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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, $(\mathrm{CH})_x$, 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 $(\mathrm{CH})_x$ 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 $(\mathrm{CH})_x$ 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:

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

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

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

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

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

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

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

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

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, $t_i^{\text{dim0}}(2N) = b + (-1)^i\delta_{2N}$ and $t_i^{\text{dim1}}(2N) = b + (-1)^{i+1}\delta_{2N}$, with $\delta_{2N} \to \delta_0$ 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 $N \to \infty$ (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 $T_{\text{dim0}}(2N)$ and $T_{\text{dim1}}(2N)$ 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 $\tau_k : \mathbb{C}^N \to \mathbb{C}^N$ 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 $\mathbf{t}(2N+1) = (t_i(2N+1))_{1\le i\le 2N+1}$ 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*

$$\sum_{i\ge 1} |t_i^\infty - b - (-1)^{i+\tau}\delta_0|^2 = \sum_{i\le 0} |t_i^\infty - b + (-1)^{i+\tau}\delta_0|^2 < \infty\,. \tag{2}$$

*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 $N \to \infty$:*

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

*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*

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

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

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

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

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

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

*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

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

Using this notation we get

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

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

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

Hence,

$$\begin{aligned}
2\mathrm{Tr}_{C^{2N}}(\Gamma_{\mathrm{dim1}}T_{\mathrm{dim1}}) - 2\mathrm{Tr}_{\mathbb{C}^{2N+1}}(\Gamma_{\mathrm{test}}T_{\mathrm{test}}) &= 2\Gamma^{1,0}_{\mathrm{dim1}}T^{0,1}_{\mathrm{dim1}} + 2\Gamma^{0,1}_{\mathrm{dim1}}T^{1,0}_{\mathrm{dim1}} \\
&= 4\Re(\Gamma^{1,0}_{\mathrm{dim1}})T^{0,1}_{\mathrm{dim1}} \\
[0 \le \Gamma_{\mathrm{dim1}} \le 1 \Rightarrow] \qquad &\le 4T^{0,1}_{\mathrm{dim1}} \\
&= 4(b - \delta_{2N}) \\
&< 4b
\end{aligned}$$

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

$$\frac{g}{2}\sum_{i}^{2N+1}(t_i^{\mathrm{test}} - b)^2 - \frac{g}{2}\sum_{i}^{2N+1}(t_i^{\mathrm{dim1}} - b)^2 = 0,$$

which together with the previous estimates implies that

$$H^{(2N+1)}(\mathbf{t}^{\mathrm{test}}) - H^{(2N)}(\mathbf{t}^{\mathrm{dim1}}(2N)) \le 4b \tag{3}$$

Now let $\boldsymbol{\xi} = (\xi_i) \in \mathbb{C}^{2N+1}$. Since $0 \le \Gamma_{\mathrm{dim1}}(2N) \le 1$ we obtain

$$\begin{aligned}
\langle \boldsymbol{\xi}, \Gamma_{\mathrm{test}}(2N+1)\boldsymbol{\xi}\rangle &= \sum_{1\le i,j\le 2N+1} \Gamma^{i,j}_{\mathrm{test}}\xi_i\overline{\xi}_j \\
&= \sum_{1\le i,j\le 2N} \Gamma^{i,j}_{\mathrm{dim1}}(2N)\xi_i\overline{\xi}_j \in \left[0, \sum_{i=1}^{2N}|\xi_j|^2\right] \subset \left[0, \|\boldsymbol{\xi}\|_2^2\right],
\end{aligned}$$

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

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

and by (3) the Lemma is proved. □

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

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

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

$$z = x^2 + \frac{1}{N}\sum s_i s_{i+1} \ge x^2 - \frac{1}{N}\sum s_i^2 = 2x^2 - y^2. \tag{4}$$

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

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

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

*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

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

The function $\phi_N$ is strictly jointly convex in $X, Y$ in the sense that $\mathrm{Hess}(\phi_N) > 0$ 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 $(X_{min}, Y_{min}) = (x^2_{min}(N), y^2_{min}(N)) = (b_N^2, b_N^2 + \delta_N^2)$ 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

$$f_{b,\delta} : [0,\pi] \to \mathbb{R}$$
$$s \mapsto \frac{\cos^2 s}{\sqrt{b^2 \sin^2 s + \delta^2 \cos^2 s}},$$

then the generalized dimerization equation is given by

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

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 $\mathscr{C}^1$ 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

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

Now, the fonction $0 < \delta \mapsto \frac{1}{\pi} \int_0^{\pi} f_{b,\delta}(s) ds$ is of class $\mathscr{C}^1$ 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.

□

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 $\mathbf{t}(2N+1)$:

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

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

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

and that

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

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

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

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

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

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

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

*Proof.* Denoting by $(x^{min}_{2N+1}, y^{min}_{2N+1}, z^{min}_{2N+1}) = (b_{2N+1}, b^2_{2N+1} + \delta^2_{2N+1}, b^2_{2N+1} - \delta^2_{2N+1})$ the unique minimizer of $\psi_{2N+1}$ over $D$ we rewrite estimate (9) in the following way

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

For any $(x,y,z) \in D$ we let $\bar{z} := 2x^2 - y^2 > 0$. Since the function $z \mapsto -\frac{1}{N}\mathrm{Tr}(2y^2 + z\Omega)$ 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 $\bar{z}^{min}_{2N+1} = z^{min}_{2N+1} = b^2_{2N+1} - \delta^2_{2N+1}$ 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 $|z_{2N+1} - z_{\mathrm{dim}}| = O(1/N)$.

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

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

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

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

From the expression

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

we deduce that

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

where

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

and

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

Note that these three quantities are convergent Riemann sums, hence

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

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 $\mathrm{v} = (h,k)^T \in \mathbb{R}^2$ we have that

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

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

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

But we have seen that for large enough $N$, $C_N \ge C_\infty/2$. 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*

$$Tr\left(T^4(2N+1) - \langle T^2(2N+1)\rangle^2\right) \le M$$

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

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

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

$$\|T(2N+1)\|^{-3}\mathrm{Tr}\left[T^4(2N+1) - \langle T^2(2N+1)\rangle^2\right] \le C,$$

but

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

From the equalities (see [4])

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

and

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

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

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

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

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

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

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

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

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

Finally, we have proved

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

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):

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

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 $i \in [I, J]$:*

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

*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 $0 \leq i_N^1 < i_N^2 < \cdots < i_N^p < 2N+1$ , such that:

1. $\lim_{N\to\infty}(i_N^{k+1} - i_N^k) = \infty$ for $1 \le k \le p-1$, $\lim_{N\to\infty}(i_N^1 + 2N + 1 - i_N^p) = \infty$

2. $\rho_{i_N^k}(N) > \gamma$

3. There is a constant $\Delta > 0$ such that, if $dist(i\,,\,\{i_N^1,\cdots,i_N^p\}+(2N+1)\mathbb{Z}) \ge \Delta$, then $\rho_i(N) \le \gamma$.

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

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

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 $\{i \in \mathbb{Z}\,:\,dist(i\,,\,\{i_N^1,\cdots,i_N^p\}+(2N+1)\mathbb{Z}) \ge \Delta\}$ 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 $1 \le k_* \le p$ 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 $\overline{R}_N \to \infty$ and, for all $\epsilon > 0$, an integer $N_\epsilon$ and a radius $\underline{R}_\epsilon > 0$ such that for all $N \ge N_\epsilon$ ,

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

and

$$(\forall N \ge N_\epsilon) \begin{cases} \sum\limits_{-\overline{R}_N < i < -\underline{R}_\epsilon} (t_i(2N+1) - b - (-1)^i\delta_0)^2 < C\epsilon \\ \sum\limits_{\underline{R}_\epsilon < t < \overline{R}_N} (t_i(2N+1) - b - (-1)^{i+1}\delta_0)^2 < C\epsilon \end{cases} \tag{19}$$

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

We also have that

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

which implies the kink property (2) of Theorem 1. Now, the pointwise convergence $[T^2(N)]_{i,j} \to [(T^\infty)^2]_{i,j}$ obviously holds, but the pointwise convergence $|T(N)|_{i,j} \to |T^\infty|_{i,j}$ 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 $A$,

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

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 $i \to i+1$, 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 $Re(m_N(p)) \ge r$ for some positive constant $r$ independent of $N$ and $\omega$. As a consequence, there holds the estimate $|(\omega^2 + m_N(p))^{-1}| \le \frac{1}{r+\omega^2}$ 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

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

As a consequence,

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

Similarly, for $N$ infinite we have

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

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 $\omega \ge \omega_0$ :*

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

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

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

$$(\forall\, i, j \in \mathbb{Z}) \;:\; \big|\big[(\omega^2 + S^2)^{-1}\big]_{i,j}\big| \le \frac{C}{\omega^2}\, e^{-\rho\,|i-j|}\,. \tag{21}$$

*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 $\eta : \mathbb{R} \to [0,1]$ satisfying $\eta(0) = 0$, $\eta(1) = \frac{1}{2}$, $\eta(2) = 1$ and $0 \le \eta'(t) \le 1$ for all $t$.

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

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 $V_i = \big[(\omega^2 + S^2)^{-1}\big]_{i,j}$. Now, for each integer $m \ge 1$ we define the vector $V^m$ of coordinates $V_i^m = \eta_{m,R}(i-j)V_i$. We have $\eta_{m,R}(i-j)\big[(\omega^2 + S^2)V\big]_i = 0$, hence

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

with

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

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

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

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

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

Finally, we get the estimate

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

and for all $m \ge 2$

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

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

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

Assuming $\omega \ge \omega_0$ and choosing $R > 8\,M^2/\omega_0^2$ 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 $N \to \infty$. Then:*

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

*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 $i, j \in \mathbb{Z}$,

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

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 $\sigma_N : (z_i) \to (z_{i-N})$. 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 $N \to \infty$. So, writing

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

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

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 $N \to \infty$. 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

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

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

□

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

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

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 $T^2_{dim}(2N) = 2(b^2+\delta_{2N}^2)\mathbf{1} + (b^2-\delta_{2N}^2)\Omega_{2N}$, with $\delta_{2N} \to \delta_0$ as $N$ goes to infinity. Similarly, for the infinite chain $T^2_{dim} = 2(b^2+\delta_0^2)\mathbf{1} + (b^2-\delta_0^2)\Omega$.

**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 $(s_i^2+s_{i-1}^2-2b^2-2\delta_0^2)^2+2(s_is_{i+1}-b^2+\delta_0^2)^2 \le \kappa\ (\forall i)$, 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, $T^2_{dim}$ 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 $T^2_{dim}$ has operator norm $1/\delta_0^2$. Now, if $\kappa$ is chosen small enough, then the hypothesis on $\mathbf{s}$ implies that $\|S^2 - T^2_{dim}\| \le \delta_0^2/2$, hence the lemma. □

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 $\chi_{[0,\delta_0^2/4]}(T^2_\infty)$ is at most $D$.*

*Proof.* We first treat the case of an infinite chain, which is easier. We consider a normalized eigenvector $V$ of $T^2_\infty$ with eigenvalue $\lambda \le \delta_0^2/4$. 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 $m \ge 1$. We know that there is $\tau \in \{0,1\}$ such that $t_i^\infty - b - (-1)^{i+\tau}\delta_0 \to 0$ as $i \to \infty$. Now, we take a large integer $R_0$ and we define $s_i := b + (-1)^{i+\tau}\delta_0 (\forall i < R_0)$ and $s_i := t_i^\infty\ (\forall i \ge R_0)$. Then, if $R_0$ is chosen large enough,

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

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 $\|(S^2-\lambda)V_i^1\|_2 \le O(1/R)$, $\|(S^2-\lambda)V_i^m\|_2 \le O(1/R)\|V_i^{m-1}\|_2\ (\forall m \ge 2)$. 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 $|V_i| \le C\, e^{-\alpha\, i}$. 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 $|V_i| \le C\, e^{-\alpha|i|}$

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 $0 = i_N^0 < i_N^1 < \cdots < i_N^{p_\epsilon} = N$ such that:

1. $\lim_{N\to\infty}(i_N^{k+1} - i_N^k) = \infty$ 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 $dist(i, \{i_N^k, i_N^{k+1}\}) \geq A_\epsilon$ 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

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

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*

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

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

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

*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:

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

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

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

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.

□

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

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

and finally

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

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 $\mathrm{tr}((T^\infty+U)Q) \geq 0$. Moreover the diagonal coefficients of $U$ are zero, so $\mathrm{tr}(U) = 0$ . As a consequence,

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

and finally

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

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

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

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

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