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# Existence of kink solutions in a discrete model of the polyacetylene molecule

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## Abstract

This paper deals with the proof of the existence of kink states in the discrete model of the polyacetylene molecule. We use ideas from Kennedy and Lieb [4] to study finite, odd chains of polyacetylene, and then we consider the limit as the number of atoms goes to infinity. We show that, after extraction of a subsequence and up to a translation, the energy minimizers of odd chains tend to an infinite vector approaching one of the infinite dimerized states at  $+\infty$  and the other one at  $-\infty$ . This state is called a kink and its existence was strongly suggested in previous works such as [8, 5, 12], but a mathematical proof was missing, to our knowledge.

## Introduction

The first rigorous study of the discrete model of the polyacetylene molecule,  $(\text{CH})_x$ , was made by Kennedy and Lieb in [4]. They show that, under certain conditions, the energy of a chain with an even number of CH groups has exactly two minimizers, and that these minimizers are dimerized configurations, as suggested in previous works by Su, Schrieffer and Heeger [10, 9] (see also [3]). This validates the theory of the *Peierls instability* [7, 2] in one-dimensional chains.

Other works (for instance [11] and [1]) deal with the continuum approximation of the polyacetylene molecule. There, the authors obtain formal results on the existence of solutions of the Euler-Lagrange equations associated to the minimization problem of the energy of the  $(\text{CH})_x$  molecule in the continuum model. In particular, Campbell and Bishop build in [1] kink-like solutions of these equations which connect the two ground states at  $\pm\infty$ .

To our knowledge, in the discrete case no rigorous proof of the existence of kink states has been given. However, numerical calculations suggest that such kinks exist [8] and some discussions on their properties have been published [5, 12]. In the present work, we prove rigorously the existence of kinks. They appear naturally by considering the ground states of chains with  $2N + 1$  CH groups and then making  $N$  tend to infinity. The ground states converge, up to a translation and to extraction of a subsequence, to an infinite state connecting the two infinite dimerized states. This will be made more precise in section 2.

In section 1, we briefly introduce the discrete mathematical model describing the  $(\text{CH})_x$  molecule. We define the energy functional as a function of the molecule configuration, and we recall some technical aspects that will be useful further on. For a more detailed physical description of the model the reader may refer to [10, 9, 4].

The main theorem of this paper, dealing with the existence of kinks and other properties, is proved on section 2. We use mainly ideas from [4] to develop the proof of the theorem. However, our argument is also based upon the concentration-compactness principle of P.L. Lions [6].

## 1 A model for finite chains

In the whole paper,  $\chi_A$  denotes the characteristic function of the set  $A$  and  $\theta_A$  denotes the operator of multiplication by the characteristic function  $\chi_A$ , *i.e.* for any sequence  $x = (x_i)$ ,  $(\theta_A x)_i = \chi_A(i)x_i$ . We also denote by  $\sigma_p(\mathcal{X})$  the Schatten classes in a Hilbert space  $\mathcal{X}$ , and by  $\|\cdot\|_{\sigma_p}$  the associated norms.

We consider a closed chain of  $N \in \mathbb{N}$  atoms. Our model is the same as in Kennedy and Lieb (KL) in [4], except for the fact that we will not only consider chains of an even number of atoms. The underlying electronic space is  $\mathbb{C}^{\mathbb{Z}/N\mathbb{Z}}$ . To any  $N$ -tuple of real numbers  $\mathbf{t} = (t_i)_{i \in \mathbb{Z}/N\mathbb{Z}}$  we associate a Hamiltonian operator  $T$  whose coefficients are  $T_{i,i+1} = T_{i+1,i} = t_i$  and  $T_{i,j} = 0$  otherwise (here  $i, j$  are defined modulo  $N$ ). We look for minimizers of the energy, which is a function of  $T$  and of a one-body electronic density matrix  $\Gamma = (\Gamma_{i,j})_{i,j \in \mathbb{Z}/N\mathbb{Z}}$ . The matrix  $\Gamma$  has complex coefficients, is self-adjoint and satisfies  $0 \leq \Gamma \leq 1$ .

The formula for the energy is:

$$\mathcal{E}^{(N)}(\Gamma, \mathbf{t}) = \frac{1}{2}g \sum_{i=1}^N (t_i - b)^2 + 2\text{Tr}(T\Gamma).$$

If we fix  $\mathbf{t}$ , this energy is minimal when  $\Gamma = \chi_{(-\infty, 0)}(T)$  and the minimal energy is given by the following "reduced" functional

$$H^{(N)}(\mathbf{t}) = \frac{1}{2}g \sum_{i=1}^N (t_i - b)^2 - \text{Tr}(|T|).$$

If, on the contrary, we fix  $\Gamma$ , then the minimum of the energy is attained by a unique vector  $\mathbf{t}(\Gamma)$  of coordinates  $t_i = b - \frac{4}{g}\text{Re}(\Gamma_{i,i+1})$  and the minimal energy is given by the following "reduced" functional

$$F^{(N)}(\Gamma) = 2b\text{Tr}(T^1\Gamma) - \frac{8}{g} \sum_{i=1}^N (\text{Re}(\Gamma_{i,i+1}))^2,$$

where  $T^1$  is the Hamiltonian associated to the constant sequence  $t_i = 1$ , *i.e.*  $T_{i,i+1}^1 = (T^1)_{i+1,i} = 1$  and  $T_{i,j}^1 = 0$  otherwise, hence  $2b\text{Tr}(T^1\Gamma) = 4b \sum_{i=1}^N \text{Re}(\Gamma_{i,i+1})$ .

In the rest of the paper, we make the assumption  $gb > 1$ . The authors KL define the following variables associated to the vector  $\{t_i\}$

$$x := \frac{1}{N} \sum_{i=1}^N t_i \quad y^2 := \frac{1}{N} \sum_{i=1}^N t_i^2 \quad z := \frac{1}{N} \sum_{i=1}^N t_i t_{i+1}, \quad (1)$$

and they denote by  $\langle T^2 \rangle$  the mean of  $T^2$  under translations. This mean matrix can be written as  $\langle T^2 \rangle = 2y^2 + z\Omega$ , where  $\Omega$  is the matrix whose only nonzero elements are  $\Omega_{i,i+2} = \Omega_{i+2,i} = 1$ .

They show rigorously in the even case that the minimum of  $H^{(2N)}$ , in the class of  $2N$ -periodic vectors  $\mathbf{t}$ , is attained by exactly two configurations,  $t_i^{\text{dim}0}(2N) = b + (-1)^i \delta_{2N}$  and  $t_i^{\text{dim}1}(2N) = b + (-1)^{i+1} \delta_{2N}$ , with  $\delta_{2N} \rightarrow \delta_0$  as  $N$  goes to infinity. The assumption  $gb > 1$  corresponds to realistic data from physics, as explained by Kennedy-Lieb. It implies that  $b > \delta_0$ , where  $\delta_0$  is the unique positive solution of the dimerization equation in the limit  $N \rightarrow \infty$  (see (5))

$$\frac{1}{\pi} \int_0^\pi \frac{\cos^2 s}{\sqrt{b^2 \sin^2 s + \delta^2 \cos^2 s}} ds = \frac{1}{2} g.$$

Note that the dimerized ground state operators  $T_{\text{dim}0}(2N)$  and  $T_{\text{dim}1}(2N)$  have the same square, which we shall denote by  $T_{\text{dim}}^2(2N)$ . Similarly we shall denote by  $|T_{\text{dim}}(2N)|$  their common absolute value, which is the square root of  $T_{\text{dim}}^2(2N)$ , and we shall denote by  $e(2N)$  their common energy, which is the minimum of  $H^{(2N)}$ .

## 2 The *kink* problem in odd chains

Firstly, we note that the model is invariant under translations in the sense that if we let  $\tau_k : \mathbb{C}^N \rightarrow \mathbb{C}^N$  be defined by  $(\tau_k v)_i = v_{i+k}$ , then for any given vector  $\mathbf{t} = (t_i)_{i \in \mathbb{Z}/N\mathbb{Z}}$  we get  $H^{(N)}(\tau_k \mathbf{t}) = H^{(N)}(\mathbf{t})$ . The main goal of this paper is to prove the following

**Theorem 1.** *Suppose that  $gb > 1$  and let  $\mathbf{t}(2N+1) = (t_i(2N+1))_{1 \leq i \leq 2N+1}$  be a global minimizer of  $H^{(2N+1)}$ . Then, up to a translation  $i \mapsto i + k_N$ , the following properties hold:*

*After extraction of a subsequence,  $t_i(2N+1)$  converges to a limit  $t_i^\infty$ , for every  $i \in \mathbb{Z}$ . The infinite sequence  $\mathbf{t}^\infty := (t_i^\infty)_{i \in \mathbb{Z}}$  obtained in this way is a kink connecting the two dimerized states. More precisely, there is  $\tau \in \{0, 1\}$  such that*

$$\sum_{i \geq 1} |t_i^\infty - b - (-1)^{i+\tau} \delta_0|^2 = \sum_{i \leq 0} |t_i^\infty - b + (-1)^{i+\tau} \delta_0|^2 < \infty. \quad (2)$$

*Moreover, denoting by  $T^\infty$  the operator in  $l_2(\mathbb{Z})$  associated with the sequence  $\mathbf{t}^\infty$ , the coefficients of  $|T(2N+1)|$  converge pointwise to those of  $|T^\infty|$  as  $N \rightarrow \infty$ :*

$$|T(2N+1)|_{i,j} \rightarrow |T^\infty|_{i,j} \quad (\forall i, j)$$

and  $\mathbf{t}^\infty$  is a relative energy minimizer. By relative minimizer we mean the following:

Given any sequence  $\mathbf{u} = (u_i)_{i \in \mathbb{Z}}$  in  $l_1(\mathbb{Z})$  and setting  $U$  the associated operator, the difference  $|T^\infty| - |T^\infty + U|$  is trace-class and

$$\Delta H(\mathbf{u}) := \frac{1}{2}g \sum_{i \in \mathbb{Z}} (u_i + 2t_i^\infty - 2b)u_i + \text{Tr}(|T^\infty| - |T^\infty + U|) \geq 0.$$

As a consequence, denoting  $\Gamma^\infty := \chi_{(-\infty, 0)}(T^\infty)$ , the following self-consistent equations hold:

$$t_i^\infty = b - \frac{4}{g} \text{Re}(\Gamma_{i, i+1}^\infty).$$

To prove Theorem 1, we start with some *a priori* estimates which use results from [4].

**Lemma 1.** For all  $N \geq 1$ ,

$$H^{(2N+1)}(\mathbf{t}(2N+1)) - H^{(2N)}(\mathbf{t}^{\text{dim1}}(2N)) \leq 4b.$$

*Proof.* First of all we define the test vector  $\mathbf{t}^{\text{test}} \in \mathbb{C}^{\mathbb{Z}/(2N+1)\mathbb{Z}}$  by

$$t_i^{\text{test}} = \begin{cases} b + (-1)^{i+1} \delta_{2N} & 1 \leq i \leq 2N \\ b & i = 2N + 1 \end{cases},$$

and we denote by  $T_{\text{test}}$  the associated operator. Recalling that  $T_{\text{dim1}}(2N)$  is the operator on  $\mathbb{C}^{\mathbb{Z}/2N\mathbb{Z}}$  associated to the dimerized configuration  $\mathbf{t}^{\text{dim1}}(2N) = \{b + (-1)^{i+1} \delta_{2N}\}_{i \in \mathbb{Z}/2N\mathbb{Z}}$ , let  $\Gamma_{\text{dim1}}(2N) = \chi_{(-\infty, 0)}(T_{\text{dim1}}(2N))$ .

Now let us define the operator  $\Gamma_{\text{test}}$  acting on  $\mathbb{C}^{\mathbb{Z}/(2N+1)\mathbb{Z}}$  by

$$\Gamma_{\text{test}}^{i,j} = \begin{cases} \Gamma_{\text{dim1}}(2N)^{i,j} & \text{if } 1 \leq i \leq 2N \text{ and } 1 \leq j \leq 2N \\ 0 & \text{if } i = 2N + 1 \text{ or } j = 2N + 1 \end{cases}.$$

Using this notation we get

$$\begin{aligned} 2\text{Tr}_{\mathbb{C}^{2N+1}}(\Gamma_{\text{test}} T_{\text{test}}) &= 2 \sum_{i=1}^{2N+1} (\Gamma_{\text{test}}^{i, i+1} T_{\text{test}}^{i+1, i} + \Gamma_{\text{test}}^{i, i-1} T_{\text{test}}^{i-1, i}) \\ &= 2\Gamma_{\text{dim1}}^{1,2} T_{\text{dim1}}^{2,1} + 2\Gamma_{\text{dim1}}^{2N, 2N-1} T_{\text{dim1}}^{2N-1, 2N} \\ &\quad + 2 \sum_{i=2}^{2N-1} (\Gamma_{\text{dim1}}^{i, i+1} T_{\text{dim1}}^{i+1, i} + \Gamma_{\text{dim1}}^{i, i-1} T_{\text{dim1}}^{i-1, i}). \end{aligned}$$

And, omitting the argument  $(2N)$  from our notation, we obtain

$$2\text{Tr}_{\mathbb{C}^{2N}}(\Gamma_{\text{dim1}} T_{\text{dim1}}) = 2 \sum_{i=1}^{2N} (\Gamma_{\text{dim1}}^{i, i+1} T_{\text{dim1}}^{i+1, i} + \Gamma_{\text{dim1}}^{i, i-1} T_{\text{dim1}}^{i-1, i}).$$

Hence,

$$\begin{aligned}
2\mathrm{Tr}_{\mathbb{C}^{2N}}(\Gamma_{\dim 1} T_{\dim 1}) - 2\mathrm{Tr}_{\mathbb{C}^{2N+1}}(\Gamma_{\mathrm{test}} T_{\mathrm{test}}) &= 2\Gamma_{\dim 1}^{1,0} T_{\dim 1}^{0,1} + 2\Gamma_{\dim 1}^{0,1} T_{\dim 1}^{1,0} \\
&= 4\Re(\Gamma_{\dim 1}^{1,0}) T_{\dim 1}^{0,1} \\
[0 \leq \Gamma_{\dim 1} \leq 1 \Rightarrow] &\leq 4T_{\dim 1}^{0,1} \\
&= 4(b - \delta_{2N}) \\
&< 4b
\end{aligned}$$

On the other hand, from the definition of  $\mathbf{t}^{\mathrm{test}}$  we see that

$$\frac{g}{2} \sum_i^{2N+1} (t_i^{\mathrm{test}} - b)^2 - \frac{g}{2} \sum_i^{2N+1} (t_i^{\dim 1} - b)^2 = 0,$$

which together with the previous estimates implies that

$$H^{(2N+1)}(\mathbf{t}^{\mathrm{test}}) - H^{(2N)}(\mathbf{t}^{\dim 1}(2N)) \leq 4b \quad (3)$$

Now let  $\boldsymbol{\xi} = (\xi_i) \in \mathbb{C}^{2N+1}$ . Since  $0 \leq \Gamma_{\dim 1}(2N) \leq 1$  we obtain

$$\begin{aligned}
\langle \boldsymbol{\xi}, \Gamma_{\mathrm{test}}(2N+1)\boldsymbol{\xi} \rangle &= \sum_{1 \leq i, j \leq 2N+1} \Gamma_{\mathrm{test}}^{i,j} \xi_i \bar{\xi}_j \\
&= \sum_{1 \leq i, j \leq 2N} \Gamma_{\dim 1}^{i,j}(2N) \xi_i \bar{\xi}_j \in \left[ 0, \sum_{i=1}^{2N} |\xi_i|^2 \right] \subset [0, \|\boldsymbol{\xi}\|_2^2],
\end{aligned}$$

so that  $0 \leq \Gamma_{\mathrm{test}}(2N+1) \leq 1$ . Hence we conclude that

$$H^{(2N+1)}(\mathbf{t}^{\mathrm{test}}(2N+1)) \geq H^{(2N+1)}(\mathbf{t}(2N+1)),$$

and by (3) the Lemma is proved.  $\square$

We now apply some ideas from the proof of Kennedy-Lieb's theorem in [4] to study the following function

$$\psi_N(x, y, z) := \frac{1}{2}g(y^2 - 2bx + b^2) - \frac{1}{N}\mathrm{Tr}_{\mathbb{C}^N} [(2y^2 + z\Omega_N)^{1/2}],$$

defined for every  $(x, y, z) \in \mathbb{R}^3$ . The matrix  $\Omega_N \in \mathcal{M}_{N \times N}$  has been defined in the introduction. Notice that the analysis of  $\psi_N$  made in [4] is valid for any  $N$ , excepting the physical interpretation which makes no sense in the odd case.

To any given sequence  $\mathbf{t} = (t_i)_{i \in \mathbb{Z}/N\mathbb{Z}}$  we associate the vector  $(x, y, z)$  using (1). Now, defining as in [4] the variable  $s_i = x - t_i$ , we have  $y^2 = x^2 + \frac{1}{N} \sum s_i^2$  and by the Cauchy-Schwartz inequality Kennedy and Lieb obtain

$$z = x^2 + \frac{1}{N} \sum s_i s_{i+1} \geq x^2 - \frac{1}{N} \sum s_i^2 = 2x^2 - y^2. \quad (4)$$

Note that the inequality  $x^2 \leq y^2$  also holds so that it is natural to study  $\psi_N$  on the domain  $D := \{(x, y, z) \in \mathbb{R}^3 \mid z \geq 2x^2 - y^2; y^2 \geq x^2; y \geq 0\}$  of  $\mathbb{R}^3$ . We do so in the following

**Lemma 2.** For large enough  $N$  the function  $\psi_N : \mathbb{R}^3 \rightarrow \mathbb{R}$  defined by

$$\psi_N(x, y, z) := \frac{1}{2}g(y^2 - 2bx + b^2) - \frac{1}{N} \text{Tr}_{\mathbb{C}^N} [(2y^2 + z\Omega_N)^{1/2}]$$

has a unique minimizer in the region  $D = \{(x, y, z) \in \mathbb{R}^3 \mid z \geq 2x^2 - y^2; y^2 \geq x^2; y \geq 0\}$ .

*Proof.* As noticed by Kennedy and Lieb, the function  $\psi_N$  is increasing in  $|z|$ . Hence, we get the lower bound  $\psi_N(x, y, z) \geq \psi_N(x, y, 0)$ . Also, we remark that

$$\inf_{2x^2 - y^2 \leq 0} \psi_N(x, y, 0) = \inf_{2x^2 = y^2} \psi_N(x, y, 0) \geq \inf_D \psi_N(x, y, z) + e,$$

with  $e > 0$ , so the case  $2x^2 - y^2 \leq 0$  is not optimal and we should restrict ourselves to the subregion of  $D$  where  $2x^2 - y^2 > 0$ . Furthermore, using again the fact that  $\psi_N$  is an increasing function of  $|z|$ , in the latter subregion we have that  $\psi_N(x, y, z) \geq \psi_N(x, y, 2x^2 - y^2)$ . Hence the minimum of  $\psi_N$  on  $D$  is actually attained in the subregion  $D' := \{2x^2 - y^2 > 0; z = 2x^2 - y^2\} \cap D$ . We suppose from now on that  $(x, y, z) \in D'$ .

As a function of the variables  $X := x^2$  and  $Y := y^2$ ,  $\psi_N(x, y, 2x^2 - y^2)$  is written as

$$\phi_N(X, Y) := \frac{1}{2}g(Y - 2b\sqrt{X} + b^2) - \frac{1}{N} \text{Tr} \left[ (2Y + (2X - Y)\Omega)^{1/2} \right].$$

The function  $\phi_N$  is strictly jointly convex in  $X, Y$  in the sense that  $\text{Hess}(\phi_N) > 0$  at any point  $(X, Y)$  in the convex domain  $\{2X > Y \geq X > 0\}$ . Moreover, we have that

$$\inf_{2X=Y} \phi_N(X, Y) \geq \inf_{2X>Y} \phi_N(X, Y) + e',$$

with  $e' > 0$ .

Thus there is a unique minimizer  $(X_{min}, Y_{min}) = (x_{min}^2(N), y_{min}^2(N)) = (b_N^2, b_N^2 + \delta_N^2)$  of  $\phi_N$  in the region  $\{2X > Y\}$ , and  $\min_{\{2X>Y\}} \phi_N = \min \psi_N$ . Here,  $\delta_N$  is the unique positive solution to the generalized dimerization equation that we recall below. Let us first define, for  $\delta > 0$ , the function

$$f_{b,\delta} : [0, \pi] \rightarrow \mathbb{R}$$

$$s \mapsto \frac{\cos^2 s}{\sqrt{b^2 \sin^2 s + \delta^2 \cos^2 s}},$$

then the generalized dimerization equation is given by

$$\frac{1}{2}g = \frac{1}{N} \sum_{k=1}^N f_{b,\delta} \left( \frac{\pi k}{N} \right). \quad (5)$$

Notice that the couple  $(b_N^2, b_N^2 + \delta_N^2)$  indeed belongs to the domain  $\{2X > Y \geq X > 0\}$  when  $N$  is large enough, for the following two reasons. On the one hand we have assumed that  $gb > 1$ , which implies that  $b > \delta_0$ ; and on the second hand, we have that

$b_N = b + O(1/N)$  and  $\delta_N = \delta_0 + O(1/N)$ . To prove the latter equality we notice that, for any  $\delta > 0$ , the function  $f_{b,\delta}$  is of class  $\mathcal{C}^1$  and its derivative is bounded independently of  $\delta$ , when  $\delta$  stays bounded away from zero. Hence

$$\left| \frac{1}{N} \sum_{k=1}^N f_{b,\delta} \left( \frac{\pi k}{N} \right) - \frac{1}{\pi} \int_0^\pi f_{b,\delta}(s) ds \right| = O(1/N).$$

By the definition of  $\delta_N$  and  $\delta_0$ , we know that

$$\frac{1}{2N} \sum_{k=1}^{2N} f_{b,\delta_N} \left( \frac{\pi k}{2N} \right) = \frac{1}{\pi} \int_0^\pi f_{b,\delta_0}(s) ds,$$

thus

$$\left| \frac{1}{\pi} \int_0^\pi f_{b,\delta_N}(s) ds - \frac{1}{\pi} \int_0^\pi f_{b,\delta_0}(s) ds \right| = O(1/N). \quad (6)$$

Now, the fonction  $0 < \delta \mapsto \frac{1}{\pi} \int_0^\pi f_{b,\delta}(s) ds$  is of class  $\mathcal{C}^1$  and its derivative is strictly negative. So (6) implies that  $\delta_N = \delta_0 + O(1/N)$ . A similar argument shows that  $b_N = b + O(1/N)$ , so the lemma follows.  $\square$

Notice that Lemma 1, together with KL's Lemma proved in [4], imply the following inequalities, where we put  $T(2N+1) = T$  and for the sake of simplicity, and let  $(x_{2N+1}, y_{2N+1}, z_{2N+1})$  be the vector associated to  $\mathbf{t}(2N+1)$ :

$$\begin{aligned} 4b &\geq H^{(2N+1)}(\mathbf{t}(2N+1)) - H^{(2N)}(\mathbf{t}^{dim1}(2N)) \\ &\geq \frac{1}{2}g \sum_{i=1}^{2N+1} (t_i - b)^2 - \text{Tr}(\langle T^2 \rangle^{1/2}) + \frac{1}{8} \|T\|^{-3} \text{Tr} \left[ (T^2 - \langle T^2 \rangle)^2 \right] - 2N \min_D \psi_{2N} \\ &= (2N+1) \left( \psi_{2N+1}(x_{2N+1}, y_{2N+1}, z_{2N+1}) - \min_D \psi_{2N+1} \right) \end{aligned} \quad (7)$$

$$+ \frac{1}{8} \|T\|^{-3} \text{Tr} \left[ (T^2 - \langle T^2 \rangle)^2 \right] + (2N+1) \min_D \psi_{2N+1} - 2N \min_D \psi_{2N}. \quad (8)$$

Since  $(2N+1) \min_D \psi_{2N+1} - 2N \min_D \psi_{2N} = O(1)$ , we get from the latter estimate that there exists a constant  $C > 0$  such that

$$C \geq (2N+1) \left( \psi_{2N+1}(x_{2N+1}, y_{2N+1}, z_{2N+1}) - \min_D \psi_{2N+1} \right) \quad (9)$$

and that

$$C \geq \frac{1}{8} \|T\|^{-3} \text{Tr} \left[ T^4 - \langle T^2 \rangle^2 \right], \quad (10)$$

after applying the general equality  $\text{Tr}((A - \langle A \rangle)^2) = \text{Tr}(A^2 - \langle A \rangle^2)$  to  $A = T^2$  in line (8).

We use the latter estimates to prove the following two lemmas.



**Lemma 3.** *The sequences  $x_{2N+1} = \frac{1}{2N+1} \sum t_i(2N+1)$ ,  $y_{2N+1}^2 = \frac{1}{2N+1} \sum t_i^2(2N+1)$ , and  $z_{2N+1} = \frac{1}{2N+1} \sum t_i(2N+1)t_{i+1}(2N+1)$  converge to  $x_{dim}$ ,  $y_{dim}^2$ , and  $z_{dim}$  respectively, with*

$$\begin{cases} x_{dim} := b \\ y_{dim}^2 := \frac{1}{2} [(b + \delta_0)^2 + (b - \delta_0)^2] = b^2 + \delta_0^2 \\ z_{dim} := (b + \delta_0)(b - \delta_0) = b^2 - \delta_0^2. \end{cases}$$

*The convergence takes place at speed  $O(\frac{1}{N})$  for  $z_{2N+1}$ , and at speed  $O(\frac{1}{\sqrt{N}})$  for  $x_{2N+1}$  and  $y_{2N+1}^2$ . As a consequence,*

$$\|\langle T(2N+1)^2 \rangle - (2y_{2N+1}^2 + z_{2N+1}\Omega_{2N+1})\|_{\sigma_2} = O(1)_{N \rightarrow \infty}.$$

*Proof.* Denoting by  $(x_{2N+1}^{min}, y_{2N+1}^{min}, z_{2N+1}^{min}) = (b_{2N+1}, b_{2N+1}^2 + \delta_{2N+1}^2, b_{2N+1}^2 - \delta_{2N+1}^2)$  the unique minimizer of  $\psi_{2N+1}$  over  $D$  we rewrite estimate (9) in the following way

$$\begin{aligned} \frac{C}{2N+1} &\geq \psi_{2N+1}(x_{2N+1}, y_{2N+1}, z_{2N+1}) - \min_D \psi_{2N+1} \\ &= \psi_{2N+1}(x_{2N+1}, y_{2N+1}, z_{2N+1}) - \psi_{2N+1}(x_{2N+1}^{min}, y_{2N+1}^{min}, z_{2N+1}^{min}) \end{aligned} \quad (11)$$

For any  $(x, y, z) \in D$  we let  $\bar{z} := 2x^2 - y^2 > 0$ . Since the function  $z \mapsto -\frac{1}{N}\text{Tr}(2y^2 + z\Omega)$  is differentiable, convex, even, and increasing in  $|z|$ , this is also true for the function  $z \mapsto \psi_N(x, y, z)$  with  $x, y$  fixed, so we infer that

$$\forall z > 0, \quad \frac{\partial}{\partial z} \psi_N(x, y, z) \geq \frac{\psi_N(x, y, z) - \psi_N(x, y, 0)}{z} > 0.$$

Thus, if  $z > \bar{z} > 0$ , we have

$$\psi_N(x, y, z) - \psi_N(x, y, \bar{z}) \geq \frac{\partial}{\partial z} \psi_N(x, y, \bar{z})(z - \bar{z}) = \beta(z - \bar{z}),$$

with  $\beta > 0$ .

But  $\bar{z}_{2N+1}^{min} = z_{2N+1}^{min} = b_{2N+1}^2 - \delta_{2N+1}^2$  and from the proof of Lemma 2 we have that  $b_{2N+1} = b + O(1/N)$  and that  $\delta_{2N+1} = \delta_0 + O(1/N)$ . Hence, from (11) and the latter estimates we conclude that  $|z_{2N+1} - z_{dim}| = O(1/N)$ .

Now, using the analysis made of the functions  $\psi_N$  and  $\Phi_N$  in the proof of Lemma 2 we will prove that there exist two positive constants  $\alpha$  and  $r$  independent of  $N$ , such that

$$\begin{aligned} \psi_N(x, y, 2x^2 - y^2) - \psi_N(x_{2N+1}^{min}, y_{2N+1}^{min}, 2x_{2N+1}^{min} - (y_{2N+1}^{min})^2) \\ \geq \alpha \min\left\{ \left[ (x^2 - (x_{2N+1}^{min})^2)^2 + (y^2 - (y_{2N+1}^{min})^2)^2 \right], r^2 \right\}. \end{aligned} \quad (12)$$

To prove this estimate, we just need to bound the least eigenvalue of  $\text{Hess}_{(X,Y)}(\phi_N)$  from below by  $\alpha$ , for all  $X, Y$  such that  $(X - (x_{2N+1}^{min})^2)^2 + (Y - (y_{2N+1}^{min})^2)^2 \leq r^2$ . To obtain this bound we proceed as follows.

The eigenvalues of  $\Omega$  are  $\lambda_k = 2 \cos(4\pi k/N)$  (with eigenvectors  $v_k = ((w_k)^n)_{n \in \mathbb{Z}/N\mathbb{Z}}$ , where  $w_k = e^{i\frac{2\pi k}{N}}$ ) for  $0 \leq k \leq N-1$ . So, for  $0 < X < Y$ , we have

$$\begin{aligned} K_N(X, Y) &:= -\frac{1}{N} \operatorname{Tr} \left( (2Y + (2X - Y)\Omega)^{1/2} \right) \\ &= -\frac{\sqrt{2}}{N} \sum_{k=0}^{N-1} (2 \cos(4\pi k/N)X + (1 - \cos(4\pi k/N))Y)^{1/2} \end{aligned}$$

From the expression

$$\Phi_N(X, Y) = \frac{1}{2}g(Y - 2b\sqrt{X} + b^2) + K_N(X, Y),$$

we deduce that

$$\operatorname{Hess}_{(X,Y)}(\Phi_N) = \begin{pmatrix} \frac{b}{2X^{3/2}} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} A_N & B_N \\ B_N & C_N \end{pmatrix},$$

where

$$\begin{aligned} A_N &= \frac{\partial^2}{\partial X^2} K_N(X, Y) \\ &= \frac{\sqrt{2}}{N} \sum_{k=0}^{N-1} [2 \cos(4\pi k/N)X + (1 - \cos(4\pi k/N))Y]^{-3/2} \cos^2(4\pi k/N), \\ B_N &= \frac{\partial^2}{\partial X \partial Y} K_N(X, Y) \\ &= \frac{\sqrt{2}}{2N} \sum_{k=0}^{N-1} [2 \cos(4\pi k/N)X + (1 - \cos(4\pi k/N))Y]^{-3/2} \cos(4\pi k/N)(1 - \cos(4\pi k/N)), \end{aligned}$$

and

$$\begin{aligned} C_N &= \frac{\partial^2}{\partial Y^2} K_N(X, Y) \\ &= \frac{\sqrt{2}}{4N} \sum_{k=0}^{N-1} [2 \cos(4\pi k/N)X + (1 - \cos(4\pi k/N))Y]^{-3/2} (1 - \cos(4\pi k/N))^2. \end{aligned}$$

Note that these three quantities are convergent Riemann sums, hence

$$A_N \rightarrow A_\infty, \quad B_N \rightarrow B_\infty, \quad \text{and} \quad C_N \rightarrow C_\infty,$$

as  $N$  goes to infinity, with  $A_\infty, C_\infty > 0$ . Therefore, for large enough  $N$ ,  $C_N \geq C_\infty/2$ .

Now, for each  $N$  and for any vector  $v = (h, k)^T \in \mathbb{R}^2$  we have that

$$\langle \operatorname{Hess}_{(X,Y)}(K_N)v, v \rangle = A_N h^2 + 2B_N h k + C_N k^2 \geq 0. \quad (13)$$

We choose  $r = x_{\dim}^2/2 = b^2/2$ . If  $|X - x_{\dim}^2| \leq r$  then  $\frac{b}{2X^{3/2}} \geq \frac{\sqrt{2}}{b^2}$ . Let  $\epsilon_0 := \frac{\sqrt{2}-1}{b^2}$ .

$$\begin{aligned}
\langle \text{Hess}_{(X,Y)}(\Phi_N)\mathbf{v}, \mathbf{v} \rangle &= \left( \frac{b}{2X^{3/2}} - \epsilon_0 \right) h^2 + (A_N + \epsilon_0)h^2 + 2B_Nhk + C_Nk^2 \\
&\geq \frac{1}{b^2}h^2 \\
&\quad + A_N \left( \frac{\sqrt{A_N + \epsilon_0}}{\sqrt{A_N}}h \right)^2 + 2B_N \left( \frac{\sqrt{A_N + \epsilon_0}}{\sqrt{A_N}}h \right) \left( \frac{\sqrt{A_N}}{\sqrt{A_N + \epsilon_0}}k \right) + C_N \left( \frac{\sqrt{A_N}}{\sqrt{A_N + \epsilon_0}}k \right)^2 \\
&\quad + C_N \left( 1 - \frac{A_N}{A_N + \epsilon_0} \right) k^2 \\
[(13) \Rightarrow] &\geq \frac{1}{b^2}h^2 + C_N \left( \frac{\epsilon_0}{A_N + \epsilon_0} \right) k^2.
\end{aligned}$$

But we have seen that for large enough  $N$ ,  $C_N \geq C_\infty/2$ . So there is  $\alpha > 0$  independent of  $N$ , such that (12) holds.

Consequently, we have proved that  $x_{2N+1} - x_{\dim} = O(1/\sqrt{N})$  and  $y_{2N+1}^2 - y_{\dim}^2 = O(1/\sqrt{N})$  and the lemma follows.  $\square$

Let us apply all the above results to prove

**Lemma 4.** *The estimate*

$$\text{Tr} \left( T^4(2N+1) - \langle T^2(2N+1) \rangle^2 \right) \leq M$$

holds for some constant  $M$  independent of  $N$ . Hence

$$\|T^2(2N+1) - (2y_{2N+1}^2 + z_{2N+1}\Omega_{2N+1})\|_{\sigma_2} = O(1)_{N \rightarrow \infty}.$$

*Proof.* From inequality (10) there is  $C > 0$  such that

$$\|T(2N+1)\|^{-3} \text{Tr} [T^4(2N+1) - \langle T^2(2N+1) \rangle^2] \leq C,$$

but

$$\begin{aligned}
\|T(2N+1)\|^3 &= \|T^4(2N+1)\|^{3/4} \\
&\leq \left( \left\| T^4(2N+1) - \langle T^2(2N+1) \rangle^2 \right\| + \left\| \langle T^2(2N+1) \rangle \right\|^2 \right)^{3/4} \\
&\leq \left\| T^4(2N+1) - \langle T^2(2N+1) \rangle^2 \right\|^{3/4} + \left\| \langle T^2(2N+1) \rangle \right\|^2 \right)^{3/4}
\end{aligned}$$

From the equalities (see [4])

$$\langle T^2(2N+1) \rangle = 2y_{2N+1}^2 + z_{2N+1}\Omega_{2N+1}$$

and

$$\sigma(\langle T^2(2N+1) \rangle) = \{2y_{2N+1}^2 + 2z_{2N+1} \cos 2\theta, \theta \in \Theta\},$$

for a certain set of angles  $\Theta$  of no importance here, we infer that

$$\begin{aligned} \|\langle T^2(2N+1) \rangle\| &= \sup \sigma(\langle T^2(2N+1) \rangle) \leq 2y_{2N+1}^2 + 2|z_{2N+1}| \\ &\rightarrow 2y_{dim}^2 + 2z_{dim} \\ &= 2b^2 + 2\delta_0^2 + 2b^2 - 2\delta_0^2 \\ &= 4b^2. \end{aligned}$$

Hence, the sequence  $(\|\langle T^2(2N+1) \rangle\|)_{N \geq 0}$  is bounded. Let  $B$  be its upper bound and set  $\eta_N := \text{Tr}[T^4(2N+1) - \langle T^2(2N+1) \rangle^2]$ . We have

$$C \geq \|T(2N+1)\|^{-3} \text{Tr}[T^4(2N+1) - \langle T^2(2N+1) \rangle^2] \geq \frac{\eta_N}{\eta_N^{3/4} + B^{3/2}}.$$

It follows that there is  $M < +\infty$  such that  $\eta_N \leq M$  for all  $N$ .  $\square$

We notice that Lemma 4 tells us that

$$\sum_i \left[ (t_i^2(2N+1) + t_{i+1}^2(2N+1) - 2y_{dim}^2)^2 + 2(t_i(2N+1)t_{i+1}(2N+1) - z_{dim})^2 \right] \leq M, \quad (14)$$

by the definition of  $T^2$  and  $\langle T^2 \rangle$  in terms of the variables  $x, y, z$ .

Now, we have

$$\begin{aligned} z_{2N+1} - \bar{z}_{2N+1} &= \frac{1}{2N+1} \sum s_i s_{i+1} + \frac{1}{2N+1} \sum s_i^2 \\ &= \frac{1}{4N+2} \sum (s_i + s_{i+1})^2 \\ &= \frac{1}{4N+2} \sum (t_i(2N+1) + t_{i+1}(2N+1) - 2x_{2N+1})^2. \end{aligned}$$

This, together with the estimate  $z_{2N+1} - \bar{z}_{2N+1} = O(1/N)$  from Lemma 3, implies that

$$\sum (t_i(2N+1) + t_{i+1}(2N+1) - 2x_{2N+1})^2 = O(1)_{N \rightarrow \infty}.$$

Finally, we have proved

$$\begin{aligned} \sum (t_i(2N+1) + t_{i+1}(2N+1) - 2b)^2 &= \sum (t_i(2N+1) + t_{i+1}(2N+1) - 2x_{2N+1})^2 \\ &\quad + (2N+1)(2x_{2N+1} - 2b)^2 \\ &= O(1) \end{aligned} \quad (15)$$

Furthermore, denoting

$$\rho_i(N) := (t_i(2N+1) + t_{i+1}(2N+1) - 2b)^2 + (t_i(2N+1)t_{i+1}(2N+1) - z_{dim})^2$$

we get from (14) and (15):

$$\sum_{i=1}^{2N+1} \rho_i(N) < M'. \quad (16)$$

The next lemma tells us that the smallness of  $\rho(N)$  on an interval implies that  $\mathbf{t}(2N+1)$  is close to one of the two dimerized states on this interval.

**Lemma 5.** *There exist  $\gamma > 0$  and  $C > 0$  such that: given  $N \geq 1$  and any pair of integers  $I < J \in \mathbb{Z}$ , if*

$$\forall i \in [I, J-1], \rho_i(N) \leq \gamma$$

*then there is  $\tau_N \in \{0, 1\}$  such that for all  $i \in [I, J]$ :*

$$|t_i(2N+1) - b - (-1)^{i+\tau_N} \delta_0|^2 \leq C \rho_i(N).$$

*We shall say that  $[I, J]$  is of type 1 when  $\tau_N = 0$ , of type 2 when  $\tau_N = 1$ .*

*Proof.* In the interval  $[I, J]$  each couple  $(t_i(2N+1), t_{i+1}(2N+1))$  solves the second-degree equation  $X^2 - S_i(N)X + P_i(N) = 0$ , where

$$\begin{aligned} S_i(N) &= t_i(2N+1) + t_{i+1}(2N+1) = 2b + \lambda_i(N) \\ P_i(N) &= t_i(2N+1)t_{i+1}(2N+1) = z_{dim} + \mu_i(N) \\ \rho_i(N) &= \lambda_i^2(N) + \mu_i^2(N) \leq \gamma \end{aligned}$$

Hence,  $\{t_i(2N+1), t_{i+1}(2N+1)\} = \left\{ \frac{S_i(N) \pm \sqrt{\Delta_i(N)}}{2} \right\}$ , with  $\Delta_i(N) = S_i^2(N) - 4P_i(N)$ .

Note that the roots  $\frac{S_i(N) \pm \sqrt{\Delta_i(N)}}{2}$  are differentiable functions of  $(\lambda_i(N), \mu_i(N))$  near  $(0, 0)$ , taking distinct values  $b \pm \delta_0$  at  $(0, 0)$ . So, for  $\gamma$  small enough, there is a constant  $C$  such that *exactly one* of the following two estimates holds:

$$|t_i(2N+1) - b - (-1)^i \delta_0| + |t_{i+1}(2N+1) - b - (-1)^{i+1} \delta_0| \leq \sqrt{C \rho_i(N)}$$

or

$$|t_i(2N+1) - b - (-1)^{i+1} \delta_0| + |t_{i+1}(2N+1) - b - (-1)^{i+2} \delta_0| \leq \sqrt{C \rho_i(N)}.$$

Assume, for instance, that the first estimate holds for  $i = I$ . Then the same estimate holds for any  $i \in [I, J]$ , by induction on  $i$ . In this case we define  $\tau_N = 0$ . Similarly, if the second estimate holds for  $i = I$  then it holds everywhere in the interval, and we define  $\tau_N = 1$ . In both cases, Lemma 5 is true. □

Now, the estimate (16) gives us a bound  $M'$  independent of  $N$  on the  $l_1$  norms of the  $(2N+1)$ -tuples  $\rho(N) := (\rho_i(N))_{i \in \mathbb{Z}/(2N+1)\mathbb{Z}}$ . By an easy argument in the spirit of the concentration-compactness method, we find, up to extraction of a subsequence, a nonnegative integer  $p < M'/2\gamma$ , and  $p$  sequences of integers  $0 \leq i_N^1 < i_N^2 < \dots < i_N^p < 2N+1$ , such that:

1.  $\lim_{N \rightarrow \infty} (i_N^{k+1} - i_N^k) = \infty$  for  $1 \leq k \leq p-1$ ,  $\lim_{N \rightarrow \infty} (i_N^1 + 2N + 1 - i_N^p) = \infty$
2.  $\rho_{i_N^k}(N) > \gamma$
3. There is a constant  $\Delta > 0$  such that, if  $\text{dist}(i, \{i_N^1, \dots, i_N^p\} + (2N+1)\mathbb{Z}) \geq \Delta$ , then  $\rho_i(N) \leq \gamma$ .

A priori  $p$  might be zero (this is called "vanishing" in the concentration-compactness theory). In such a case, for all  $i \in \mathbb{Z}$ ,  $\rho_i(N) \leq \gamma$ . By Lemma 5, this would imply the existence of  $\tau_N$  such that for all integers  $i \in \mathbb{Z}$ ,

$$|t_i(2N+1) - b - (-1)^{i+\tau_N} \delta_0| \leq \sqrt{C\rho_i(N)}.$$

Taking  $\gamma$  small enough we see that this is impossible since for every  $i$  we have  $t_{i+2N+1}(2N+1) = t_i(2N+1)$  and  $\rho(N)_{i+2N+1} = \rho(N)_i$ . So vanishing is excluded and  $p$  must be positive.

Now, for  $N$  large enough, the set  $\{i \in \mathbb{Z} : \text{dist}(i, \{i_N^1, \dots, i_N^p\} + (2N+1)\mathbb{Z}) \geq \Delta\}$  consists of intervals separating the integers  $i_N^k + (2N+1)m$ , and, by Lemma 5, each interval must be either of type 1 or of type 2. Using once again an odd-period argument, we see that there are necessarily two intervals of different types, hence the existence of  $1 \leq k_* \leq p$  and  $m_* \in \{0, 1\}$  such that  $i_N := i_N^{k_*} + (2N+1)m_*$  has an interval of type 1 immediately to its left side, and an interval of type 2 immediately to its right side. Then we may shift the  $(2N+1)$ -tuple  $\mathbf{t}(2N+1)$  so that  $i_N$  becomes zero for all  $N$ . We finally get the following estimates (after shifting and extraction):

$$\rho_0(N) > \gamma \tag{17}$$

There is a sequence  $\bar{R}_N \rightarrow \infty$  and, for all  $\epsilon > 0$ , an integer  $N_\epsilon$  and a radius  $\underline{R}_\epsilon > 0$  such that for all  $N \geq N_\epsilon$ ,

$$\sum_{\underline{R}_\epsilon < |i| < \bar{R}_N} \rho_i(N) < \epsilon \tag{18}$$

and

$$(\forall N \geq N_\epsilon) \begin{cases} \sum_{-\bar{R}_N < i < -\underline{R}_\epsilon} (t_i(2N+1) - b - (-1)^i \delta_0)^2 < C\epsilon \\ \sum_{\underline{R}_\epsilon < i < \bar{R}_N} (t_i(2N+1) - b - (-1)^{i+1} \delta_0)^2 < C\epsilon \end{cases} \tag{19}$$

Now, the estimate (16) gives us a bound  $M'$  independent of  $N$  on the  $l_1$  norms of the  $(2N+1)$ -tuples  $\rho(N) := (\rho_i(N))_{i \in \mathbb{Z}/(2N+1)\mathbb{Z}}$ . It also provides a uniform  $l_\infty$  bound on the  $(2N+1)$ -tuples  $\mathbf{t}(2N+1)$ . So, after extraction of a subsequence, we may impose

the pointwise convergence  $t_i(2N+1) \rightarrow t_i^\infty$ , and, denoting  $\rho_i^\infty := (t_i^\infty + t_{i+1}^\infty - 2b)^2 + (t_i^\infty t_{i+1}^\infty - z_{dim})^2$ , Fatou's lemma guarantees that  $\sum_{i \in \mathbb{Z}} \rho_i^\infty \leq M'$ .

We also have that

$$\begin{cases} \forall i \geq \Delta, & |t_i^\infty - b - (-1)^{i+1} \delta_0| \leq \sqrt{C \rho_i^\infty} \\ \forall i \leq -\Delta, & |t_i^\infty - b - (-1)^i \delta_0| \leq \sqrt{C \rho_i^\infty}, \end{cases}$$

which implies the kink property (2) of Theorem 1. Now, the pointwise convergence  $[T^2(N)]_{i,j} \rightarrow [(T^\infty)^2]_{i,j}$  obviously holds, but the pointwise convergence  $|T(N)|_{i,j} \rightarrow |T^\infty|_{i,j}$  is less obvious. In order to study the absolute values of  $T(N)$  and  $T^\infty$ , we shall use the classical formula for the absolute value of a self-adjoint operator  $A$ ,

$$|A| = \frac{1}{\pi} \int_{\mathbb{R}} A^2(\omega^2 + A^2)^{-1} d\omega. \quad (20)$$

To exploit this formula, we shall need a decay estimate on the coefficients of the matrices  $(\omega^2 + T^2)^{-1}$  away from the diagonal.

Note that  $T_{dim}^2(2N)$  commutes with the translation  $i \rightarrow i+1$ , and in the Fourier domain it is a multiplication operator by a nonzero  $2\pi$ -periodic scalar function  $m_N(p)$ , which is a complex-analytic function of the frequency  $p$  in a strip of the form  $\{p : |Im(p)| < \rho\}$  for some  $\rho > 0$  independent of  $N$  and  $\omega$ . Moreover, there is an estimate in this strip of the form  $Re(m_N(p)) \geq r$  for some positive constant  $r$  independent of  $N$  and  $\omega$ . As a consequence, there holds the estimate  $|(\omega^2 + m_N(p))^{-1}| \leq \frac{1}{r+\omega^2}$  in the complex strip. So the Fourier coefficients  $c_l$  of the analytic and periodic function  $(\omega^2 + m_N(p))^{-1}$  satisfy a decay estimate of the form

$$|c_l| \leq \frac{C}{1+\omega^2} e^{-\rho l}, \quad l \in \mathbb{Z}.$$

As a consequence,

$$|[(\omega^2 + T_{dim}^2(N))^{-1}]_{i,j}| \leq \frac{C}{1+\omega^2} e^{-\rho \text{dist}(i-j, 2N\mathbb{Z})}.$$

Similarly, for  $N$  infinite we have

$$|[(\omega^2 + T_{dim}^2)^{-1}]_{i,j}| \leq \frac{C}{1+\omega^2} e^{-\rho|i-j|}.$$

For arbitrary  $N$ -tuples  $\mathbf{s}$ , we are able to prove the following (weaker) estimate:

**Lemma 6.** *Let  $M, \omega_0 > 0$ . Then there are two constants  $C, \rho > 0$  depending only on  $M$  and  $\omega_0$ , such that, for any  $\omega \geq \omega_0$ :*

1. *For all  $N \geq 1$ , if  $\mathbf{s} \in \mathbb{R}^{\mathbb{Z}/N\mathbb{Z}}$  satisfies  $(\forall 1 \leq i \leq N) : |s_i| \leq M$ , then*

$$(\forall i, j \in \mathbb{Z}) : |[(\omega^2 + S^2)^{-1}]_{i,j}| \leq \frac{C}{\omega^2} e^{-\rho \text{dist}(i-j, N\mathbb{Z})}.$$

2. For an infinite chain, if  $\mathbf{s} \in \mathbb{R}^{\mathbb{Z}}$  satisfies  $(\forall i \in \mathbb{Z}) : |s_i| \leq M$ , then

$$(\forall i, j \in \mathbb{Z}) : \left| [(\omega^2 + S^2)^{-1}]_{i,j} \right| \leq \frac{C}{\omega^2} e^{-\rho|i-j|}. \quad (21)$$

*Proof.* The proofs for finite and infinite chains are similar, so we only treat the case of an infinite chain:  $\mathbf{s} \in \mathbb{R}^{\mathbb{Z}}$  and  $S$  acts in  $l_2(\mathbb{Z}, \mathbb{C})$ .

We first introduce a smooth function  $\eta : \mathbb{R} \rightarrow [0, 1]$  satisfying  $\eta(0) = 0$ ,  $\eta(1) = \frac{1}{2}$ ,  $\eta(2) = 1$  and  $0 \leq \eta'(t) \leq 1$  for all  $t$ .

Given  $m \in \mathbb{N}$  and  $R \geq 4$ , let  $\eta_{m,R}(t) := \eta\left(\frac{|t-mR|}{R}\right)$ . This function of  $t$  is even and satisfies  $\eta_{m,R} \equiv 0$  on  $[-mR, mR]$ ,  $\frac{1}{2} \leq \eta_{m,R} \leq 1$  on  $[(m+1)R, (m+2)R]$ ,  $\eta_{m,R} \equiv 1$  on  $[(m+2)R, \infty]$ . Moreover,  $|\eta'_{m,R}| \leq \frac{1}{R}$ , hence  $|\eta_{m,R}(t+2) - \eta_{m,R}(t)| \leq \frac{2}{R}$ .

Take an arbitrary  $j \in \mathbb{Z}$ . Let  $e_j = (\delta_{i,j})_{i \in \mathbb{Z}}$  and consider the vector  $V := (\omega^2 + S^2)^{-1} e_j$ . The coordinates of  $V$  are  $V_i = [(\omega^2 + S^2)^{-1}]_{i,j}$ . Now, for each integer  $m \geq 1$  we define the vector  $V^m$  of coordinates  $V_i^m = \eta_{m,R}(i-j)V_i$ . We have  $\eta_{m,R}(i-j)[(\omega^2 + S^2)V]_i = 0$ , hence

$$[(\omega^2 + S^2)V^m]_i = \xi_i^m$$

with

$$\begin{aligned} \xi_i^m &:= s_i s_{i+1} \left( (\eta_{m,R}(i+2-j) - \eta_{m,R}(i-j)) V_{i+2} \right. \\ &\quad \left. + s_i s_{i-1} \left( (\eta_{m,R}(i-2-j) - \eta_{m,R}(i-j)) V_{i-2} \right) \right) \end{aligned}$$

hence, remembering that  $|s_{i-1}|, |s_i|, |s_{i+1}| \leq M$ , we get

$$|\xi_i^m| \leq \frac{2M^2}{R} (|V_{i+2}| + |V_{i-2}|).$$

When  $m \geq 2$ , we see that  $\xi_i^m = 0$  when  $|i-j| \leq mR - 2$ , while for all  $(i, j)$  such that  $|i-j| \geq mR - 2$  we have  $\eta_{m-1,R}(i \pm 2 - j) \geq \frac{1}{2}$ , since  $R \geq 4$ . As a consequence,

$$|\xi_i^m| \leq \frac{4M^2}{R} (|V_{i+2}^{m-1}| + |V_{i-2}^{m-1}|).$$

Finally, we get the estimate

$$\|(\omega^2 + S^2)V^1\|_2 \leq \frac{4M^2}{R} \|V\|_2$$

and for all  $m \geq 2$

$$\|(\omega^2 + S^2)V^m\|_2 \leq \frac{8M^2}{R} \|V^{m-1}\|_2.$$

Clearly,  $\|(\omega^2 + S^2)^{-1}\| \leq \frac{1}{\omega^2}$ , hence  $\|V\|_2 \leq \frac{1}{\omega^2}$  and, by induction on  $m \geq 1$ :

$$\|V^m\|_2 \leq \frac{1}{2\omega^2} \left( \frac{8M^2}{\omega^2 R} \right)^m.$$

Assuming  $\omega \geq \omega_0$  and choosing  $R > 8M^2/\omega_0^2$  we easily derive the decay estimate (21).  $\square$



Thanks to Lemma 6, we are now able to prove the desired pointwise convergence result:

**Lemma 7.** *Take a finite constant  $M$ . Assume that we are given a sequence of  $N$ -tuples  $\mathbf{s}(N) \in \mathbb{R}^{\mathbb{Z}/N\mathbb{Z}}$  such that for all  $i, N$ :  $|s_i(N)| \leq M$ . Assume, moreover, that for each  $i \in \mathbb{Z}$ , the sequence  $s_i(N)$  has a limit  $s_i^\infty$  as  $N \rightarrow \infty$ . Then:*

$$\forall i, j \in \mathbb{Z}, |S(N)|_{i,j} \rightarrow |S^\infty|_{i,j}.$$

*Proof.* First of all, note that for any bounded, self-adjoint operator  $A$ , the integrand in  $|A| = \frac{1}{\pi} \int_{\mathbb{R}} A^2(\omega^2 + A^2)^{-1} d\omega$  has operator norm  $\|A^2(\omega^2 + A^2)^{-1}\| \leq \min\{1, \|A\|^2/\omega^2\}$ . So, by Lebesgue's dominated convergence theorem, we just have to prove that for each  $\omega > 0$  and any  $i, j \in \mathbb{Z}$ ,

$$[(\omega^2 + S^2(N))^{-1}]_{i,j} \rightarrow [(\omega^2 + (S^\infty)^2)^{-1}]_{i,j} \text{ as } N \rightarrow \infty.$$

So, from now on, we fix  $\omega > 0$ . We denote  $L(N) := (\omega^2 + S^2(N))^{-1}$  (acting in  $\mathbb{C}^{\mathbb{Z}/N\mathbb{Z}}$ ) and  $L^\infty := (\omega^2 + (S^\infty)^2)^{-1}$  (acting in  $l_2(\mathbb{Z}, \mathbb{C})$ ).

For each positive integer  $N$ , we consider the infinite sequence  $(s_i^{\infty, N})$  such that  $s_{i+N}^{\infty, N} = s_i^{\infty, N}$  ( $\forall i \in \mathbb{Z}$ ) and  $s_i^{\infty, N} = s_i^\infty$  when  $0 < i \leq N$ . Let  $(S_{i,j}^{\infty, N})_{i,j \in \mathbb{Z}}$  be the associated operator. By construction,  $S^{\infty, N}$ , considered as an operator in  $l_2(\mathbb{Z}, \mathbb{C})$ , commutes with the shift  $\sigma_N : (z_i) \rightarrow (z_{i-N})$ . So the operator  $L^{\infty, N} := (\omega^2 + (S^{\infty, N})^2)^{-1}$  also commutes with  $\sigma_N$ . Again by construction, the coefficients of  $S^{\infty, N}$  converge pointwise to those of  $S^\infty$  as  $N \rightarrow \infty$ . So, writing

$$[L^{\infty, N} - L^\infty]_{i,j} = [L^{\infty, N}((S^\infty)^2 - (S^{\infty, N})^2)L^\infty]_{i,j}$$

one easily proves, thanks to Lemma 6, that the coefficients of  $L^{\infty, N}$  converge pointwise to those of  $L^\infty$  as  $N \rightarrow \infty$ .

Now, for each  $N \geq 1$  we define a new matrix  $(\tilde{S}_{i,j}(N))_{i,j \in \mathbb{Z}/N\mathbb{Z}}$  by the formula  $\tilde{S}_{i,j}(N) := \sum_{m \in \mathbb{Z}} S_{i+Nm, j}^{\infty, N}$ . Note that only a finite number of terms in this series are nonzero, so that there is no problem of convergence. Similarly, we define  $\tilde{L}_{i,j}(N) := \sum_{m \in \mathbb{Z}} L_{i+Nm, j}^{\infty, N}$ . This time we have an infinite series, but thanks to Lemma 6 its terms decay exponentially, and the coefficients of  $\tilde{L}(N) - L^{\infty, N}$  converge pointwise to zero as  $N \rightarrow \infty$ . By construction,  $\tilde{L}(N)$ , considered as an operator in  $\mathbb{C}^{\mathbb{Z}/N\mathbb{Z}}$ , coincides with  $(\omega^2 + (\tilde{S}(N))^2)^{-1}$ . Our last step is to write

$$[L(N) - \tilde{L}(N)]_{i,j} = [L(N) (\tilde{S}^2(N) - S^2(N)) \tilde{L}(N)]_{i,j}.$$

From this we see, thanks once again to Lemma 6, that the coefficients of  $L(N) - \tilde{L}(N)$  converge pointwise to zero as  $N \rightarrow \infty$ . Combining the successive pointwise convergence results obtained above, we finally get the desired convergence  $L_{i,j}(N) \rightarrow L_{i,j}^\infty$ .  $\square$

We recall that the assumptions of Lemma 7 are satisfied by our minimizers  $\mathbf{t}(2N+1)$ , up to extraction of a subsequence. So we can conclude that

$$\forall i, j \in \mathbb{Z}, |T(2N+1)|_{i,j} \rightarrow |T^\infty|_{i,j}.$$

Now, our goal is to prove that  $\mathbf{t}^\infty$  is a relative energy minimizer. For this purpose, we need a better understanding of the possible lack of invertibility of  $T^2(2N+1)$  and  $(T^\infty)^2$ . We recall that  $T_{dim}^2(2N) = 2(b^2 + \delta_{2N}^2)\mathbf{1} + (b^2 - \delta_{2N}^2)\Omega_{2N}$ , with  $\delta_{2N} \rightarrow \delta_0$  as  $N$  goes to infinity. Similarly, for the infinite chain  $T_{dim}^2 = 2(b^2 + \delta_0^2)\mathbf{1} + (b^2 - \delta_0^2)\Omega$ .

**Lemma 8.** *There is a positive constant  $\kappa$  such that, when  $N$  is large enough or in the case of the infinite chain, if  $\mathbf{s}$  satisfies  $(s_i^2 + s_{i-1}^2 - 2b^2 - 2\delta_0^2)^2 + 2(s_i s_{i+1} - b^2 + \delta_0^2)^2 \leq \kappa (\forall i)$ , then  $S$  is invertible and its inverse has operator norm less than  $2/\delta_0^2$ .*

*Proof.* We only give the proof in the case  $\mathbf{s} \in \mathbb{C}^{\mathbb{Z}}$ , the case “ $N$  large” being similar. In the Fourier domain,  $T_{dim}^2$  is a multiplication operator by a function of the form  $b^2 \cos^2(k) + \delta_0^2 \sin^2(k)$ . Since  $\delta_0 < b$ , the smallest value of this multiplier is  $\delta_0^2$ , so the inverse of  $T_{dim}^2$  has operator norm  $1/\delta_0^2$ . Now, if  $\kappa$  is chosen small enough, then the hypothesis on  $\mathbf{s}$  implies that  $\|S^2 - T_{dim}^2\| \leq \delta_0^2/2$ , hence the lemma.  $\square$

The next lemma tells us that  $T^2(2N+1)$  has a bounded inverse with bound at most  $4/\delta_0^2$  on the orthogonal complement of a subspace of  $\mathbb{C}^{\mathbb{Z}/(2N+1)\mathbb{Z}}$  the dimension of which is bounded independently of  $N$ .

**Lemma 9.** *There is a finite constant  $D$  such that, if  $N$  is large enough, then the rank of  $\chi_{[0, \delta_0^2/4]}(T^2(2N+1))$  is at most  $D$ . Similarly, the rank of  $\chi_{[0, \delta_0^2/4]}(T_\infty^2)$  is at most  $D$ .*

*Proof.* We first treat the case of an infinite chain, which is easier. We consider a normalized eigenvector  $V$  of  $T_\infty^2$  with eigenvalue  $\lambda \leq \delta_0^2/4$ . We follow the same kind of strategy as in the proof of Lemma 6, in order to get a decay estimate on the components of  $V$ . We shall only prove the decay for positive values of  $i$ , the case of negative values being similar. We take the same function  $\eta$  as in the proof of Lemma 6, but our definition of  $\eta_{m,R}$  is slightly different: we take  $\eta_{m,R}(t) := \eta(\frac{t-mR}{R})$ , so that  $\eta_{m,R}$  vanishes on the whole interval  $(-\infty, mR]$ . We define a sequence of vectors  $V^m$  by  $V_i^m = \eta_{m,R}(i)V_i$  for  $m \geq 1$ . We know that there is  $\tau \in \{0, 1\}$  such that  $t_i^\infty - b - (-1)^{i+\tau}\delta_0 \rightarrow 0$  as  $i \rightarrow \infty$ . Now, we take a large integer  $R_0$  and we define  $s_i := b + (-1)^{i+\tau}\delta_0 (\forall i < R_0)$  and  $s_i := t_i^\infty (\forall i \geq R_0)$ . Then, if  $R_0$  is chosen large enough,

$$(s_i^2 + s_{i-1}^2 - 2b^2 - 2\delta_0^2)^2 + 2(s_i s_{i+1} - b^2 + \delta_0^2)^2 \leq \kappa (\forall i).$$

So Lemma 8 tells us that  $S^2$  is invertible and that the operator norm of its inverse is less than  $2/\delta_0^2$ . We now take  $R > R_0$ . Proceeding as in the proof of Lemma 6 we find estimates of the form  $\|(S^2 - \lambda)V_i^1\|_2 \leq O(1/R)$ ,  $\|(S^2 - \lambda)V_i^m\|_2 \leq O(1/R)\|V_i^{m-1}\|_2 (\forall m \geq 2)$ . But the norm operator of  $(S^2 - \lambda)^{-1}$  is less than  $4/\delta_0^2$ . So, choosing  $R$  large enough, we get a decay estimate of the form  $|V_i| \leq C e^{-\alpha i}$ . The positive constants  $C, \alpha$  do not depend on  $\lambda$ , and arguing in the same way for negative values of  $i$ , we get the estimate  $|V_i| \leq C e^{-\alpha|i|}$

for all normalized vectors in the range of  $\chi_{[0, \delta_0^2/4]}(T_\infty^2)$ . This implies that the unit ball of this range is compact, so  $\chi_{[0, \delta_0^2/4]}(T_\infty^2)$  has finite rank.

Now, we shortly explain how these ideas can be adapted to the case of a large finite chain. Combining Lemmas 4 and 5 we find that for any  $\epsilon > 0$ , there are a positive constant  $A_\epsilon$ , an integer  $p_\epsilon \geq 1$  independent of  $N$  (for  $N$  large enough) and  $p_\epsilon + 1$  sequences of integers  $0 = i_N^0 < i_N^1 < \dots < i_N^{p_\epsilon} = N$  such that:

1.  $\lim_{N \rightarrow \infty} (i_N^{k+1} - i_N^k) = \infty$  for  $0 \leq k \leq p_\epsilon - 1$ .
2. For each  $0 \leq k \leq p_\epsilon - 1$  there is  $\tau_k \in \{0, 1\}$ , such that, when  $i$  varies in the interval  $(i_N^k, i_N^{k+1})$ , if  $\text{dist}(i, \{i_N^k, i_N^{k+1}\}) \geq A_\epsilon$  then  $|t_i(2N+1) - b - (-1)^{i+\tau_k} \delta_0| < \epsilon$ .

Now, we fix a small enough value of  $\epsilon$ , and we denote  $P = p_\epsilon$ . By arguments similar to those used for the infinite chain, we can get a decay estimate of the form

$$|V_i| \leq C \exp[-\alpha \text{dist}(|i|, \{i_N^0, i_N^1, \dots, i_N^P\}) + (2N+1)\mathbb{Z}]$$

for all normalized vectors  $V$  in the range of  $\chi_{[0, \delta_0^2/4]}(T^2(2N+1))$ . This implies that for any  $r > 0$ , the unit ball of this range can be covered by a finite number  $q(r)$  of balls of radius  $r$  where  $q(r)$  is independent of  $N$ . So there is a constant  $D$  such that for any  $N$ , the rank of  $\chi_{[0, \delta_0^2/4]}(T^2(N))$  is at most  $D$ . □

Now we consider a sequence  $\mathbf{u} \in l_1(\mathbb{Z}, \mathbb{R})$ . Given  $N \geq 1$ , we call  $\mathbf{u}(N)$  the  $N$ -periodic sequence such that  $u_i(N) = u_i$  ( $\forall 1 \leq i \leq N$ ). We have the following result:

**Lemma 10.** *The difference  $(|T^\infty + U| - |T^\infty|)$  is a trace-class operator in  $l_2(\mathbb{Z}, \mathbb{C})$ , and for any  $\epsilon > 0$  there is  $\Delta_\epsilon$  such that, for any  $N$  large enough, denoting*

$$\mathcal{J}_\epsilon := \{i \in \mathbb{Z} : \text{dist}(i, (2N+1)\mathbb{Z}) \geq \Delta_\epsilon\},$$

and recalling our notation  $\theta_A$  for the operator of multiplication by  $\chi_A$ , we have

$$\|(|T(2N+1) + U(2N+1)| - |T(2N+1)|)\theta_{\mathcal{J}_\epsilon}\|_{\sigma_1(\mathbb{C}^{\mathbb{Z}/(2N+1)\mathbb{Z}})} \leq \epsilon. \quad (22)$$

*Proof.* We take  $\omega_0 > 0$  (to be chosen later), we denote  $S(2N+1) := T(2N+1) + U(2N+1)$  and using (20) we write  $|S(2N+1)| - |T(2N+1)| = \frac{1}{\pi}(A(2N+1) + B(2N+1) + C(2N+1))$  where, omitting temporarily the  $(2N+1)$  argument, we have:

$$A := \int_{|\omega| \geq \omega_0} \omega^2 (\omega^2 + S^2)^{-1} (S^2 - T^2) (\omega^2 + T^2)^{-1} d\omega \quad (23)$$

$$B := \int_{|\omega| \leq \omega_0} (S^2 (\omega^2 + S^2)^{-1} - T^2 (\omega^2 + T^2)^{-1}) \chi_{[0, \delta_0^2/4]}(T^2) d\omega \quad (24)$$

$$C := \int_{|\omega| \leq \omega_0} \omega^2 (\omega^2 + S^2)^{-1} (S^2 - T^2) (\omega^2 + T^2)^{-1} \chi_{(\delta_0^2/4, \infty)}(T^2) d\omega \quad (25)$$

The operator norms of  $\omega^2(\omega^2 + S^2(2N + 1))^{-1}$ ,  $S^2(2N + 1)(\omega^2 + S^2(2N + 1))^{-1}$ ,  $T^2(2N + 1)(\omega^2 + T^2(2N + 1))^{-1}$  are at most 1, and the operator norm of  $(\omega^2 + T^2(2N + 1))^{-1}\chi_{(\delta_0^2/4, \infty)}(T^2(2N + 1))$  is at most  $4/\delta_0^2$ . Moreover the trace norm of  $S^2(2N + 1) - T^2(2N + 1)$  is bounded independently of  $N$ , and  $\|\chi_{[0, \delta_0^2/4]}(T^2(2N + 1))\|_{\sigma_1} \leq D$  thanks to Lemma 9. So, choosing  $\omega_0$  small enough (independently of  $N$ ), we can impose  $\|B(2N + 1)\|_{\sigma_1} + \|C(2N + 1)\|_{\sigma_1} \leq \epsilon/2$ . It remains to study  $A(2N + 1)$ . Since  $\omega_0$  is now fixed, we can apply Lemma 6 to  $(\omega^2 + S^2(2N + 1))^{-1}$  and  $(\omega^2 + T^2(2N + 1))^{-1}$ , and we easily find  $\Delta_\epsilon$  such that

$$\|A(2N + 1)\theta_{\mathcal{J}_\epsilon}\|_{\sigma_1(\mathbb{C}^{\mathbb{Z}/(2N+1)\mathbb{Z}})} \leq \epsilon/2.$$

This proves (22). Using a similar decomposition  $|T^\infty + U^\infty| - |T^\infty| = \frac{1}{\pi}(A^\infty + B^\infty + C^\infty)$ , one shows in the same way that this operator is trace-class, and the lemma is proved.  $\square$

Now, by Lemma 7 applied to  $T(2N + 1)$  and  $T(2N + 1) + U(2N + 1)$ , we see that for each  $i \in \mathbb{Z}$ ,  $(|T(2N + 1) + U(2N + 1)| - |T(2N + 1)|)_{i,i} \rightarrow (|T^\infty + U^\infty| - |T^\infty|)_{i,i}$ . Combining this with the uniform estimate (22), we conclude that

$$\text{Tr}(|T(2N + 1)| - |T(2N + 1) + U(2N + 1)|) \rightarrow \text{Tr}(|T^\infty| - |T^\infty + U|) \text{ as } N \rightarrow \infty$$

and finally

$$H^{(2N+1)}(\mathbf{t}(2N + 1) + \mathbf{u}(2N + 1)) - H^{(2N+1)}(\mathbf{t}(2N + 1)) \rightarrow \Delta H(\mathbf{u}).$$

But  $\mathbf{t}(2N + 1)$  is an energy minimizer, so

$$H^{(2N+1)}(\mathbf{t}(2N + 1) + \mathbf{u}(2N + 1)) - H^{(2N+1)}(\mathbf{t}(2N + 1)) \geq 0 \ (\forall N),$$

hence  $\Delta H(\mathbf{u}) \geq 0$ . We have proved that  $\mathbf{t}^\infty$  is a relative minimizer.

Our last task is to prove that  $\mathbf{t}^\infty$  satisfies the self-consistent equations. We recall that  $\Gamma^\infty := \chi_{(-\infty, 0)}(T^\infty)$ . Taking as before  $\mathbf{u} \in l_1(\mathbb{Z}, \mathbb{R})$ , we denote  $Q := \Gamma^\infty - \chi_{(-\infty, 0)}(T^\infty + U)$ . We know that  $U$  and  $(|T^\infty| - |T^\infty + U|)$  are trace-class. But  $|T^\infty| = T^\infty(1 - 2\Gamma^\infty)$  and  $|T^\infty + U| = (T^\infty + U)(1 - 2\Gamma^\infty + 2Q)$ , hence

$$|T^\infty| - |T^\infty + U| = -U + 2U\Gamma^\infty - 2(T^\infty + U)Q.$$

Remembering that  $\Gamma^\infty$  is a projector, we see that  $\text{tr}((T^\infty + U)Q) \geq 0$ . Moreover the diagonal coefficients of  $U$  are zero, so  $\text{tr}(U) = 0$ . As a consequence,

$$2\text{tr}(U\Gamma^\infty) \geq \text{tr}(|T^\infty| - |T^\infty + U|)$$

and finally

$$\frac{1}{2}g \sum_{i \in \mathbb{Z}} (u_i + 2t_i^\infty - 2b)u_i + 2\text{tr}(U\Gamma^\infty) \geq \Delta H(\mathbf{u}) \geq 0.$$

But  $\text{tr}(U\Gamma^\infty) = 2 \sum_{i \in \mathbb{Z}} \text{Re}(\Gamma_{i,i+1}^\infty)u_i$ , hence

$$\sum_{i \geq 1} \frac{1}{2}gu_i^2 + (4\text{Re}(\Gamma_{i,i+1}^\infty) + g(t_i^\infty - b))u_i \geq 0.$$

Varying  $\mathbf{u}$ , we conclude that  $4\text{Re}(\Gamma_{i,i+1}^\infty) + g(t_i^\infty - b) = 0 \ (\forall i)$ . This ends the proof of Theorem 1.

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