i.e., a vector of \( s + s' \) components if \( j \) and \( j' \) have, respectively, \( s \) and \( s' \) components, which has as first \( s \) components those of \( j \), then those of \( j' \).

**Lemma 6** Let \( \tau = (\tau^{(1)}, \ldots, \tau^{(S_1)}) \) be a \( s + s' \)-admissible collection of indices and let \( J(\tau) \) be the set of vectors \( J \) such that
\[ J_l = J_{l'} \iff \exists i \text{ s.t. } l, l' \in \text{supp}(\tau^{(i)}). \] (34)
Then there exist \( K, N_0 > 0 \) such that, for any \( s \) and \( s' \), any \( \alpha, \alpha' \), any \( \tau \), and any \( J \in J(\tau) \), one has for \( N > N_0 \)
\[ \left| \langle y_{j,\alpha} y_{j',\alpha'} \rangle - \langle y_{j,\alpha} \rangle \langle y_{j',\alpha'} \rangle \right| \leq K^{s+s'} \beta^{-(s+s')/2} \prod_{i=1}^{S_1} \sqrt{n_i!}, \] (35)
in which \( n_i \) denotes the cardinality of \( \text{supp}(\tau^{(i)}) \). Moreover, if \( (\tau^{(1)}, \ldots, \tau^{(S_1)}) \in \bar{T} \) then
\[ \left| \langle y_{j,\alpha} y_{j',\alpha'} \rangle - \langle y_{j,\alpha} \rangle \langle y_{j',\alpha'} \rangle \right| \leq \frac{1}{N} K^{s+s'} \beta^{-(s+s')/2} \prod_{i=1}^{S_1} \sqrt{n_i!}. \] (36)

This lemma is a minor modification of Lemma 4 of [6] and consists in a simple adaptation of standard probabilistic arguments, which are not reported here.

We pass from the variables \((\xi^\pm, \eta^\pm)\) to \((p^\pm, q^\pm)\) by using (6), then apply (28,32) of Appendix A to pass to the variables \((p_j, r_j)\), thus getting
\[ \Xi_{\sigma,k,l} = \sum_{\alpha,\beta} c_{k,\alpha,\sigma,l,\hat{\tau}} \sum_{j_1, \ldots, j_s=1} y_{j,\alpha} e^{i\hat{\kappa}_1 j_1} \cdots e^{i\hat{\kappa}_s j_s}, \quad \text{with } |c_{k,\alpha,\sigma,l,\tau}| \leq 1, \] 25
Lemma 7

where $\tilde{\tau} = (\tilde{\tau}_1, \ldots, \tilde{\tau}_s)$, $\tilde{\tau}_i = \pm 1$. Hence follows that

$$
\left| \langle \Xi_{\sigma,k,l}^{s',k',l'} - \langle \Xi_{\sigma,k,l}^{s',k',l'} \rangle \right| \leq \frac{1}{2^{(s+s')/2}N(s+s')/2} \sum_{\alpha,\alpha'} \sum_{\tilde{\tau},\tilde{\tau}'} 
\sum_{j_1, \ldots, j_s, j'_1, \ldots, j'_{s'}} e^{i\tilde{\tau}_1j_1} \cdots e^{i\tilde{\tau}_sj_s} \left( \langle y_{j_1,\alpha}y_{j'_1,\alpha'} \rangle - \langle y_{j_1,\alpha} \rangle \langle y_{j'_1,\alpha'} \rangle \right).
$$

(37)

The sum in the second line has $N^{s+s'}$ terms, which, however, contain the oscillating factors $e^{iks}$. The key remark here is that the property of exchangeability of the variables $y_{j,\alpha}$ entails that the terms in brackets take always the same value, but for some very peculiar cases, so that almost all oscillating sums vanish. In fact, let us consider the sequences of complex numbers $B_J$, with $J = (j_1, \ldots, j_r)$, having the following property:

**Definition 3 (Property A)** Let $\{i_1, \ldots, i_r\}$ be a permutation of $\{1, \ldots, r\}$ and let the values of the indices $j_{i_1}, \ldots, j_{i_r}$ be fixed, for $n < r$, while the remaining indices have the same value $j_{i_{n+1}} = \ldots = j_{i_r} = \bar{j}$. We say that the sequence $B_J$ possesses Property A if and only if it takes the same value for all values of $\bar{j} \neq j_{i_l}$, for any $l \leq n$.

Because of exchangeability $\langle y_{j,\alpha}y_{j',\alpha'} \rangle - \langle y_{j,\alpha} \rangle \langle y_{j',\alpha'} \rangle$ has precisely this property, for $J = (j, j')$, $r = s + s'$ and any $\alpha, \alpha'$. For this reason, in its estimate we can use the following

Lemma 7

Let $B_J$ be a sequence satisfying Property A and let

$$
\hat{B}_K^\tau = \sum_J B_J e^{i\tilde{\tau}_1j_1} \cdots e^{i\tilde{\tau}_rj_r}.
$$

Then

$$
\hat{B}_K^\tau = \sum_{S_1=1}^{r} N^{S_1} \sum_{(\tau(1), \ldots, \tau(S_1)) \in T_{\bar{n}_1, \ldots, n_{S_1}}} \sum_{\delta^{\tau(1),K}_{\tau(S_1),K}} \sum_{i=1}^{S_1} \sum_{S_2(i)=1}^{n_i} \sum_{(\tau(1), \ldots, \tau(S_2(i))) \in T_{n_i}(\tau(i))} \sum_{j_{S_2(i)}=1}^{c_{\tau(S_1)}S_1} \left( \delta^{\tau(1),K}_{\tau(S_1),K} \right)
$$

(38)
where $n_i$ is the cardinality of $\text{supp}(\tau^{(i)})$, $\mathcal{T}_n(\tau^{(i)})$ is the set of vectors in $\mathbb{Z}_3^n$ which are $n_i$-admissible on the support of $\tau^{(i)}$ and vanishing outside it, while

$$\tau = (\tau^{(1,1)}, \ldots, \tau^{(1,S_2(1))}, \ldots, \tau^{(S_1,1)}, \ldots, \tau^{(S_1,S_2(1))}) \in \mathcal{T}_r.$$ 

For the constants $c^\tau_{S_1} > 0$ it holds

$$c^\tau_{S_1} \leq \sup_{J \in J(\tau)} |B_J| \prod_{i=1}^{S_1} (S_2(i) - 1)! ,$$

in which $J(\tau)$ is the set of vectors $J$ defined by (34).

The proof of the previous lemma is performed by summing over all $j$, from $j_r$ down to $j_1$, and observing by induction on $0 \leq R < r$ that the terms obtained by summing over $j_r, \ldots, j_{r-R}$ have a peculiar form which we detail now. First of all, let us denote by $\mathcal{T}_r^R$ the set of $(\tau^{(1)}, \ldots, \tau^{(r-R+S_1)}) \in \mathcal{T}_r$ such that $\text{supp}(\tau^{(i)}) \cap \{1, \ldots, r-R\} = i$ for $i \leq r-R$ and with $\mathcal{T}_n(\tau^{(i)})$ the analogous of $\mathcal{T}_n(\tau^{(i)})$, with $\mathcal{T}_r$ replaced by $\mathcal{T}_r^R$; let us put

$$\tau_R \stackrel{\text{def}}{=} (\tau^{(1,1)}, \ldots, \tau^{(1,S_2(1))}, \ldots, \tau^{(r-R+S_1,1)}, \ldots, \tau^{(r-R+S_1,S_2(r-R+S_1))}) .$$

The inductive hypothesis is the following

$$\tilde{B}^\tau_{K} = \sum_{(\tau^{(1)}, \ldots, \tau^{(r-R+S_1)}) \in \mathcal{T}_r^R, j_1, \ldots, j_{r-R}} e^{i2\pi j_1 K \cdot \tau^{(1)}/N} \ldots e^{i2\pi j_{r-R} K \cdot \tau^{(r-R)}/N} \prod_{S=0}^{r-R} N^{R} \sum_{n_1, \ldots, n_{S_1}} \delta^{n_1}_{\tau^{(r-R+1)}, K} \cdots \delta^{n_{S_1}}_{\tau^{(r-R+S_1)}, K}$$

$$\sum_{i=1}^{r-R+S_1} \sum_{S_2(i)=1} n_i \sum_{\tau^{(i)}(1,1)+\ldots+\tau^{(i)}(1,S_2(i))=\tau^{(i)}} B^\tau_{j_1, \ldots, j_{r-R}} ,$$

in which the coefficients $B^\tau_{j_1, \ldots, j_{r-R}}$ have Property A with respect to the set of indices $(j_1, \ldots, j_{r-R})$.

By the very definition of $\tilde{B}^\tau_{K}$ this is true for $R = 0$, putting $\tau^{(i)}_j = \delta_{ij} \pi_j$. Let us suppose that (40) be true up to step $R$ and prove it for the step $R+1$, by summing on $j_{r-R}$.
Since $B_{j_1, \ldots, j_{r-R}}$ has Property A, when $j_{r-R}$ varies it takes always the same value (which we will denote by $B_{r,R,S_1}$) unless the index $j_{r-R}$ coincides with at least one among $j_1, \ldots, j_{r-R-1}$. We thus write

$$B^r_{j_1, \ldots, j_{r-R}} = B^r_{j_1, \ldots, j_{r-R}} + \left( B^r_{j_1, \ldots, j_{r-R}} - B^r_{\neq} \right).$$

Moreover, since, whenever there exists $l \leq r - R - 1$ such that $j_l = j_{r-R}$,

$$1 = \sum_{l=1}^{r-1} \delta_{j_l, j_{r-R}} = \sum_{l=1}^{r-1} \frac{\delta_{j_l, j_{r-R}}}{\sum_{l'=1}^{r-1} \delta_{j_l, j_{l'}}},$$

we can also write

$$B^r_{j_1, \ldots, j_{r-R}} = B^r_{j_1, \ldots, j_{r-R}} + \sum_{l=1}^{r-1} \left( B^r_{j_1, \ldots, j_{r-R}} - B^r_{\neq} \right) \frac{\delta_{j_l, j_{r-R}}}{m^l_{j_1, \ldots, j_{r-R-1}}},$$

where, for $l \in \{1, \ldots, r - R - 1\}$ the function $m^l_{j_1, \ldots, j_{r-R-1}}$ counts the number of indices which have the same value as $j_l$. By summing over $j_{r-R}$ we get

$$\sum_{j_{r-R}} e^{i2\pi j_{r-R} K^{(1)} / N} \ldots e^{i2\pi j_{r-R} K^{(r-R) / N}} B^r_{j_1, \ldots, j_{r-R}} =$$

$$e^{i2\pi j_1 K^{(1)} / N} \ldots e^{i2\pi j_{r-R-1} K^{(r-R-1) / N}} N B^r_{\neq} \sum_{n_{S_1+1}} \delta^{n_{S_1+1}}_{(r-R).K}$$

$$+ \sum_{l=1}^{r-1} e^{i2\pi j_1 K^{(1)} / (r_{R+1}) / N} \ldots e^{i2\pi j_{r-R-1} K^{(r-R-1) / (r_{R+1}) / N}} B^r_{j_1, \ldots, j_{r-R-1}}$$

$$+ \sum_{l=1}^{r-1} e^{i2\pi j_1 K^{(1)} / (r_{R+1}) / N} \ldots e^{i2\pi j_{r-R-1} K^{(r-R-1) / (r_{R+1}) / N}} B^r_{j_1, \ldots, j_{r-R-1}} ,$$

where

$$B^r_{j_1, \ldots, j_{r-R-1}} = \frac{B^r_{j_1, \ldots, j_{r-R} \neq j_l}}{m^l_{j_1, \ldots, j_{r-R-1}}} ,$$

$$\bar{B}^r_{j_1, \ldots, j_{r-R-1}} = \frac{B^r_{\neq}}{m^l_{j_1, \ldots, j_{r-R-1}}} ,$$

28
while the collection of vectors \( \tau_{R+1}(l) \) and \( \bar{\tau}_{R+1}(l) \) are relied to \( \tau_R \) by the following relations:

\[
\tau_{R+1}^{(i,j)}(l) = \begin{cases} 
\tau^{(i,j)}(l) & \text{if } 1 \leq i \leq r - R - 1, \ i \neq l \\
\tau^{(i+1,j)}(l) & \text{if } r - R \leq i \leq r - R + 1 + S_1 \\
\tau^{(l,1)} \cup \tau^{(r-R,1)} & \text{if } i = l, \ j = 1 \\
\tau^{(l,j')} \lor \tau^{(r-R,j'')} & \text{if } i = l, \ 2 \leq j \leq S_2(l) + S_2(r-R) + 1 \\
\tau^{(i,j)}(l) & \text{if } 1 \leq i \leq r - R - 1, \ i \neq l \\
\tau^{(i+1,j)}(l) & \text{if } r - R \leq i \leq r - R + 1 + S_1 \\
\tau^{(l,1)} & \text{if } i = l, \ j = 1 \\
\tau^{(l,j')} \lor \tau^{(r-R,j'')} & \text{if } i = l, \ 2 \leq j \leq S_2(l) + S_2(r-R) + 1
\end{cases}
\]

\[
\bar{\tau}_{R+1}^{(i,j)}(l) = \begin{cases} 
\tau^{(i,j)}(l) & \text{if } 1 \leq i \leq r - R - 1, \ i \neq l \\
\tau^{(i+1,j)}(l) & \text{if } r - R \leq i \leq r - R + 1 + S_1 \\
\tau^{(l,1)} \cup \tau^{(r-R,1)} & \text{if } i = l, \ j = 1 \\
\tau^{(l,j')} \lor \tau^{(r-R,j'')} & \text{if } i = l, \ 2 \leq j \leq S_2(l) + S_2(r-R) + 1 \\
\tau^{(i,j)}(l) & \text{if } 1 \leq i \leq r - R - 1, \ i \neq l \\
\tau^{(i+1,j)}(l) & \text{if } r - R \leq i \leq r - R + 1 + S_1 \\
\tau^{(l,1)} & \text{if } i = l, \ j = 1 \\
\tau^{(l,j')} \lor \tau^{(r-R,j'')} & \text{if } i = l, \ 2 \leq j \leq S_2(l) + S_2(r-R) + 1
\end{cases}
\]

Here, \( 2 \leq j' \leq S_2(l), \ 2 \leq j'' \leq S_2(r-R) \) and \( \tau^{(l,j)}(l) \), for \( j \geq 2 > \) are so chosen that \( \min(\text{supp}(\tau^{(l,j)}(l))) \leq \min(\text{supp}(\tau^{(l,k)}(l))) \) if and only if \( j < k \), while the analogous condition holds for \( \bar{\tau}_{R+1}(l) \) (in order that such collections are admissible).

Notice that \( B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R-1}} \) and \( B^{\tau_{R+1}(l),S_1}_{j_1,\ldots,j_{r-R-1}} \) are functions of the indices \( (j_1,\ldots,j_{r-R-1}) \) only, since \( m_{j_1,\ldots,j_{r-R-1}}^{(l)} \) does. We observe further that they possess Property A with respect to the set \( (j_1,\ldots,j_{r-R-1}) \). In fact, it can be shown directly that \( m_{j_1,\ldots,j_{r-R-1}}^{(l)} \) has such a property, while \( B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R-1}} \) possess it simply because \( B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R-1}} \) has the corresponding property with respect to \( (j_1,\ldots,j_{r-R-1}) \). As for \( B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R-1}} \), we recall that, for any \( (j_1,\ldots,j_{r-R-1}) \), it is defined as the common value taken by \( B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R}} \) for all \( j_{r-R} \neq j_1 \), for \( i < r-R \). So, by fixing arbitrarily \( n < r-R-1 \) indices among \( (j_1,\ldots,j_{r-R-1}) \) and taking for the remaining indices \( j_{i_{n+1}} = \ldots = j_{i_{r-R-1}} \) the common value \( \bar{j} \), one has

\[
B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R-1},j_{r-R}} = B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R-1},j_{r-R}} , \quad \text{for any } j_{r-R} \neq j_1,\ldots,j_{i_n},\bar{j}.
\]

We fix \( j_{r-R} \) and let \( \bar{j} \) vary: by Property A for \( B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R}} \) \( B^{\tau_{R,S_1}}_{j_1,\ldots,j_{r-R}} \) takes the same value for all \( \bar{j} \neq j_1,\ldots,j_{i_n},j_{r-R} \). Then we change \( j_{r-R} \), thus showing that the same holds true for all \( \bar{j} \neq j_1,\ldots,j_{i_n}, \) i.e., exactly Property A with respect to \( (j_1,\ldots,j_{r-R-1}) \).

This way we have completed the proof of the inductive hypothesis (41) at step \( R + 1 \), and so equation (39).

In order to prove estimate (39), we use a graphical tool to keep track of the number of addenda which contribute to any collection \( \tau \).
We associate to any $\tau$ a graph in the following way: we draw $r$ points, corresponding to the indices $\{1, \ldots, r\}$ in this order, and connect them in such a way that two sites belong to the support of the same $\tau^{(i)}$ if and only if there exists at least a line joining them and that they belong to the support of the same $\tau^{(i,j)}$ if and only if they are joined by a double line. The example of Figure 1 displays a case in which $r = 8$ and $\text{supp}(\tau^{(1,1)}) = \{1, 2\}$, $\text{supp}(\tau^{(1,2)}) = \{5\}$, $\text{supp}(\tau^{(1,3)}) = \{6\}$, $\text{supp}(\tau^{(2,1)}) = \{3\}$, $\text{supp}(\tau^{(2,2)}) = \{4, 7, 8\}$. We point out that the correspondence between the collections $\tau$ and the graph is biunivocal, as the order of the $\tau^{(i,j)}$ is univoquely assigned.

The term corresponding to a given $\tau$ can come from different terms in the sum over $(j_r, \ldots, j_1)$, as we illustrate now, by constructing another type of graph, where the only difference with respect to the previous one lies in the form of the lines. For any site $r - R$, for $0 \leq R \leq r$, three alternatives are possible:

- no line pointing left comes out of the site;
- one double line pointing left comes out of the point and joins it with one site on its left;
- one simple line pointing left starts from the point and ends on one point on its left.

Such options correspond to the first, to the second and to the third term at the r.h.s. of (41), respectively. This way we associate with a bijection to any graph one single term coming from the sums on $(j_r, \ldots, j_1)$. Moreover, every graph of this kind is associated to one and only one graph of the previous type via the prescription that in the latter two points are joined by a line (be it a simple or a double line) if and only if there exists a line, or a set of lines,
Figure 2: Two different example of graphs of the second type corresponding to a single graph of the first type, namely, the graph in Figure 1.

of the same kind which connects them continuously in the former. We point out that the relation between the two types of graph is *not* biunivocal. In Figure 2 we show two examples of terms with different graphs of the second type, corresponding to the same \( \tau \) as in Figure 1.

We have reduced the estimate \((39)\) basically to the count of the number of graphs of the second type giving the same graph of the first kind. Indeed, let us remark the following facts, which can be checked from \((41)\):

1. all terms corresponding to a given \( \tau \) depend on \( B_J \) only for \( J \in J(\tau) \);

2. in the graphs of the second type, if two or more sites are connected by a chain of double lines (in such a case we will call the maximal set of sites forming one of such groups a *double chain*), a possible simple line joining a point of the double chain to a point on the left of the group can start only from the leftmost point in the double chain;

3. any line starting from a point \( m \) in a graph of the second type and ending on the point \( l < m \) implies that the corresponding term is divided by

   \[
   \sum_{j=1}^{m-1} \delta^{m}_{j,l},
   \]

   with \( \delta^{m}_{j,l} = 1 \) if \( j \) and \( l \) belong to the same double chain (or coincide), 0 otherwise.

Due to item 3 all terms linking a point, through a simple line, to a double chain on the left of the point count algebraically as one single term, whereas by item 2 the same happens for the connection between two double chains through a simple line. Still by item 3, all terms forming a double chain count algebraically as one. In order to estimate \( c_{\tau,S}^{\tau,S_i} \) it is then sufficient to count the
number of possible connections between the different double chains, in such a way that each double chain is connected with another one on its left. For any \( \tau^{(i)} \), we have \( S_2(i) \) double chains, which can be connected in \( (S_2(i) - 1)! \) ways. This completes the estimate (39) and concludes the proof of Lemma 7.

From this lemma, and in particular from equation (38), Lemma 4 immediately follows. In order to prove Lemma 5, instead, we use (39) together with Lemma 6. In our case this gives, for \( \tau \in \bar{T} \),

\[
C_{\tau,S_1}^\tau \leq \frac{K^{2s}}{N^s} \sqrt{2s! \prod_{i=1}^{S_1} (S_2(i) - 1)!}.
\]

For fixed \( \tau^{(i)} \) and \( S_2(i) \), the number \( m_{i,S_2(i)} \) of collections \( (\tau^{(i,1)}, \ldots, \tau^{(i,S_2(i))}) \) giving the same \( \tau^{(i)} \) is

\[
m_{i,S_2(i)} = \sum_{n_i=1}^{n_i} \frac{(n_i - 1)!}{(n_i - n_{i,1})!(n_{i,1} - 1)!} \cdots \sum_{n_j=1}^{n_j} \frac{(n_i - n_{i,1} - \cdots - n_{i,j-1} - 1)!}{(n_i - n_{i,1} - \cdots - n_{i,j})!(n_{i,j} - 1)!} \cdots \sum_{n_{i,S_2(i)-2}=1}^{n_{i,S_2(i)-2}} \frac{(n_i - n_{i,1} - \cdots - n_{i,S_2(i)-2} - 1)!}{(n_i - n_{i,1} - \cdots - n_{i,S_2(i)-2})!(n_{i,S_2(i)-2} - 1)!}.
\]

Due to the binomial expansion, we have

\[
\sum_{j=1}^{m-1} \frac{(m - 1)!l^{m-1-j}}{(m - j)!((j - 1)!)^l} \leq \frac{(l + 1)^{m-1}}{l}.
\]

By applying repeatedly this formula, with \( m = n_i - n_{i,1} - \cdots - n_{i,j-1} \) e \( j = n_{i,j} \), we get

\[
m_{i,S_2(i)} \leq \frac{S_2(i)^{n_i-1}}{(S_2(i) - 1)!},
\]

so that, for some suitable \( C \geq 0 \),

\[
m_i \overset{\text{def}}{=} \sum_{S_2(i)=1}^{n_i} m_{i,S_2(i)} (S_2(i) - 1)! \leq C m_i \frac{(n_i - 1)!}{n_i}.
\]
We then sum over all possible \((\tau^{(1)}, \ldots, \tau^{(S_1)})\), obtaining

\[
\sum_{(\tau^{(1)}, \ldots, \tau^{(S_1)}) \in \mathcal{T}_{2s}} \prod_{i=1}^{S_1} m_i n_i = 2^{2s-S_1+1} \sum_{n_1=1}^{2s-n_1} \frac{(2s-1)!m_1 n_1}{(2s-n_1)(n_1-1)!} \cdots \sum_{n_{S_1-1}=1}^{2s-n_{S_1-1}-S_1-1} \frac{(2s-n_1-\cdots-n_{S_1-2}-1)!m_{S_1-1} n_{S_1-1} n_{S_1-1} n_{S_1}}{(2s-n_1-\cdots-n_{S_1-1})(n_{S_1}-1)!}.
\]

Since \(m_i n_i/(n_i-1)! \leq C^{n_i}\) and \(\sum_i n_i = 2s\), we get

\[
\sum_{(\tau^{(1)}, \ldots, \tau^{(S_1)}) \in \mathcal{T}_{2s}} \prod_{i=1}^{S_1} m_i n_i \leq C^{2s}(2s)!.
\]

A last sum over \(S_1\) and a suitable choice of constants bring us to the proof of the statement of Lemma 5 for \((\tau^{(1)}, \ldots, \tau^{(S_1)}) \in \mathcal{T}\). The case of \((\tau^{(1)}, \ldots, \tau^{(S_1)}) \in \mathcal{T}^c\) is dealt with in a completely analogous way.

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