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# ON THE BOUND STATES OF NON-RELATIVISTIC KRÖNIG-PENNEY HAMILTONIANS WITH SHORT RANGE IMPURITIES

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## Abstract

It is shown that the non-relativistic Krönig-Penney Hamiltonian perturbed by a potential whose integral is different from zero and whose  $1 + \delta$ -moment is finite for some  $\delta > 0$  has at least a bound state in each sufficiently remote gap of its essential spectrum.

The uniqueness of the bound state in each sufficiently remote gap is also shown under the further assumption that the sign of the perturbing potential is constant.

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### 1) Introduction

In a recent paper (1), the present author has shown the existence of bound states of the Schrödinger Hamiltonian for a spinless particle in a Krönig-Penney crystal with an impurity given by an  $L^1(\mathbb{R})$  function whose sign is constant in each remote gap of the essential spectrum.

As is well known, the Krönig-Penney Hamiltonian for a one-dimensional lattice  $\Lambda$  is formally given by

$$H_\alpha = H_0 + \alpha V_{per} = -\frac{1}{2m} \frac{d^2}{dx^2} + \sum_{\lambda \in \Lambda} \alpha \delta(\cdot - \lambda) \quad (1.1)$$

( in units such that  $\frac{\hbar}{2\pi} = 1$  ). In the following we shall assume, without loss of generality, that  $\Lambda = (2\mathbb{Z} + 1)\pi$ .

It follows from the results of the direct integral decomposition theory that in our case the spectrum of the self-adjoint operator formally given by the right-hand side of (1.1) is

$$\left( \bigcup_{k=0}^{\infty} [E_{2k+1}^\alpha(0), E_{2k+1}^\alpha(\pi)] \right) \cup \left( \bigcup_{k=1}^{\infty} [E_{2k}^\alpha(\pi), E_{2k}^\alpha(0)] \right) \quad (1.2)$$

and that the Krönig-Penney Hamiltonian has a purely absolutely continuous spectrum ( see (2) Theor.III.2.3.3 ).

The Krönig-Penney model can be made more realistic by introducing a potential representing various types of impurities which occur in real solids.

The importance of "impurity levels" in solids is due to the fact that such bound states reduce the width of the gap in which they are situated. This feature has important consequences from the point of view of conductivity properties of solids. Furthermore, such impurity levels lead to a selective absorption of certain photon energies which is an important element in the theory of the colour of crystals ( see the introduction in (3)).

In this paper we shall consider impurities given by  $L^1(\mathbb{R})$  functions whose  $1+\delta$ -moment

( for some  $\delta > 0$  ) is finite since we want to give some general results about the number of bound states of  $H_\alpha + \lambda W$  in the gaps of its essential spectrum.

It will be shown that if the  $1 + \delta$ -moment of the potential representing the impurity is finite and the impurity has integral different from zero then there exist bound states in each sufficiently remote gap of the essential spectrum. Furthermore, if the impurity has constant sign it will be shown that there is only one bound state in each sufficiently remote gap of the essential spectrum.

Let us now give a brief description of the content of each section.

In section 2 we compute the Green's function for the Hamiltonian  $H_\alpha$  in the gaps of its spectrum by using well-known properties of second order differential equations with periodic coefficients. The expression of the Green's function of  $H_\alpha$  will be used in section 3 in order to write the Birman-Schwinger kernel  $(\operatorname{sgn} W)|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}$  explicitly for  $E$  belonging to a gap in the essential spectrum of  $H_\alpha + \lambda W$  where  $W$  is a function in  $L^1(\mathbb{R})$  with finite  $1 + \delta$ -moment and with integral different from zero.

We shall basically follow the method used by Zheludev in (4) and (5) in order to show that the Birman-Schwinger kernel diverges on a one-dimensional subspace when  $E$  approaches either endpoint of the gap. This fact will be crucial in the proof of Theorem 3.2. in which the existence of bound states of  $H_\alpha + \lambda W$  in every gap sufficiently far out will be established.

In section 4 we shall be concerned with the number of bound states of  $H_\alpha + \lambda W$  located in the gaps of its essential spectrum when  $W$  has a definite sign. In particular, it will be shown that there is only one bound state in every sufficiently remote gap of the essential spectrum of such an operator. Furthermore, estimates on the number of bound states in each gap of  $\sigma_{ess}(H_\alpha - \lambda W)$ ,  $(\lambda > 0, W \geq 0)$  will be given. Finally, the number of bound



states in the unbounded interval  $(-\infty, E_1^\alpha(0))$  will be estimated and it will be shown that for  $\alpha = 0$  one obtains the bound given in (6).

**2) The Green's function for  $H_\alpha = -\frac{d^2}{dx^2} + \alpha \sum_{m \in \mathbb{Z}} \delta(\cdot - (2m+1)\pi)$  inside the gaps of its essential spectrum.**

In this section we will explicitly determine the form of the Green's function  $G_\alpha(x, y; E)$  for the self-adjoint operator formally given by  $H_\alpha = -\frac{d^2}{dx^2} + \alpha \sum_{m \in \mathbb{Z}} \delta(\cdot - (2m+1)\pi)$ , ( $\alpha \in \mathbb{R}, \alpha \neq 0$ ) for  $E$  belonging to one of the gaps of the spectrum of  $H_\alpha$ .

For simplicity, let us assume  $E \in (E_{2N}^\alpha(0), E_{2N+1}^\alpha(0))$ ,  $N \in \mathbb{N}$  since everything can be carried out similarly when  $E \in (E_{2N-1}^\alpha(\pi), E_{2N}^\alpha(\pi))$ .

In order to find the Green's function for the equation

$$\left[ -\frac{d^2}{dx^2} + \alpha \sum_{m \in \mathbb{Z}} \delta(\cdot - (2m+1)\pi) \right] \phi = E\phi \quad (2.1)$$

with  $E$  belonging to the gap written above, we first notice that the gaps of the first type are characterised by having the discriminant  $D(E)$  greater than 2 at all their points, while those of the other type have  $D(E) < -2$  ( see (2),(7) and (8)).

It follows from the well-known properties of Hill's equation ( see (8)) that our problem is reduced to studying the equation

$$\begin{cases} -\frac{d^2}{dx^2} \phi + \alpha \delta(\cdot - \pi) \phi = E\phi \\ \phi(2\pi) = e^{\pm\theta} \phi(0) \\ \phi'(2\pi) = e^{\pm\theta} \phi'(0) \end{cases} \quad (2.2)$$

$\theta \in [0, 2\pi)$ , in the gaps with  $D(E) > 2$ , while in the gaps with  $D(E) < -2$  the only modification is a minus sign in front of the exponential in the boundary condition in (2.2).

Let us choose  $\phi$  of the form

$$\phi(x) = \begin{cases} A_1^{(\theta)} \cos \sqrt{E}x + B_1^{(\theta)} \sin \sqrt{E}x, & 0 \leq x \leq \pi \\ A_2^{(\theta)} \cos \sqrt{E}(x - 2\pi) + B_2^{(\theta)} \sin \sqrt{E}(x - 2\pi), & \pi \leq x \leq 2\pi \end{cases} \quad (2.3)$$

The boundary conditions on  $\phi$  and its first derivative enable us to write the coefficients  $A_2^{(\theta)}, B_2^{(\theta)}$  as functions of the coefficients  $A_1^{(\theta)}, B_1^{(\theta)}$  respectively and we have

$$\begin{cases} A_2^{(\theta)} = e^{\pm\theta} A_1^{(\theta)} \\ B_2^{(\theta)} = e^{\pm\theta} B_1^{(\theta)} \end{cases} \quad (2.4)$$

Furthermore, by imposing the continuity of the function  $\phi$  at  $x = \pi$  we obtain

$$\phi(\pi) = A_1^{(\theta)} \cos \sqrt{E}\pi + B_1^{(\theta)} \sin \sqrt{E}\pi = A_1^{(\theta)} e^{\pm\theta} \cos \sqrt{E}\pi - B_1^{(\theta)} e^{\pm\theta} \sin \sqrt{E}\pi \quad (2.5)$$

Since

$$\begin{cases} \phi'(\pi_+) = \sqrt{E} [A_1^{(\theta)} e^{\pm\theta} \sin \sqrt{E}\pi + B_1^{(\theta)} e^{\pm\theta} \cos \sqrt{E}\pi] \\ \phi'(\pi_-) = \sqrt{E} [-A_1^{(\theta)} \sin \sqrt{E}\pi + B_1^{(\theta)} \cos \sqrt{E}\pi] \end{cases} \quad (2.6)$$

the  $\delta$ -condition  $\phi'(\pi_+) - \phi'(\pi_-) = \alpha\phi(\pi)$  gives

$$\sqrt{E} [A_1^{(\theta)}(e^{\pm\theta} + 1) \sin \sqrt{E}\pi + B_1^{(\theta)}(e^{\pm\theta} - 1) \cos \sqrt{E}\pi] = \alpha A_1^{(\theta)} \left[ 1 + \frac{e^{\pm\theta} - 1}{e^{\pm\theta} + 1} \right] \cos \sqrt{E}\pi \quad (2.7)$$

which finally leads, by using (2.5), to the equation

$$\cosh \theta = \cos 2\pi\sqrt{E} + \frac{\alpha}{2\sqrt{E}} \sin 2\pi\sqrt{E} \quad (2.8)$$

The right-hand side of (2.8) is exactly  $F_\alpha(E)$  appearing in the well-known Krönig-Penney relation ( for the graph of  $F_\alpha(E)$  see (2) pag.268 ). Since  $F_\alpha(E)$  has a maximum in each gap where  $D(E) > 2$ , i.e.  $(E_{2N}^\alpha(0), E_{2N+1}^\alpha(0))$ ,  $\forall N \in \mathbb{N}$  we can split the interval into two subintervals in order to have  $F_\alpha(E)$  monotone in each of the two subintervals.

Therefore, in each subinterval we can define

$$\theta = \cosh^{-1} \left( \cos 2\pi\sqrt{E} + \frac{\alpha}{2\sqrt{E}} \sin 2\pi\sqrt{E} \right) > 0 \quad (2.9)$$

This implies that for  $E$  belonging to either subinterval we have two independent solutions of (2.2) which can be extended to the whole real axis in order to give the two independent solutions of (2.1), namely

$$\phi_{\pm,E}^{\alpha}(x) = e^{\pm m\theta} \left[ \cos \sqrt{E}(x - 2m\pi) \pm \frac{e^{\theta} - 1}{e^{\theta} + 1} \cot \sqrt{E}\pi \sin \sqrt{E}(x - 2m\pi) \right] = e^{\pm m\theta} p_{\pm}(x, E) \quad (2.10)$$

with  $p_{\pm}(x + 2\pi, E) = p_{\pm}(x, E)$ , for any  $x \in [(2m - 1)\pi, (2m + 1)\pi)$  and any  $m \in \mathbb{Z}$  with  $\theta = \theta(E)$  as defined by (2.9).

We notice that  $\phi_{+,E}^{\alpha} \in L^2(-\infty, 0)$  while  $\phi_{-,E}^{\alpha} \in L^2(0, +\infty)$ . Consequently, the function  $\phi_E^{\alpha}$  defined by

$$\phi_E^{\alpha}(x) = \begin{cases} \phi_{+,E}^{\alpha}(x) & x \leq 0 \\ \phi_{-,E}^{\alpha}(x) & x > 0 \end{cases} \quad (2.11)$$

belongs to  $L^2(\mathbb{R})$ .

In order to determine the expression of the Green's function we must compute the Wronskian related to  $\phi_{+,E}^{\alpha}$  and  $\phi_{-,E}^{\alpha}$ . Due to the form of the equation, the Wronskian is a constant given by

$$\mathcal{W}(E) = \sqrt{E} \cot \sqrt{E}\pi \frac{2 \sinh \theta}{1 + \cosh \theta} \quad (2.12)$$

Thus

$$[\mathcal{W}(E)]^{-1} = \frac{1 + \cosh \theta}{2\sqrt{E} \sinh \theta \cot \sqrt{E}\pi} \quad (2.13)$$

Therefore the Green's function related to (2.1) for  $E$  belonging to either subinterval is given by

$$G_{\alpha}(x, y; E) = \frac{(1 + \cosh \theta) \tan \pi \sqrt{E}}{2\sqrt{E} \sinh \theta} \begin{cases} \phi_{+,E}^{\alpha}(x) \phi_{-,E}^{\alpha}(y) & x \leq y \\ \phi_{-,E}^{\alpha}(x) \phi_{+,E}^{\alpha}(y) & x > y \end{cases} \quad (2.14)$$

with  $\phi_{-,E}^{\alpha}$  and  $\phi_{+,E}^{\alpha}$  defined as above.

After performing some calculations we finally get:

$$G_\alpha(x, y; E) = \frac{1}{2\sqrt{E}} e^{-|m-n|\theta} \left[ (\beta(\theta))^{-1} \tan \sqrt{E}\pi \cos \sqrt{E}(x - 2m\pi) \cos \sqrt{E}(y - 2n\pi) - \right. \\ \left. - \beta(\theta) \cot \sqrt{E}\pi \sin \sqrt{E}(x - 2m\pi) \sin \sqrt{E}(y - 2n\pi) - \sin \sqrt{E}(|x - y| - 2\pi|m - n|) \right] \quad (2.15)$$

for any  $x \in I_m = [(2m - 1)\pi, (2m + 1)\pi]$ ,  $y \in I_n = [(2n - 1)\pi, (2n + 1)\pi]$ ,  $m, n \in \mathbb{Z}$  with

$$\beta(\theta) = \frac{\sinh \theta}{1 + \cosh \theta}$$

It is not difficult to check, by using (2.8) and the relation  $\cosh^2 \theta - \sinh^2 \theta = 1$  that

$$\beta(\theta(E)) \sim \text{const} \cdot |E - E_{2N}^\alpha(0)|^{\frac{1}{2}} \quad (2.16)$$

in a right neighbourhood of  $E_{2N}^\alpha(0)$  and similarly in a left neighbourhood of the other endpoint of the gap  $(E_{2N}^\alpha(0), E_{2N+1}^\alpha(0))$ , where the constant is positive.

If  $\alpha > 0$  then  $E_{2N}^\alpha(0) = N^2$ , while when  $\alpha < 0$  we have  $E_{2N+1}^\alpha(0) = N^2$  (a complete description of  $\sigma(H_\alpha)$  can be found in (2), Chapt.III.2.3.). By using (2.16) and the behaviour of the function  $\cot \sqrt{E}\pi$  near the endpoints of the gap we obtain the following results:

a) if  $\alpha > 0$  then as  $E \rightarrow N^2_+$

$$-\beta(\theta) \cot \sqrt{E}\pi \sim -\frac{\text{const}}{(E - N^2)^{\frac{1}{2}}} \quad (2.17)$$

and as  $E \rightarrow E_{2N+1}^\alpha(0)_-$

$$-\beta(\theta) \cot \sqrt{E}\pi \sim -\text{const} \cdot (E_{2N+1}^\alpha(0) - E)^{\frac{1}{2}} \quad (2.18)$$

b) if  $\alpha < 0$  then as  $E \rightarrow E_{2N}^\alpha(0)_+$

$$-\beta(\theta) \cot \sqrt{E}\pi \sim \text{const} \cdot (E - E_{2N}^\alpha(0))^{\frac{1}{2}} \quad (2.19)$$

and as  $E \rightarrow N_-^2$

$$-\beta(\theta) \cot \sqrt{E}\pi \sim \frac{\text{const}}{(N^2 - E)^{\frac{1}{2}}} \quad (2.20)$$

where the constant is always positive.

We shall use these results in the next section.

### 3) Existence of bound states of $H_\alpha + \lambda W$ in the distant gaps of its essential spectrum.

In this section we will prove the existence of bound states of  $H_\alpha + \lambda W$  in each gap sufficiently far out under the two following assumptions on the potential  $W$  representing the impurity:

$$\int_{\mathbb{R}} (1 + |x|)^{1+\delta} |W(x)| dx < \infty \quad (3.1)$$

for some  $\delta > 0$  ( we shall see that we need the  $\delta$  in order to have only trace-class operators in the following ), and

$$\int_{\mathbb{R}} W(x) dx \neq 0 \quad (3.2)$$

The present author has shown in (1) that the Hamiltonian written above has bound states in each sufficiently remote gap of its spectrum in the case  $\alpha = 1$  assuming that  $W \in L^1(\mathbb{R})$  and has constant sign. The proof is based on the Birman-Schwinger principle, for which we refer to (7) and (9), and the Gelfand expansion for the resolvent of the unperturbed Krönig-Penney Hamiltonian ( the theorem about the existence of such an expansion for N-dimensional Schrödinger Hamiltonians with periodic potentials can also be found in (7)).

In this work we are going to use a different method which exploits the explicit expression of the Green's function  $G_\alpha(x, y; E)$  given by (2.16). This method will enable us to investigate the number of bound states in the gaps of  $\sigma(H_\alpha + \lambda W)$  in section 4.

We want to mention that the case of a Hamiltonian with a piecewise continuous periodic potential in place of the Krönig-Penney one and with an impurity  $W$  whose integral is zero has been investigated by Firsova in (10) under the further assumptions that  $W$  is reflectionless and its second moment is finite showing that in such a case there are no eigenvalues in the remote gaps of the spectrum.

Furthermore, Deift and Hempel in (3) have given results about the existence of bound states of  $H - \lambda|W|$  in the gaps of  $\sigma(H)$ ,  $H = -\frac{d^2}{dx^2} + V$  where  $V$  is not assumed to be periodic but has some "short range order", which produces gaps in  $\sigma(H)$ .

We briefly recall here that if  $W \in L^1(\mathbb{R})$  then  $H_\alpha + \lambda W$  is the self-adjoint operator defined by means of the KLMN theorem and its essential spectrum is exactly the absolutely continuous spectrum of  $H_\alpha$  since  $\lambda W$  is a compact perturbation in the sense of quadratic forms ( see (7)XIII.4 Corollary 4).

In the following we shall only consider the case  $\alpha < 0$  corresponding to the physical situation of a spinless particle of negative charge in a Krönig-Penney crystal of positive ions. Furthermore, we shall only analyse the behaviour of the Birman-Schwinger kernel in the gaps of the type  $(E_{2N}^\alpha(0), N^2)$  since everything can be carried out similarly in the case of the gaps of the other type.

By using (2.15) the Birman-Schwinger kernel can be written as follows

$$\lambda(\operatorname{sgn} W)|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}} = \lambda \sum_{l=1}^5 T_\alpha^{(l)}(E) \quad (3.3)$$

where the operators  $\{T_\alpha^{(l)}(E)\}_{l=1}^5$  are defined by means of their integral kernels for any  $x \in I_m, y \in I_n, m, n \in \mathbb{Z}$  as follows:

$$T_\alpha^{(1)}(x, y; E) = \frac{1}{2\sqrt{E}}(\beta(\theta))^{-1} \tan \sqrt{E}\pi (\operatorname{sgn} W)|W|^{\frac{1}{2}}(x) \phi_\alpha^{(1)}(x; E)|W|^{\frac{1}{2}}(y) \phi_\alpha^{(1)}(y; E) \quad (3.4)$$

with

$$\phi_{\alpha}^{(1)}(x, E) = e^{-|m|\theta} \cos \sqrt{E}(x - 2m\pi), \quad (3.5)$$

$$T_{\alpha}^{(2)}(x, y; E) = -\frac{1}{2\sqrt{E}}\beta(\theta) \cot \sqrt{E}\pi (\operatorname{sgn} W)|W|^{\frac{1}{2}}(x) \phi_{\alpha}^{(2)}(x; E)|W|^{\frac{1}{2}}(y) \phi_{\alpha}^{(2)}(y; E) \quad (3.6)$$

with

$$\phi_{\alpha}^{(2)}(x; E) = e^{-|m|\theta} \sin \sqrt{E}(x - 2m\pi), \quad (3.7)$$

$$T_{\alpha}^{(3)}(x, y; E) = \frac{1}{2\sqrt{E}}(\beta(\theta))^{-1} \tan \sqrt{E}\pi \left[ e^{-|m-n|\theta} - e^{-(|m|+|n|)\theta} \right] \cdot (\operatorname{sgn} W)|W|^{\frac{1}{2}}(x) \cos \sqrt{E}(x - 2m\pi)|W|^{\frac{1}{2}}(y) \cos \sqrt{E}(y - 2n\pi) \quad (3.8)$$

$$T_{\alpha}^{(4)}(x, y; E) = -\frac{1}{2\sqrt{E}}\beta(\theta) \cot \sqrt{E}\pi \left[ e^{-|m-n|\theta} - e^{-(|m|+|n|)\theta} \right] \cdot (\operatorname{sgn} W)|W|^{\frac{1}{2}}(x) \sin \sqrt{E}(x - 2m\pi)|W|^{\frac{1}{2}}(y) \sin \sqrt{E}(y - 2n\pi) \quad (3.9)$$

$$T_{\alpha}^{(5)}(x, y; E) = -\frac{1}{2\sqrt{E}} e^{-|m-n|\theta} (\operatorname{sgn} W)|W|^{\frac{1}{2}}(x) \sin \sqrt{E}(|x - y| - 2\pi|m - n|)|W|^{\frac{1}{2}}(y) \quad (3.10)$$

It is easy to check that the functions  $\phi_{\alpha}^{(1)}$  and  $\phi_{\alpha}^{(2)}$  belong to  $L^2(\mathbb{R}) \cap L^{\infty}(\mathbb{R})$  so that  $T_{\alpha}^{(1)}(E)$  and  $T_{\alpha}^{(2)}(E)$  are rank-one operators.

As follows from (2.19) the nonzero eigenvalue of  $T_{\alpha}^{(1)}(E)$  diverges as  $E \rightarrow E_{2N}^{\alpha}(0)_{+}$  and vanishes at  $E = N^2$  while from (2.20) we infer that the nonzero eigenvalue of  $T_{\alpha}^{(2)}(E)$  diverges as  $E \rightarrow N_{-}^2$  and vanishes at  $E = E_{2N}^{\alpha}(0)$ .

Furthermore, the operators  $T_{\alpha}^{(l)}(E), l = 3, 4, 5$  are trace-class for any  $E \in [E_{2N}^{\alpha}(0), N^2]$  for any  $N \in \mathbb{N}$  and are  $\|\cdot\|_{\mathcal{J}_1}$ -continuous functions of  $E$  on each closed interval written above as the following theorem shows.

**THEOREM 3.1.** *Let  $W$  be a real-valued function satisfying (3.1) and let  $T_\alpha^{(l)}(E), l = 3, 4, 5$  be the operator-valued functions defined as above. Then  $T_\alpha^{(3)}(E)$  and  $T_\alpha^{(4)}(E)$  have removable singularities at both endpoints of  $[E_{2N}^\alpha(0), N^2], \forall N \in \mathbb{N}$  and can be made  $\|\cdot\|_{\mathcal{J}_1}$ -continuous on every closed interval  $[E_{2N}^\alpha(0), N^2]$  by defining*

$$T_\alpha^{(3)}(E_{2N}^\alpha(0)) = \|\cdot\|_{\mathcal{J}_1} - \lim_{E \rightarrow E_{2N}^\alpha(0)^+} T_\alpha^{(3)}(E) = \frac{\tan \sqrt{E_{2N}^\alpha(0)}\pi}{\sqrt{E_{2N}^\alpha(0)}} R(E_{2N}^\alpha(0)) \quad (3.11)$$

$$T_\alpha^{(3)}(N^2) = \|\cdot\|_{\mathcal{J}_1} - \lim_{E \rightarrow N^2} T_\alpha^{(3)}(E) = 0 \quad (3.12)$$

where  $R(E_{2N}^\alpha(0))$  is the trace-class operator with integral kernel given by

$$R(x, y; E_{2N}^\alpha(0)) = (\operatorname{sgn} W) |W|^{\frac{1}{2}}(x) \cos \sqrt{E_{2N}^\alpha(0)}(x - 2m\pi) [|m| + |n| - |m - n|] \cdot \\ \cdot |W|^{\frac{1}{2}}(y) \cos \sqrt{E_{2N}^\alpha(0)}(y - 2n\pi) \quad (3.13)$$

for any  $x \in I_m, y \in I_n, \forall m, n \in \mathbb{Z}$  and

$$T_\alpha^{(4)}(E_{2N}^\alpha(0)) = \|\cdot\|_{\mathcal{J}_1} - \lim_{E \rightarrow E_{2N}^\alpha(0)^+} T_\alpha^{(4)}(E) = 0, \quad (3.14)$$

$$T_\alpha^{(4)}(N^2) = \|\cdot\|_{\mathcal{J}_1} - \lim_{E \rightarrow N^2} T_\alpha^{(4)}(E) = \frac{|\alpha|}{2N^2} S(N^2) \quad (3.15)$$

where  $S(N^2)$  is the trace-class operator whose integral kernel on  $I_m \times I_n, \forall m, n \in \mathbb{Z}$  is given by

$$S(x, y; N^2) = (\operatorname{sgn} W) |W|^{\frac{1}{2}}(x) \sin Nx [|m| + |n| - |m - n|] |W|^{\frac{1}{2}}(y) \sin Ny \quad (3.16)$$

$T_\alpha^{(5)}(E)$  is  $\|\cdot\|_{\mathcal{J}_1}$ -continuous on  $[E_{2N}^\alpha(0), N^2], \forall N \in \mathbb{N}$ .

**PROOF:** It is not difficult to check that the operators  $T_\alpha^{(l)}(E), l = 3, 4, 5$  are Hilbert-Schmidt for any  $E \in (E_{2N}^\alpha(0), N^2), \forall N \in \mathbb{N}$  and that they are  $\mathcal{J}_2$ -continuous functions in each gap we are considering. Let us first show that (3.11) holds with respect to the Hilbert-Schmidt norm.



Since  $\theta \rightarrow 0_+$  as  $E$  approaches either endpoint of  $(E_{2N}^\alpha(0), N^2)$ ,  $\forall N \in \mathbb{N}$  we have

$$\frac{e^{-|m-n|\theta} - e^{-(|m|+|n|)\theta}}{\sinh \theta} \leq |m| + |n| - |m - n| \quad (3.17)$$

and

$$\lim_{\theta \rightarrow 0_+} \frac{e^{-|m-n|\theta} - e^{-(|m|+|n|)\theta}}{\sinh \theta} = |m| + |n| - |m - n| \quad (3.18)$$

Thus we have

$$\begin{aligned} & \left| (\operatorname{sgn} W) |W|^{\frac{1}{2}}(x) \cos \sqrt{E}(x - 2m\pi) \frac{e^{-|m-n|\theta} - e^{-(|m|+|n|)\theta}}{\sinh \theta} \right. \\ & \left. \cdot |W|^{\frac{1}{2}}(y) \cos \sqrt{E}(y - 2n\pi) \right| \leq |W|^{\frac{1}{2}}(x) [|m| + |n| - |m - n|] |W|^{\frac{1}{2}}(y) \end{aligned} \quad (3.19)$$

for any  $E$  in a right neighbourhood of  $E_{2N}^\alpha(0)$  or in a left neighbourhood of  $N^2$ .

The right-hand side of (3.19) belongs to  $L^2(\mathbb{R} \times \mathbb{R})$  since

$$\begin{aligned} & \sum_{m,n \in \mathbb{Z}} \iint_{I_m \times I_n} |W(x)| [|m| + |n| - |m - n|]^2 |W(y)| \, dx dy \leq \\ & \leq 4 \sum_{m,n \in \mathbb{Z}} \iint_{I_m \times I_n} |W(x)| [\min\{|m|, |n|\}]^2 |W(y)| \, dx dy \leq \\ & \leq 4 \sum_{m,n \in \mathbb{Z}} \iint_{I_m \times I_n} |W(x)| |m| |n| |W(y)| \, dx dy \leq \\ & \leq \frac{4}{\pi^2} \sum_{m,n \in \mathbb{Z}} \iint_{I_m \times I_n} |W(x)| |x| |y| |W(y)| \, dx dy = \frac{4}{\pi^2} \|xW\|_1^2 \end{aligned} \quad (3.20)$$

Therefore, by means of the dominated convergence theorem we get

$$\lim_{E \rightarrow E_{2N}^\alpha(0)_+} \left\| T_\alpha^{(3)}(\cdot, \cdot; E) - \frac{\tan \sqrt{E_{2N}^\alpha(0)} \pi}{\sqrt{E_{2N}^\alpha(0)}} R(\cdot, \cdot; E_{2N}^\alpha(0)) \right\|_{L^2(\mathbb{R} \times \mathbb{R})} = 0 \quad (3.21)$$

which implies that

$$\lim_{E \rightarrow E_{2N}^\alpha(0)_+} \left\| T_\alpha^{(3)}(E) - \frac{\tan \sqrt{E_{2N}^\alpha(0)} \pi}{\sqrt{E_{2N}^\alpha(0)}} R(E_{2N}^\alpha(0)) \right\|_{\mathcal{J}_2} = 0 \quad (3.22)$$

and similarly

$$\lim_{E \rightarrow N_-^2} \|T_\alpha^{(3)}(E)\|_{\mathcal{J}_2} = 0 \quad (3.23)$$

Let us show that  $T_\alpha^{(3)}(E)$  is trace-class for any  $E \in (E_{2N}^\alpha(0), N^2)$ ,  $\forall N \in \mathbb{N}$ .

First of all, we notice that the trace-class norm of  $T_\alpha^{(3)}(E)$  is equal to that of the self-adjoint operator  $(\operatorname{sgn} W)T_\alpha^{(3)}(E)$  which implies

$$\begin{aligned} \|T_\alpha^{(3)}(E)\|_{\mathcal{J}_1} &= \|(\operatorname{sgn} W)T_\alpha^{(3)}(E)\|_{\mathcal{J}_1} = \operatorname{tr} \left( [(\operatorname{sgn} W)T_\alpha^{(3)}(E)]_+ \right) + \operatorname{tr} \left( [(\operatorname{sgn} W)T_\alpha^{(3)}(E)]_- \right) = \\ &= 2 \operatorname{tr} \left( [(\operatorname{sgn} W)T_\alpha^{(3)}(E)]_+ \right) + \operatorname{tr} \left( [(\operatorname{sgn} W)T_\alpha^{(3)}(E)]_- - [(\operatorname{sgn} W)T_\alpha^{(3)}(E)]_+ \right) = \\ &= 2 \operatorname{tr} \left( [(\operatorname{sgn} W)T_\alpha^{(3)}(E)]_+ \right) - \operatorname{tr} \left( (\operatorname{sgn} W)T_\alpha^{(3)}(E) \right) \end{aligned} \quad (3.24)$$

At this point we are going to show that the operator

$$\sum_{m,n} e^{-|m-n|\theta} |W|^{\frac{1}{2}} \chi_m \cos \sqrt{E}(\cdot - 2m\pi) \left( \cos \sqrt{E}(\cdot - 2n\pi) |W|^{\frac{1}{2}} \chi_n \right),$$

$\chi_m$  being the characteristic function of  $I_m$ , is a positive trace-class operator for any  $\theta > 0$ .

First of all, let us set

$$\int_{I_m} f(x) |W(x)|^{\frac{1}{2}} \cos \sqrt{E}(x - 2m\pi) dx = C_m \quad (3.25)$$

where  $f$  is a generic  $L^2(\mathbb{R})$ -function.

The sequence  $\{C_m\}_{m \in \mathbb{Z}}$  belongs to  $l_1(\mathbb{Z})$  since

$$\begin{aligned} \sum_{m \in \mathbb{Z}} \left| \int_{I_m} f(x) |W(x)|^{\frac{1}{2}} \cos \sqrt{E}(x - 2m\pi) dx \right| &\leq \sum_{m \in \mathbb{Z}} \int_{I_m} |f(x)| |W(x)|^{\frac{1}{2}} dx = \\ &= \int_{\mathbb{R}} |f(x)| |W(x)|^{\frac{1}{2}} dx \leq \|f\|_2 \|W\|_1^{\frac{1}{2}} \end{aligned} \quad (3.26)$$

Thus, for any  $\theta > 0$  we have

$$\begin{aligned} \sum_{m,n \in \mathbb{Z}} \iint_{I_m \times I_n} \overline{f(x)} |W(x)|^{\frac{1}{2}} \cos \sqrt{E}(x - 2m\pi) e^{-|m-n|\theta} |W(y)|^{\frac{1}{2}} \cos \sqrt{E}(y - 2n\pi) f(y) dx dy = \\ \sum_{m,n \in \mathbb{Z}} \bar{C}_m e^{-|m-n|\theta} C_n = \left( \{C_m\}, \{e^{-|m|\theta}\} * C_m \right)_{l_2(\mathbb{Z})} = \end{aligned}$$

$$\begin{aligned}
&= (2\pi)^{\frac{1}{2}} \left( \mathcal{F}^{-1}\{C_m\}, \mathcal{F}^{-1}\{e^{-|m|\theta}\} \mathcal{F}^{-1}\{C_m\} \right)_{L^2(-\pi, \pi)} = \\
&= \int_{-\pi}^{\pi} \frac{e^{2\theta} - 1}{e^{2\theta} - 2e^{\theta} \cos p + 1} |\mathcal{F}^{-1}\{C_m\}(p)|^2 dp \geq 0
\end{aligned} \tag{3.27}$$

The finiteness of the trace-class norm is guaranteed by condition (3.1) as follows from an estimate completely analogous to the one we shall use in section 4 for the estimate of the trace-class norm of  $T_{\alpha}^{(5)}(N^2)$ .

Since the operator is positive its trace-class norm is given by its trace which is simply equal to the sum of the traces of the rank-one summands on the diagonal due to the fact that the off-diagonal summands are nilpotent rank-one operators.

Since  $\beta(\theta) > 0$  for any  $\theta > 0$  and  $\tan \pi \sqrt{E}$  is negative in every gap of the type  $(E_{2N}^{\alpha}(0), N^2)$  we see that the operator  $(\operatorname{sgn} W)T_{\alpha}^{(3)}(E)$  is the sum of a positive rank-one operator and a negative trace-class operator for any  $E$  in such gaps and consequently its spectrum has infinitely many negative eigenvalues clustering at 0 and may have an additional positive eigenvalue. Therefore we obtain that the second summand in (3.24) is equal to

$$-\frac{(1 + \cosh \theta) \tan \sqrt{E} \pi}{2\sqrt{E}} \sum_{m \in \mathbb{Z}} \int_{I_m} |W(x)| \frac{1 - e^{-2|m|\theta}}{\sinh \theta} \cos^2 \sqrt{E}(x - 2m\pi) dx \tag{3.28}$$

Since

$$\begin{aligned}
&-\frac{(1 + \cosh \theta) \tan \sqrt{E} \pi}{2\sqrt{E}} \frac{1 - e^{-2|m|\theta}}{\sinh \theta} \int_{I_m} |W(x)| \cos^2 \sqrt{E}(x - 2m\pi) dx \leq \\
&\quad -\frac{C_1 \tan \sqrt{E_{2N}^{\alpha}(0)} \pi}{\sqrt{E_{2N}^{\alpha}(0)}} |m| \int_{I_m} |W(x)| dx
\end{aligned} \tag{3.29}$$

for any  $E$  in a right neighbourhood of  $E_{2N}^{\alpha}(0)$  (where  $C_1$  is an upper bound for  $(1 + \cosh \theta)$  in that neighbourhood) and the sequence on the right-hand side of (3.29) belongs to  $l^1(\mathbb{Z})$ , due to the finiteness of the first moment of  $W$ , it follows from the dominated convergence theorem that the second summand in (3.24) is a continuous function of  $E$  in any open right neighbourhood of the left endpoint of the gap being considered with a removable singularity

at  $E = E_{2N}^\alpha(0)$  since

$$\lim_{E \rightarrow E_{2N}^\alpha(0)+} \left( (\operatorname{sgn} W) T_\alpha^{(3)}(E) \right) = - \frac{2 \tan \sqrt{E_{2N}^\alpha(0)} \pi}{\sqrt{E_{2N}^\alpha(0)}} \sum_{m \in \mathbb{Z}} \int_{I_m} |m| |W(x)| dx \quad (3.30)$$

Therefore the second summand on the right-hand side of (3.24) can be made continuous as a function of  $E$  in any closed right neighbourhood of  $E_{2N}^\alpha(0)$ ,  $\forall N \in \mathbb{N}$ .

Furthermore, since we have already shown the continuity of the operator-valued function  $T_\alpha^{(3)}(E)$  in any closed right neighbourhood of  $E_{2N}^\alpha(0)$  with respect to the  $\mathcal{J}_2$ -norm it follows that each eigenvalue of  $(\operatorname{sgn} W) T_\alpha^{(3)}(E)$  is a continuous function of  $E$  converging to the respective eigenvalue of the limit operator at  $E = E_{2N}^\alpha(0)$ . In particular, the possible positive eigenvalue  $\lambda_{\alpha,+}^{(3)}(E)$  is continuous as a function of  $E$  in any closed right neighbourhood of  $E = E_{2N}^\alpha(0)$  which implies together with the continuity of the second summand of the right-hand side of (3.24) that the trace-class norm of  $T_\alpha^{(3)}(E)$  is a continuous function of  $E$  in any closed right neighbourhood of  $E_{2N}^\alpha(0)$ .

This fact and the  $\mathcal{J}_2$ -continuity of  $T_\alpha^{(3)}(E)$  in any closed right neighbourhood of  $E_{2N}^\alpha(0)$  imply by means of Grümmer's convergence theorem ( see (11)) that  $T_\alpha^{(3)}(E)$  is  $\mathcal{J}_1$ -continuous in any open right neighbourhood of  $E_{2N}^\alpha(0)$ .

Furthermore, the limit operator with respect to the  $\mathcal{J}_2$ -norm topology is trace-class since

$$\sup_{E \in (E_{2N}^\alpha(0), \tilde{E})} \|T_\alpha^{(3)}(E)\|_{\mathcal{J}_1} < \infty$$

( see (7) and (12)). Thus, in order to apply Grümmer's theorem again and obtain the  $\mathcal{J}_1$ -continuity of  $T_\alpha^{(3)}(E)$  at  $E_{2N}^\alpha(0)_+$  we need only show that

$$\lim_{E \rightarrow E_{2N}^\alpha(0)+} \|T_\alpha^{(3)}(E)\|_{\mathcal{J}_1} = - \frac{\tan \sqrt{E_{2N}^\alpha(0)} \pi}{\sqrt{E_{2N}^\alpha(0)}} \|R(E_{2N}^\alpha(0))\|_{\mathcal{J}_1} \quad (3.31)$$

First of all, we claim that  $(\operatorname{sgn} W) R(E_{2N}^\alpha(0))$  is a positive operator.

This can be seen by noticing that  $|m| + |n| - |m - n|$  is equal to zero if  $m$  and  $n$  have different sign and equal to  $2 \min\{|m|, |n|\}$  if their sign is the same. By setting

$$\int_{I_m} f(x) |W(x)|^{\frac{1}{2}} \cos \sqrt{E_{2N}^\alpha(0)}(x - 2m\pi) dx = \gamma_m \quad (3.32)$$

for any  $f \in L^2(\mathbb{R})$  we have

$$\begin{aligned} (f, (\operatorname{sgn} W) R(E_{2N}^\alpha(0)) f) &= \sum_{m, n \in \mathbb{Z}} \bar{\gamma}_m [|m| + |n| - |m - n|] \gamma_n = \\ &2 \sum_{m, n > 0} \bar{\gamma}_m [\min\{m, n\}] \gamma_n \geq 0 \end{aligned} \quad (3.33)$$

The last inequality is due to

$$\sum_{m, n=0}^N \min\{m, n\} \bar{\gamma}_m \gamma_n = \sum_{n=0}^N \left| \sum_{j \geq n} \gamma_j \right|^2 \geq 0 \quad (3.34)$$

(the kernel  $\min\{m, n\}$  has been investigated in the context of the theory of Brownian motion, see (13) for example ).

Thus, the possible positive eigenvalue of  $(\operatorname{sgn} W) T_\alpha^{(3)}(E)$  converges to zero as  $E \rightarrow E_{2N}^\alpha(0)$  and the trace-class norm of the limit operator is given by the sum of the traces of the positive rank-one operators on the diagonal since the off-diagonal summands are nilpotent rank-one operators. Therefore, the trace-class norm of the limit is exactly given by the right-hand side of (3.30) and consequently we are allowed to use Gr\"umm's theorem to get (3.11).

The same argument can be repeated at the right endpoint of the gap in order to get (3.12).

By rewriting the integral kernel of  $(\operatorname{sgn} W) T_\alpha^{(4)}(E)$  as

$$\begin{aligned} &-\frac{\sinh \theta \beta(\theta) \cot \sqrt{E} \pi}{2\sqrt{E}} |W(x)|^{\frac{1}{2}} \sin \sqrt{E}(x - 2m\pi) \frac{e^{-|m-n|\theta} - e^{-(|m|+|n|)\theta}}{\sinh \theta} \\ &\cdot |W(y)|^{\frac{1}{2}} \sin \sqrt{E}(y - 2n\pi) \end{aligned} \quad (3.35)$$

and noticing that

$$\lim_{E \rightarrow E_{2N}^\alpha(0)+} \frac{-\sinh^2 \theta \cot \sqrt{E} \pi}{2(1 + \cosh \theta) \sqrt{E}} = 0 \quad (3.36)$$

and

$$\begin{aligned} & \lim_{E \rightarrow N_-^2} -\frac{\sinh^2 \theta \cot \sqrt{E} \pi}{2(1 + \cosh \theta) \sqrt{E}} = \\ & \lim_{E \rightarrow N_-^2} \frac{\left[ \left(1 - \frac{\alpha^2}{4E}\right) \sin 2\sqrt{E} \pi - \frac{\alpha}{\sqrt{E}} \cos 2\sqrt{E} \pi \right] \cos^2 \pi \sqrt{E}}{(1 + \cosh \theta) \sqrt{E}} = \frac{|\alpha|}{2N^2} \end{aligned} \quad (3.37)$$

we obtain (3.14) and (3.15) by using the previous method since the spectrum of the operator  $(\operatorname{sgn} W)T_\alpha^{(4)}(E)$  contains infinitely many positive eigenvalues clustering at 0 and only one possible negative eigenvalue.

From the expression of the integral kernel of  $T_\alpha^{(5)}(E)$  we easily get that  $T_\alpha^{(5)}(E)$  is Hilbert-Schmidt for any  $E \in [E_{2N}^\alpha(0), N^2]$ ,  $\forall N \in \mathbb{N}$  and is  $\mathcal{J}_2$ -continuous on those intervals as a  $\mathcal{J}_2$ -valued function of  $E$ .

It follows from (11) Prop.5.6. ( whose proof is substantially based on the method we are going to use in the next section in order to estimate the trace-class norm of  $T_\alpha^{(5)}(N^2)$ ) that  $T_\alpha^{(5)}(E)$  is trace-class for any  $E \in [E_{2N}^\alpha(0), N^2]$ ,  $\forall N \in \mathbb{N}$  if  $W$  satisfies assumption (3.1) since

$$T_\alpha^{(5)}(E) = \sum_{m \neq n} T_\alpha^{(5)}(E) |_{I_m \times I_n} + \sum_{m \in \mathbb{Z}} T_\alpha^{(5)}(E) |_{I_m \times I_m} \quad (3.38)$$

and there is a constant  $C$  independent of  $E$  such that

$$\left\| T_\alpha^{(5)}(E) |_{I_m \times I_n} \right\|_{\mathcal{J}_1} \leq C \left( \int_{I_m} |W(x)| dx \right)^{\frac{1}{2}} \left( \int_{I_n} |W(x)| dx \right)^{\frac{1}{2}} \quad (3.39)$$

for any  $m, n \in \mathbb{Z}$  and the sequence on the right-hand side of (3.39) is summable as long as  $W$  satisfies (3.1).

Furthermore, the off-diagonal restrictions of  $T_\alpha^{(5)}(E)$  are rank-two operators and therefore their  $\mathcal{J}_2$ -continuity as functions of  $E$  implies their  $\mathcal{J}_1$ -continuity. As a consequence of

the method we shall use in the proof of Proposition 4.2., the restrictions on the diagonal, namely  $T_\alpha^{(5)}(E)|_{I_m \times I_m}$  are also  $\mathcal{J}_1$ -continuous since they can be written as the product of two Hilbert-Schmidt operators which are both  $\mathcal{J}_2$ -continuous as functions of  $E$ , i.e.

$$T_\alpha^{(5)}(E)|_{I_m \times I_m} = \left[ |W|^{\frac{1}{2}} \chi_m \left( -i \frac{d}{dx} - i\sqrt{E} \right)^{-1} \right] \cdot K_{\alpha,m}(E) \quad (3.40)$$

The  $\mathcal{J}_1$ -continuity of the restrictions together with (3.39) imply the  $\mathcal{J}_1$ -continuity of  $T_\alpha^{(5)}(E)$  on  $[E_{2N}^\alpha(0), N^2]$ ,  $\forall N \in \mathbb{N}$ . ■

As a consequence of Theorem 3.1. we have

$$\lim_{N \rightarrow \infty} \max_{E_N \in [E_{2N}^\alpha(0), N^2]} \|T_\alpha^{(l)}(E_N)\|_{\mathcal{J}_1} = 0 \quad (3.41)$$

for  $l = 3, 4, 5$ .

We briefly recall here that according to the Birman-Schwinger principle the eigenvalues of  $H_\alpha + \lambda W$  are given by those  $E \in \rho(H_\alpha) \cap \mathbb{R}$  for which there exists a nonzero  $\psi \in L^2(\mathbb{R})$  satisfying the following equation

$$\lambda(\operatorname{sgn} W)|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}\psi = -\psi \quad (3.42)$$

which is equivalent to saying that the eigenvalues are those  $E$ 's in the gaps ( including the unbounded gap on the left of the lowest band ) for which

$$\left( I + \lambda(\operatorname{sgn} W)|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}} \right)^{-1}$$

does not exist as a bounded operator on  $L^2(\mathbb{R})$ .

Therefore, since  $(\operatorname{sgn} W)|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}$  is trace-class  $\forall E \in (E_{2N}^\alpha(0), N^2)$ ,  $\forall N \in \mathbb{N}$  ( and in all the gaps of the other type ), the eigenvalues of  $H_\alpha + \lambda W$  are given by those  $E$ 's inside each gap of  $\sigma_{ess}(H_\alpha + \lambda W) = \sigma(H_\alpha)$  for which the following equation is satisfied

$$\det \left( I + \lambda(\operatorname{sgn} W)|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}} \right) = 0 \quad (3.43)$$

At this point we are able to prove the main theorem of this section concerning the existence of bound states of  $H_\alpha + \lambda W$  in every remote gap of its essential spectrum under the assumptions (3.1) and (3.2) on  $W$ .

**THEOREM 3.2.** *If  $W$  satisfies (3.1) and (3.2) then there exists a band of  $\sigma_{ess}(H_\alpha + \lambda W) = \sigma(H_\alpha)$  such that  $H_\alpha + \lambda W$  has at least an eigenvalue in each gap on the right of that band.*

**PROOF:** As usual, we will give the proof only for the gaps of the type  $(E_{2N}^\alpha(0), N^2)$  since the proof for those of the other type is completely similar.

First of all, we notice that if  $N$  is sufficiently large the integrals

$$\int_{\mathbb{R}} W(x) dx, \int_{\mathbb{R}} W(x) [\phi_\alpha^{(1)}(x; E_N)]^2 dx, \int_{\mathbb{R}} W(x) [\phi_\alpha^{(2)}(x; E_N)]^2 dx$$

have the same sign for any  $E_N \in (E_{2N}^\alpha(0), N^2)$ ,  $\forall N \in \mathbb{N}$  as follows by using the explicit expressions of the functions  $\phi_\alpha^{(l)}(\cdot; E)$ ,  $l = 1, 2$  given in (3.5), (3.7), the identities  $\cos^2 x = \frac{1}{2}(1 + \cos 2x)$ ,  $\sin^2 x = \frac{1}{2}(1 - \cos 2x)$  and the Riemann-Lebesgue lemma in order to show that

$$\lim_{N \rightarrow \infty} \sum_{m \in \mathbb{Z}} \int_{I_m} W(x) e^{-2|m|\theta(E_N)} \cos \sqrt{E_N}(x - 2m\pi) dx = 0 \quad (3.44)$$

Furthermore, due to (3.41) the operator  $\left(I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N)\right)$  is invertible for  $N$  sufficiently large so that

$$\det \left( I + \lambda (\operatorname{sgn} W) |W|^{\frac{1}{2}} (H_\alpha - E_N)^{-1} |W|^{\frac{1}{2}} \right) = \det \left( I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right) \cdot \det \left( I + \lambda \sum_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) \quad (3.45)$$

and consequently if  $N$  is sufficiently large equation (3.43) is equivalent to

$$\det \left( I + \lambda \sum_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) = 0 \quad (3.46)$$



Since the second summand inside the determinant in (3.46) is a rank-two operator with eigenvalues  $\lambda \mu_\alpha^{(l)}(E_N)$ ,  $l = 1, 2$  we can write the determinant as follows

$$\begin{aligned} \det \left( I + \lambda \sum_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) &= [1 + \lambda \mu_\alpha^{(1)}(E_N)] [1 + \lambda \mu_\alpha^{(2)}(E_N)] = \\ &= 1 + \lambda \operatorname{tr} \left( \sum_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) + \lambda^2 \mu_\alpha^{(1)}(E_N) \mu_\alpha^{(2)}(E_N) \end{aligned} \quad (3.47)$$

If we call  $\lambda \gamma_\alpha^{(l)}(E_N)$ ,  $l = 1, 2$  the nonzero eigenvalue of

$$\lambda T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1}, \quad l = 1, 2$$

by using the linearity of the trace we can rewrite the right-hand side of (3.47) as follows

$$1 + \lambda \sum_{l=1}^2 \gamma_\alpha^{(l)}(E_N) + \lambda^2 \mu_\alpha^{(1)}(E_N) \mu_\alpha^{(2)}(E_N) \quad (3.48)$$

Furthermore, the last summand of (3.48) can be expressed as follows

$$\begin{aligned} \lambda^2 \mu_\alpha^{(1)}(E_N) \mu_\alpha^{(2)}(E_N) &= \frac{\lambda^2}{2} \left[ \operatorname{tr} \left( \sum_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) \right]^2 - \\ &\quad - \frac{\lambda^2}{2} \operatorname{tr} \left[ \left( \sum_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right] \right)^2 \right] = \\ &= \lambda^2 \left\{ \gamma_\alpha^{(1)}(E_N) \gamma_\alpha^{(2)}(E_N) - \operatorname{tr} \left( \prod_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) \right\} \end{aligned} \quad (3.49)$$

where we have exploited the property  $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ ,  $\forall A, B \in \mathcal{J}_1$  ( see (14)).

Let us consider each summand on the right-hand side of (3.49) separately. For the first one we have

$$\begin{aligned} \lambda^2 \gamma_\alpha^{(1)}(E_N) \gamma_\alpha^{(2)}(E_N) &= \\ &= -\frac{\lambda^2}{4E_N} \prod_{l=1}^2 \left( |W|^{\frac{1}{2}} \phi_\alpha^{(l)}(E_N), \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} (\operatorname{sgn} W) |W|^{\frac{1}{2}} \phi_\alpha^{(l)}(E_N) \right) \end{aligned} \quad (3.50)$$

Due to (3.41), for any  $\lambda > 0$  there exists  $\tilde{N}$  such that  $\forall N > \tilde{N}$  we have

$$\max_{E_N \in [E_{2N}^\alpha(0), N^2]} \left\| \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right\|_{\mathcal{J}_1} < \frac{1}{2\lambda} \quad (3.51)$$

and consequently for any  $N > \tilde{N}$  we get

$$\left\| \left( I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right)^{-1} \right\| < 2 \quad (3.52)$$

which implies

$$\left( \sup_{E_N \in (E_{2N}^\alpha(0), N^2)} \left| \gamma_\alpha^{(1)}(E_N) \gamma_\alpha^{(2)}(E_N) \right| \right) \leq \frac{1}{E_{2N}^\alpha(0)} \|W\|_1^2 \rightarrow 0 \quad (3.53)$$

as  $N \rightarrow \infty$ .

Similarly, since

$$\begin{aligned} & \operatorname{tr} \left( \prod_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) = \\ &= -\frac{1}{4E_N} \left( |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_N), \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} (\operatorname{sgn} W) |W|^{\frac{1}{2}} \phi_\alpha^{(2)}(E_N) \right) \\ & \cdot \left( |W|^{\frac{1}{2}} \phi_\alpha^{(2)}(E_N), \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} (\operatorname{sgn} W) |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_N) \right) \end{aligned} \quad (3.54)$$

we obtain

$$\sup_{E_N \in (E_{2N}^\alpha(0), N^2)} \left| \operatorname{tr} \left( \prod_{l=1}^2 T_\alpha^{(l)}(E_N) \left[ I + \lambda \sum_{l=3}^5 T_\alpha^{(l)}(E_N) \right]^{-1} \right) \right| \leq \frac{1}{E_{2N}^\alpha(0)} \|W\|_1^2 \rightarrow 0 \quad (3.55)$$

as  $N \rightarrow \infty$ .

Therefore, the quadratic term in (3.48) is uniformly small for  $E_N \in (E_{2N}^\alpha(0), N^2)$  when  $N$  is sufficiently large.

Since all the quantities involved are real it is clear that the determinant on the left-hand side of (3.46) is a real-valued continuous function of  $E_N$  in each gap  $(E_{2N}^\alpha(0), N^2)$  for any  $N$  sufficiently large.

By using (3.41) it follows that for  $N$  sufficiently large the sign of

$$\left( |W|^{\frac{1}{2}} \phi_{\alpha}^{(l)}(E_N), \left[ I + \lambda \sum_{l=3}^5 T_{\alpha}^{(l)}(E_N) \right]^{-1} (\operatorname{sgn} W) |W|^{\frac{1}{2}} \phi_{\alpha}^{(l)}(E_N) \right), \quad l = 1, 2$$

is equal to the sign of

$$\left( |W|^{\frac{1}{2}} \phi_{\alpha}^{(l)}(E_N), (\operatorname{sgn} W) |W|^{\frac{1}{2}} \phi_{\alpha}^{(l)}(E_N) \right), \quad l = 1, 2$$

whose sign is in both cases equal to the sign of

$$\int_{\mathbb{R}} W(x) dx$$

when  $N$  is sufficiently large as shown at the beginning of the proof.

Thus, provided  $N$  is sufficiently large the right-hand side of (3.47) diverges with opposite signs at the endpoints of each gap  $(E_{2N}^{\alpha}(0), N^2)$ .

Therefore, the Intermediate Value Theorem enables us to conclude that for  $N$  sufficiently large the determinant has at least a zero in each gap of the type being considered which implies the existence of at least a bound state of  $H_{\alpha} + \lambda W$  in each gap  $(E_{2N}^{\alpha}(0), N^2)$  for  $N$  sufficiently large. ■

**4) The number of bound states of  $H_{\alpha} + \lambda W$  in the gaps of its essential spectrum when  $W$  has a definite sign.**

The main goal of this section will be to prove the uniqueness of the bound state of  $H_{\alpha} + \lambda W$  in each sufficiently remote gap of its essential spectrum if  $W$  satisfies (3.1) and has a definite sign.

In order to achieve this we shall estimate the number of bound states of  $H_{\alpha} + \lambda W$  in each gap of its essential spectrum and show that there is only one bound state in each gap on the right of a certain band, precisely the bound state arising from the divergence at the endpoints of each gap of one of the two rank-one operators  $T_{\alpha}^{(l)}(E)$ ,  $l = 1, 2$  of section 3.

In the second part of this section we shall give an estimate on the number of bound states occurring in the unbounded interval  $(-\infty, E_1^\alpha(0))$ .

Before stating and proving Theorem 4.1. we would like to point out that the reason of the uniqueness of the bound state of the Hamiltonian being considered is basically the factor  $\frac{1}{\sqrt{E}}$  in the Green's function which is typical of the non-relativistic one-dimensional case.

At this point we state and prove Theorem 4.1. which constitutes the main result of this section.

**THEOREM 4.1.** *If  $W$  is a function of definite sign satisfying (3.1) then there exists a band of  $\sigma_{ess}(H_\alpha + \lambda W)$ ,  $\lambda > 0$  on the right of which each gap contains exactly one bound state.*

**PROOF:** First of all, we notice that if  $W$  is a function of definite sign the Birman-Schwinger kernel is self-adjoint and (3.42) becomes

$$\lambda |W|^{\frac{1}{2}} (H_\alpha - E)^{-1} |W|^{\frac{1}{2}} \psi = \pm \psi \quad (4.1)$$

with the positive sign on the right-hand side if  $W \leq 0$  and the negative one if  $W \geq 0$ . According to the Birman-Schwinger principle the number of bound states of  $H_\alpha + \lambda W$  inside a gap is equal to the number of  $E$ 's belonging to that gap for which (4.1) is satisfied.

For simplicity, let us only consider the case when  $\alpha$  is negative and the perturbing potential is non-positive, that is to say the Hamiltonian is given by  $H_\alpha - \lambda |W|$ ,  $\alpha < 0$ ,  $\lambda > 0$ . Such a Hamiltonian represents the energy operator for a spinless particle of negative charge in a Krönig-Penney crystal with an attractive impurity.

As usual, we shall give the proof only for the gaps of the type  $(E_{2N}^\alpha(0), N^2)$  since the argument can easily be repeated for the gaps of the other type.

First of all, we know that the nonzero eigenvalues of  $\lambda|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}$  are strictly increasing functions of  $E$  inside each gap ( see (9) Lemma 2.1 ). This implies that for any  $E \in (E_{2N}^\alpha(0), N^2)$  we have

$$\dim_{(E_{2N}^\alpha(0), E)}(H_\alpha - \lambda|W|) = \dim_{(1, \infty)} \left( \lambda|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}} \right) \quad (4.2)$$

As follows from what has been seen in section 3, the operator  $T_\alpha^{(1)}(E) + T_\alpha^{(3)}(E)$  ( $T_\alpha^{(l)}(E)$ ,  $l = 1, 2, 3, 4, 5$  being the operators of section 3 with  $\text{sgn} W = 1$ ) is a negative trace-class operator for any  $E \in (E_{2N}^\alpha(0), N^2)$ . Therefore, we can neglect it in counting the eigenvalues of  $\lambda|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}$  that are greater than one since its presence can only lower the positive eigenvalues of the operator given by the sum of the remaining three operators so that the right-hand side of (4.2) is bounded by

$$\dim_{(1, \infty)} \left( \lambda T_\alpha^{(2)}(E) + \lambda T_\alpha^{(4)}(E) + \lambda T_\alpha^{(5)}(E) \right) \quad (4.3)$$

Furthermore, due to the divergence of the positive rank-one operator  $\lambda T_\alpha^{(2)}(E)$  at the right endpoint of each gap of the type being considered we can repeat the argument of (11) Theorem 7.5. in order to get that (4.3) is bounded by

$$1 + \dim_{(1, \infty)} \left( \lambda T_\alpha^{(4)}(N^2) + \lambda T_\alpha^{(5)}(N^2) \right) \quad (4.4)$$

As shown in section 3,  $T_\alpha^{(4)}(E)$  and  $T_\alpha^{(5)}(E)$  are trace-class  $\forall E \in [E_{2N}^\alpha(0), N^2]$ ,  $\forall N \in \mathbb{N}$  so that the second summand in (4.4) is bounded by

$$\lambda \left( \|T_\alpha^{(4)}(N^2)\|_{\mathcal{J}_1} + \|T_\alpha^{(5)}(N^2)\|_{\mathcal{J}_1} \right) \rightarrow 0 \quad (4.5)$$

as  $N \rightarrow \infty$ , as follows from (3.41). Therefore, if  $N$  is sufficiently large the upper bound for the number of bound states of the Hamiltonian in the gap  $(E_{2N}^\alpha(0), N^2)$  is less than two while the lower bound is equal to one due to Theorem 3.2, which completes the proof in the case of a potential with finite  $1 + \delta$ -moment. ■

**Remark.** In the case  $\delta = 0$ ,  $T_\alpha^{(5)}(N^2)$  is no longer trace-class but is only Hilbert-Schmidt so that we must use the Hilbert-Schmidt norms as a bound for the sum of the positive eigenvalues of  $\lambda \left( T_\alpha^{(4)}(N^2) + T_\alpha^{(5)}(N^2) \right)$  that are greater than one. It is immediate to show that

$$\|T_\alpha^{(5)}(N^2)\|_{\mathcal{J}_2} \rightarrow 0 \quad (4.6)$$

as  $N \rightarrow \infty$  so that the assertion holds also in this case but we must use (1) Theorem 2.2 for the existence of bound states in each sufficiently remote gap of the essential spectrum.

Before considering the number of bound states occurring in the unbounded interval on the left of the essential spectrum of the perturbed Hamiltonian we want to give an explicit upper bound for the number of bound states inside the gap  $(E_{2N}^\alpha(0), N^2)$ ,  $\forall N \in \mathbb{N}$  ( of course, a similar bound can be found for the gaps of the other type ).

**PROPOSITION 4.2.** *If  $\alpha < 0$  and  $W \leq 0$  satisfies (3.1), the following estimate holds*

$$\begin{aligned} \mathcal{N}_{(E_{2N}^\alpha(0), N^2)}(H_\alpha - \lambda|W|) &\leq 1 + \lambda \left[ \frac{|\alpha|}{\pi N^2} \|xW\|_1 + \right. \\ &\left. + \left( \frac{3\pi}{2N} \right)^{\frac{1}{2}} \left( 1 + \sum_{m \neq 0} \frac{1}{[1 + (2|m| - 1)\pi]^{1+\delta}} \right) \left\| (1 + |x|)^{1+\delta} W \right\|_1 \right] \end{aligned} \quad (4.7)$$

where  $\mathcal{N}_{(E_{2N}^\alpha(0), N^2)}(H_\alpha - \lambda|W|)$  is the number of bound states of  $H_\alpha - \lambda|W|$  in the gap  $(E_{2N}^\alpha(0), N^2)$ .

**PROOF:** According to (4.6), we have to estimate the trace-class norms of the operators  $T_\alpha^{(4)}(N^2)$  and  $T_\alpha^{(5)}(N^2)$ .

As follows from what has been shown in the proof of Theorem 3.1.,  $T_\alpha^{(4)}(N^2)$  is positive and

$$\left\| \lambda T_\alpha^{(4)}(N^2) \right\|_{\mathcal{J}_1} = \frac{\lambda|\alpha|}{N^2} \sum_{m \in \mathbb{Z}} \int_{I_m} |m| |W(x)| \sin^2 Nx \, dx \leq \frac{\lambda|\alpha|}{\pi N^2} \|xW\|_1 \quad (4.8)$$

For the trace-class norm of  $\lambda T_\alpha^{(5)}(N^2)$  we have

$$\left\| \lambda T_\alpha^{(5)}(N^2) \right\|_{\mathcal{J}_1} = \lambda \left\| \sum_{m,n} T_\alpha^{(5)}(N^2) |_{I_m \times I_n} \right\|_{\mathcal{J}_1} \leq \lambda \sum_{m,n \in \mathbb{Z}} \left\| T_\alpha^{(5)}(N^2) |_{I_m \times I_n} \right\|_{\mathcal{J}_1} \quad (4.9)$$

where the summands are the restrictions of  $T_\alpha^{(5)}(N^2)$  to the sets  $I_m \times I_n$ .

If  $m \neq n$ ,  $T_\alpha^{(5)}(N^2) |_{I_m \times I_n}$  is a rank-two operator with trace-class norm bounded by

$$\frac{1}{N} \left( \int_{I_m} |W(x)| dx \right)^{\frac{1}{2}} \left( \int_{I_n} |W(x)| dx \right)^{\frac{1}{2}} \quad (4.10)$$

Now we must estimate the trace-class norm of  $T_\alpha^{(5)}(N^2) |_{I_m \times I_m}$ ,  $\forall m \in \mathbb{Z}$ .

For any  $m \in \mathbb{Z}$  we can write

$$T_\alpha^{(5)}(N^2) |_{I_m \times I_m} = -\frac{1}{2} \left( |W|^{\frac{1}{2}} \chi_m \right) \left[ f_N * |W|^{\frac{1}{2}} \chi_m \right] \quad (4.11)$$

where  $\chi_m$  is the characteristic function of the set  $I_m$  and  $f_N$  is the function defined as follows

$$f_N(x) = \begin{cases} \frac{1}{N} \sin N|x| & |x| \leq \frac{5}{2}\pi \\ \frac{1}{N} \sin^2 Nx & \frac{5}{2}\pi \leq |x| \leq 3\pi \\ 0 & |x| \geq 3\pi \end{cases} \quad (4.12)$$

It is easy to check that  $f_N \in H^{2,1}(\mathbb{R})$  and that

$$\left\| \frac{d}{dx} f_N \right\|_2^2 + \|N f_N\|_2^2 < 6\pi \quad (4.13)$$

for any  $N \in \mathbb{N}$ .

Therefore we have

$$T_\alpha^{(5)}(N^2) = |W|^{\frac{1}{2}} \chi_m \left( -i \frac{d}{dx} - iN \right)^{-1} K_m(N^2) \quad (4.14)$$

in which  $K_m(N^2)$  is the integral operator with kernel given by

$$-\frac{1}{2} \left[ \left( -i \frac{d}{dx} - iN \right) f_N(|x-y|) \right] \chi_m(y) |W(y)|^{\frac{1}{2}} \quad (4.15)$$

The two factors are Hilbert-Schmidt and we have the following bounds for their Hilbert-Schmidt norms

$$\begin{aligned} & \left\| |W|^{\frac{1}{2}} \chi_m \left( -i \frac{d}{dx} - iN \right)^{-1} \right\|_{\mathcal{J}_2} = \\ & = \left\| |W|^{\frac{1}{2}} \chi_m \left( -\frac{d^2}{dx^2} + N^2 \right)^{-1} |W|^{\frac{1}{2}} \chi_m \right\|_{\mathcal{J}_1}^{\frac{1}{2}} = \frac{1}{(2N)^{\frac{1}{2}}} \left\| |W|^{\frac{1}{2}} \chi_m \right\|_2, \end{aligned} \quad (4.16)$$

$$\begin{aligned} \|K_m(N^2)\|_{\mathcal{J}_2}^2 &= \frac{1}{4} \left\| \left( \frac{d}{dx} f_N + N f_N \right)^2 * |W| \chi_m \right\|_1 \leq \\ &\leq \frac{1}{2} \left( \left\| \frac{d}{dx} f_N \right\|_2^2 + \|N f_N\|_2^2 \right) \left\| |W|^{\frac{1}{2}} \chi_m \right\|_2^2 < 3\pi \left\| |W|^{\frac{1}{2}} \chi_m \right\|_2^2 \end{aligned} \quad (4.17)$$

( in (4.17) we have used Young's inequality and (4.13) ). Consequently,

$$\|T_\alpha^{(5)}(N^2) |_{I_m \times I_m}\|_{\mathcal{J}_1} \leq \left( \frac{3\pi}{2N} \right)^{\frac{1}{2}} \left( \int_{I_m} |W(x)| dx \right) \quad (4.18)$$

Therefore, the right-hand side of (4.10) is bounded by

$$\lambda \left( \frac{3\pi}{2N} \right)^{\frac{1}{2}} \left[ \sum_{m \in \mathbf{Z}} \left( \int_{I_m} |W(x)| dx \right)^{\frac{1}{2}} \right]^2 \quad (4.19)$$

Since

$$\int_{I_m} |W(x)| dx \leq \frac{1}{[1 + (2|m| - 1)\pi]^{1+\delta}} \int_{I_m} (1 + |x|)^{1+\delta} |W(x)| dx \quad (4.20)$$

for any  $m \neq 0$ , and

$$\int_{I_0} |W(x)| dx \leq \int_{I_0} (1 + |x|)^{1+\delta} |W(x)| dx \quad (4.21)$$

we get

$$\begin{aligned} & \sum_{m \in \mathbf{Z}} \left( \int_{I_m} |W(x)| dx \right)^{\frac{1}{2}} \leq \\ & \leq \left( 1 + \sum_{m \neq 0} \frac{1}{[1 + (2|m| - 1)\pi]^{1+\delta}} \right)^{\frac{1}{2}} \left( \sum_{m \in \mathbf{Z}} \int_{I_m} (1 + |x|)^{1+\delta} |W(x)| dx \right)^{\frac{1}{2}} = \\ & = \left( 1 + \sum_{m \neq 0} \frac{1}{[1 + (2|m| - 1)\pi]^{1+\delta}} \right)^{\frac{1}{2}} \left\| (1 + |x|)^{1+\delta} W \right\|_1^{\frac{1}{2}} \end{aligned} \quad (4.22)$$



Thus the quantity in (4.19) is bounded by

$$\lambda \left( \frac{3\pi}{2N} \right)^{\frac{1}{2}} \left( 1 + \sum_{m \neq 0} \frac{1}{[1 + (2|m| - 1)\pi]^{1+\delta}} \right) \left\| (1 + |x|)^{1+\delta} W \right\|_1 \quad (4.23)$$

which together with (4.8) yields (4.7) ■

Finally, we conclude this section by estimating the number of bound states of  $H_\alpha + \lambda W$  in the unbounded interval  $(-\infty, E_1^\alpha(0))$  for the case  $\alpha < 0$  ( we recall that in this case  $E_1^\alpha(0) < 0$ ).

First of all, it is clear that there will be no bound states in that interval if  $W \geq 0$  due to the positivity of the Birman-Schwinger kernel for any  $E < E_1^\alpha(0)$ .

If  $W \leq 0$  we have the following result.

**THEOREM 4.3.** *If  $W \leq 0$  and satisfies (3.1) then*

$$\begin{aligned} 1 \leq \mathcal{N}_{(-\infty, E_1^\alpha(0))}(H_\alpha - \lambda|W|) &\leq 1 + \lambda \frac{\tanh |E_1^\alpha(0)|^{\frac{1}{2}} \pi}{|E_1^\alpha(0)|^{\frac{1}{2}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)) \right\|_2^2} \\ &\left( \sum_{m, n \in \mathbb{Z}} \iint_{I_m \times I_n} |W(x)| \left[ \phi_\alpha^{(1)}(x; E_1^\alpha(0)) \right]^2 |m - n| |W(y)| \left[ \phi_\alpha^{(1)}(y; E_1^\alpha(0)) \right]^2 dx dy \right) + \\ &+ \frac{\lambda}{2|E_1^\alpha(0)|^{\frac{1}{2}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)) \right\|_2^2} \left( \sum_{m, n \in \mathbb{Z}} \iint_{I_m \times I_n} |W(x)| \phi_\alpha^{(1)}(x; E_1^\alpha(0)) \cdot \right. \\ &\quad \left. \cdot \sinh |E_1^\alpha(0)|^{\frac{1}{2}} (|x - y| - 2|m - n|\pi) |W(y)| \phi_\alpha^{(1)}(y; E_1^\alpha(0)) dx dy \right) \end{aligned} \quad (4.24)$$

In particular, for  $\alpha = 0$  we have the bound given by Klaus in (6), i.e.

$$1 \leq \mathcal{N}_{(-\infty, 0)}(H_0 - \lambda|W|) \leq 1 + \frac{\lambda}{2\|W\|_1} \left( \iint_{\mathbb{R}^2} |W(x)| |x - y| |W(y)| dx dy \right) \quad (4.25)$$

PROOF: By using the same method of section 1 we can determine the Green's function for  $H_\alpha$  in the unbounded interval  $(-\infty, E_1^\alpha(0))$  obtaining

$$\begin{aligned} G_\alpha(x, y; E) = \\ = \frac{1}{2|E|^{\frac{1}{2}}} e^{-|m-n|\theta} \left[ (\beta(\theta))^{-1} \tanh |E|^{\frac{1}{2}} \pi \cosh |E|^{\frac{1}{2}}(x - 2m\pi) \cosh |E|^{\frac{1}{2}}(y - 2n\pi) + \right. \\ \left. - \beta(\theta) \coth |E|^{\frac{1}{2}} \pi e^{-|m-n|\theta} \sinh |E|^{\frac{1}{2}}(x - 2m\pi) \sinh |E|^{\frac{1}{2}}(y - 2n\pi) + \right. \\ \left. - \sinh |E|^{\frac{1}{2}}(|x - y| - 2|m - n|\pi) \right] \end{aligned} \quad (4.26)$$

for any  $x \in I_m, y \in I_n, \forall m, n \in \mathbb{Z}$  with  $\beta(\theta)$  defined as in section 1.

It follows from (4.26) that

$$|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}} = \sum_{l=1}^4 T_\alpha^{(l)}(E) \quad (4.27)$$

where

$$T_\alpha^{(1)}(E) = \frac{1}{2|E|^{\frac{1}{2}}} (\beta(\theta))^{-1} \tanh |E|^{\frac{1}{2}} \pi |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E) \left( |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E), \cdot \right) \geq 0 \quad (4.28)$$

with

$$\phi_\alpha^{(1)}(x; E) = e^{-|m|\theta} \cosh |E|^{\frac{1}{2}}(x - 2m\pi) \quad (4.29)$$

for any  $x \in I_m, \forall m \in \mathbb{Z}$  and  $T_\alpha^{(l)}(E), l = 2, 3, 4$  are the operators with integral kernels given by

$$\begin{aligned} T_\alpha^{(2)}(x, y; E) = \frac{1}{2|E|^{\frac{1}{2}}} (\beta(\theta))^{-1} \tanh |E|^{\frac{1}{2}} \pi |W(x)|^{\frac{1}{2}} \cosh |E|^{\frac{1}{2}}(x - 2m\pi) \cdot \\ \cdot \left[ e^{-|m-n|\theta} - e^{-(|m|+|n|)\theta} \right] |W(y)| \cosh |E|^{\frac{1}{2}}(y - 2n\pi) \end{aligned} \quad (4.30)$$

$$\begin{aligned} T_\alpha^{(3)}(x, y; E) = \\ = - \frac{\beta(\theta) \coth |E|^{\frac{1}{2}} \pi}{2|E|^{\frac{1}{2}}} |W(x)|^{\frac{1}{2}} \sinh |E|^{\frac{1}{2}}(x - 2m\pi) e^{-|m-n|\theta} |W(y)|^{\frac{1}{2}} \sinh |E|^{\frac{1}{2}}(y - 2n\pi) \end{aligned} \quad (4.31)$$

$$T_{\alpha}^{(4)}(x, y; E) = -\frac{1}{2|E|^{\frac{1}{2}}} e^{-|m-n|\theta} |W(x)|^{\frac{1}{2}} \sinh |E|^{\frac{1}{2}} (|x-y| - 2|m-n|\pi) |W(y)|^{\frac{1}{2}} \quad (4.32)$$

for any  $x \in I_m, y \in I_n, \forall m, n \in \mathbb{Z}$ .

Since the Krönig-Penney relation in  $(-\infty, E_1^{\alpha}(0))$  is given by

$$\cosh \theta = \cosh 2\pi |E|^{\frac{1}{2}} + \frac{\alpha}{2|E|^{\frac{1}{2}}} \sinh 2\pi |E|^{\frac{1}{2}} \quad (4.33)$$

it follows that

$$\theta(E) \sim \text{const} \cdot |E - E_1^{\alpha}(0)|^{\frac{1}{2}} \quad (4.34)$$

in a left neighbourhood of  $E_1^{\alpha}(0)$  while

$$\theta(E) \sim 2\pi |E|^{\frac{1}{2}} \quad (4.35)$$

as  $E \rightarrow -\infty$ .

Equation (4.35) implies that

$$\beta(\theta) \sim \text{const} \cdot |E - E_1^{\alpha}(0)|^{\frac{1}{2}} \quad (4.36)$$

Since  $\phi_{\alpha}^{(1)}(E) \in L^2(\mathbb{R}) \cap L^{\infty}(\mathbb{R}), \forall E \in (-\infty, E_1^{\alpha}(0))$  we infer from (4.36) that the nonzero eigenvalue of the positive rank-one operator  $T_{\alpha}^{(1)}(E)$  diverges as  $E$  approaches  $E_1^{\alpha}(0)$  from the left.

Due to the fact that the Krönig-Penney potential is infinitesimally small with respect to  $H_0 = -\frac{d^2}{dx^2}$  in the quadratic form sense ( see (15) ) there exists  $C_{\alpha} > 0$  such that  $H_0 - C_{\alpha} - E \leq H_{\alpha} - E$  for any  $E < E_1^{\alpha}(0)$  and therefore

$$\left\| |W|^{\frac{1}{2}} (H_{\alpha} - E)^{-1} |W|^{\frac{1}{2}} \right\|_{\mathcal{J}_1} \leq \left\| |W|^{\frac{1}{2}} (H_0 - C_{\alpha} - E)^{-1} |W|^{\frac{1}{2}} \right\|_{\mathcal{J}_1} \rightarrow 0 \quad (4.37)$$

as  $E \rightarrow -\infty$ .

Thus, the aforementioned rank-one divergence at  $E = E_1^\alpha(0)$  and (4.37) imply the existence of at least an  $\tilde{E}$  in  $(-\infty, E_1^\alpha(0))$  for which equation (4.1) is satisfied and consequently the lower bound of (4.24).

In order to find an upper bound we need to investigate the behaviour of  $\sum_{l=2}^4 T_\alpha^{(l)}(E)$  in a left neighbourhood of  $E_1^\alpha(0)$ . We are not going to repeat the proof of Theorem 3.1 to show that each summand is a continuous  $\mathcal{J}_1$ -valued function on any closed interval  $[\tilde{E}, E_1^\alpha(0)]$  since it is clear that the property is true for  $T_\alpha^{(3)}(E)$  while for  $T_\alpha^{(2)}(E)$  we can use the same argument used for  $T_\alpha^{(l)}(E)$ ,  $l = 3, 4$  in section 3 and for  $T_\alpha^{(4)}(E)$  the argument used for  $T_\alpha^{(5)}(E)$ , i.e. the estimate (4.23).

Since  $|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}$  is a positive trace-class operator for any  $E < E_1^\alpha(0)$  we can follow the method of (6) obtaining

$$\mathcal{N}_{(-\infty, E_1^\alpha(0))}(H_\alpha - \lambda|W|) \leq 1 + \lambda \lim_{E \rightarrow E_1^\alpha(0)-} \sum_{k=2}^{\infty} \mu_{\alpha,k}(E) \quad (4.38)$$

where  $\{\mu_{\alpha,k}(E)\}_{k=1}^{\infty}$  are the eigenvalues of  $|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}$  in decreasing order and the 1 is related to  $\mu_{\alpha,1}(E)$ , the greatest eigenvalue, which diverges at  $E_1^\alpha(0)$ .

First of all, we can write the series inside the limit in (4.38) as follows

$$\sum_{k=2}^{\infty} \mu_{\alpha,k}(E) = \text{tr} \left( |W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}} \right) - \mu_{\alpha,1}(E) \quad (4.39)$$

By regarding  $\sum_{l=2}^4 T_\alpha^{(l)}(E)$  as a perturbation of the dominating rank-one operator  $T_\alpha^{(1)}(E)$  we obtain

$$\begin{aligned} \mu_{\alpha,1}(E) &= (\beta(\theta))^{-1} \frac{\tanh |E|^{\frac{1}{2}} \pi}{2|E|^{\frac{1}{2}}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E) \right\|_2^2 + \\ &+ \frac{\left( |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E), \sum_{l=2}^4 T_\alpha^{(l)}(E) |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E) \right)}{\left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E) \right\|_2^2} + \gamma_\alpha(E) \end{aligned} \quad (4.40)$$

with  $\gamma_\alpha(E) \rightarrow 0$  as  $E \rightarrow E_1^\alpha(0)_-$ .

Let us first compute

$$\lim_{E \rightarrow E_1^\alpha(0)_-} \text{tr} \left( |W|^{\frac{1}{2}} (H_\alpha - E)^{-1} |W|^{\frac{1}{2}} \right) - (\beta(\theta))^{-1} \frac{\tanh |E|^{\frac{1}{2}}}{2|E|^{\frac{1}{2}}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E) \right\|_2^2 \quad (4.41)$$

By exploiting the positivity of  $|W|^{\frac{1}{2}}(H_\alpha - E)^{-1}|W|^{\frac{1}{2}}, \forall E < E_1^\alpha(0)$  we have that the limit in (4.41) is equal to

$$\begin{aligned} \lim_{E \rightarrow E_1^\alpha(0)_-} \left[ \int_{\mathbb{R}} G_\alpha(x, x; E) |W(x)| dx - (\beta(\theta))^{-1} \frac{\tanh |E|^{\frac{1}{2}}}{2|E|^{\frac{1}{2}}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E) \right\|_2^2 \right] = \\ = \frac{2 \tanh |E_1^\alpha(0)|^{\frac{1}{2}}}{|E_1^\alpha(0)|^{\frac{1}{2}}} \left( \sum_{m \in \mathbb{Z}} \int_{I_m} |m| |W(x)| \left[ \phi_\alpha^{(1)}(x; E_1^\alpha(0)) \right]^2 dx \right) \end{aligned} \quad (4.42)$$

since  $T_\alpha^{(3)}(E_1^\alpha(0)) = 0$  and  $T_\alpha^{(4)}(E)$  has trace equal to zero for any  $E$ .

From the  $\mathcal{J}_1$ -continuity of  $T_\alpha^{(l)}(E), l = 2, 3, 4$  in a left neighbourhood of  $E_1^\alpha(0)$  we get that the second summand in (4.40) has limit equal to

$$\frac{\left( |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)), \sum_{l=2}^4 T_\alpha^{(l)}(E_1^\alpha(0)) |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)) \right)}{\left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)) \right\|_2^2} \quad (4.43)$$

By means of some tedious calculations we obtain that (4.43) is equal to

$$\begin{aligned} \frac{\tanh |E_1^\alpha(0)|^{\frac{1}{2}} \pi}{|E_1^\alpha(0)|^{\frac{1}{2}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)) \right\|_2^2} \left( \sum_{m,n} \iint_{I_m \times I_n} |W(x)| \left[ \phi_\alpha^{(1)}(x; E_1^\alpha(0)) \right]^2 \times \right. \\ \left. \times [|m| + |n| - |m - n|] |W(y)| \left[ \phi_\alpha^{(1)}(y; E_1^\alpha(0)) \right]^2 dx dy \right) - \frac{1}{2|E_1^\alpha(0)|^{\frac{1}{2}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)) \right\|_2^2} \times \\ \times \left( \sum_{m,n} \iint_{I_m \times I_n} |W(x)| \phi_\alpha^{(1)}(x; E_1^\alpha(0)) \sinh |E_1^\alpha(0)|^{\frac{1}{2}} (|x - y| - 2|m - n|\pi) \times \right. \\ \left. \times |W(y)| \phi_\alpha^{(1)}(y; E_1^\alpha(0)) dx dy \right) \end{aligned} \quad (4.44)$$

By rewriting the right-hand side of (4.42) as

$$\frac{2 \tanh |E_1^\alpha(0)|^{\frac{1}{2}} \pi}{|E_1^\alpha(0)|^{\frac{1}{2}} \left\| |W|^{\frac{1}{2}} \phi_\alpha^{(1)}(E_1^\alpha(0)) \right\|_2^2} \cdot \left( \sum_{m,n} \iint_{I_m \times I_n} |m| |W(x)| \left[ \phi_\alpha^{(1)}(x; E_1^\alpha(0)) \right]^2 |W(y)| \left[ \phi_\alpha^{(1)}(y; E_1^\alpha(0)) \right]^2 dx dy \right) \quad (4.45)$$

we obtain that  $\lambda \lim_{E \rightarrow E_1^\alpha(0)-} \sum_{k=2}^{\infty} \mu_{\alpha,k}(E)$  is exactly given by the sum of the second and third summand on the right-hand side of (4.24).

By taking the limit as  $\alpha \rightarrow 0$  of the right-hand side of (4.24) we get

$$1 + \frac{\lambda}{\|W\|_1} \left( \sum_{m,n} \iint_{I_m \times I_n} \left[ \pi |m - n| + \frac{|x - y|}{2} - \pi |m - n| \right] |W(x)| |W(y)| dx dy \right) =$$

$$1 + \frac{\lambda}{2\|W\|_1} \iint_{\mathbb{R}^2} |W(x)| |x - y| |W(y)| dx dy$$

which concludes the proof of the theorem. ■

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