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The Discrete Tight Binding Approximation

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The discrete analog of the tight binding approximation is investigated. Let λ_0 be some energy level of a real discrete potential q. Then there exists an energy band for a one-dimensional $2N$-periodic chain of the same atoms which lies near λ_0. We study the asymptotic behavior of this band when N tends to infinity.

KEY WORDS: Discrete Schrödinger equation; one-dimensional chain; energy band; tight binding approximation.

INTRODUCTION

We discuss the energy band of the discrete one-dimensional Schrödinger equation with a periodic potential Q (we say: a chain of atoms) which is the sum of the shifts of the summable potential q (a single atom). Let λ_0 be an energy level of the potential energy function q. Then there exists an energy band of the potential Q which lies near λ_0. This band is described by the asymptotic formula

$$\lambda(m, N) = \lambda_0 + s(N) + \cos(2Nm)\, \delta(N)/2 + \varepsilon(m, N) \tag{1}$$

where m is a Bloch wave number or quasimomentum, $2N$ is the distance between atoms, $s(N)$ is the shift of the band relative to λ_0, $\delta(N)$ is the width of the band, and $\varepsilon(m, N)$ is a small function as $N \to +\infty$. The formula (1) is usually studied in the framework of the tight binding method,[2] but the main criticism of this method lies in the difficulty of testing its convergence. On the other hand, if the atomic stats are not well-localized, the energy band equation is quite difficult to evaluate due to the presence of three-center integrals.

The rigorous treatment of the problem in the one-dimesional case has been suggested by many authors.[4-7]

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The goal of this paper is to find conditions on the potential function q such that Eq. (1) is valid (Theorem 8.1, parts 4c, 4d) as well as to get a similar formula in the general case (Theorem 8.1, parts 1–4b). The parameter d in Theorem 8.1 can be written as $2\cos(2Nm)$.

1. SINGLE ATOM

First, on the space $l^2(\mathbf{Z})$ we consider the one-dimensional discrete Schrödinger equation

$$-y(n+1)-y(n-1)+q(n)\,y(n)=\lambda y(n), \qquad n\in\mathbf{Z} \tag{1.1}$$

for a real discrete potential function $q(n)$ such that

$$\sum_{n=-\infty}^{+\infty} |q(n)|<\infty \tag{1.2}$$

The spectrum $\sigma(q)\subset\mathbf{R}$ of this atom consists of the interval $[-2, 2]$ and a number of energy levels which lie beyond this interval.

Let $\lambda_0\notin[-2, 2]$ be an eigenvalue and let $\theta(n)$ be a solution of Eq. (1.1) with $\lambda=\lambda_0$ such that

$$\sum_{n=-\infty}^{+\infty} \theta^2(n)=1 \tag{1.3}$$

i.e., $\theta(n)$ is a normalized eigenfunction.

Let $\varphi(n)$ be another solution of Eq. (1.1) with $\lambda=\lambda_0$. The discrete Wronskian[1] of those solutions is

$$W[\theta, \varphi]=\theta(n)\,\varphi(n+1)-\theta(n+1)\,\varphi(n)\equiv 1 \tag{1.4}$$

It is worthwhile noting that the solution $\varphi(n)$ is defined by the relation (1.4) only up to a term proportional to $\theta(n)$. However, this ambiguity does not affect the results of this paper.

It is convenient to introduce following notations:

$$\xi=[|\lambda_0|+(\lambda_0^2-4)^{1/2}]/2 \qquad \text{and} \qquad \delta=\xi-\xi^{-1}=(\lambda_0^2-4)^{1/2}$$

It can be established that there are positive constants C_θ and C_φ such that

$$|\theta(n)|\leqslant C_\theta\xi^{-|n|}, \qquad |\varphi(n)|\leqslant C_\varphi\xi^{|n|}, \qquad n\in\mathbf{Z} \tag{1.5}$$

We will need the $|n|\to+\infty$ asymptotic behavior of the solutions $\theta(n)$ and $\varphi(n)$.

For $n \in \mathbf{Z}$ let us define the following finite sets of integers: $J(n) \equiv \{ j \in \mathbf{Z}: n - |n| < 2j \leqslant n + |n| \}$ and $Y(n) \equiv J(n) \cup J(-n)$. For every $N > 0$ we introduce the function

$$p(N) = \sum_{n \in \mathbf{Z} \setminus Y(N)} |q(n)| + \xi^{-2N} \tag{1.6}$$

It follows from (1.2) that $p(N)$ tends to zero as N tends to infinity. Using this function we shall get the required estimates of the solutions $\theta(n)$ and $\varphi(n)$.

Lemma 1.1. There are some constants $C_{\pm} \neq 0$ such that at $n \to \pm\infty$ we have

$$\begin{aligned} \theta(n) &= C_{\pm} \xi^{-|n|} [1 + O(p(|n|))] \\ \varphi(n) &= \pm (C_{\pm} \delta)^{-1} \xi^{|n|} [1 + O(p(|n|/2))] \\ \sum_{k \in J(n)} \theta(k)\, \varphi(k) &= (n/\delta)[1 + o(1)] \end{aligned} \tag{1.7}$$

Proof. One can find the necessary arguments in ref. 5.

For later use we will need the following combination of two functions $f(n)$ and $g(n)$:

$$[f, g](n) = f(n)\, g(-n+1) - f(n+1)\, g(-n) \tag{1.8}$$

Then for those solutions $\theta(n)$ and $\varphi(n)$ of Eq. (1.1) chosen earlier we get asymptotic formulas with $n \to \pm\infty$, which follows from Lemma 1.1:

$$a(n) = [\varphi, \varphi](n) = \pm (\delta C_+ C_-)^{-1} \xi^{2|n|} [1 + O(p(|n|/2))] \tag{1.9}$$

$$b(n) = [\theta, \varphi](n) = O(p(|n|/2)) \tag{1.10}$$

$$c(n) = [\theta, \theta](n) = \pm \delta C_+ C_- \xi^{-2|n|} [1 + O(p(|n|))] \tag{1.11}$$

2. PERIODIC CHAIN OF IDENTICAL ATOMS

For some fixed $N > 0$, using the potential $q(n)$, we consider the periodic potential $Q(n, N)$ [in shortened form $Q(n)$ or Q] with period $2N$, defined by

$$Q(n, N) = \sum_{k=-\infty}^{+\infty} q(n + 2Nk) \tag{2.1}$$

The convergence of the series in (2.1) is guaranteed by the condition (1.2).

We now consider the Schrödinger equation

$$-y(n+1)-y(n-1)+Q(n,N)\,y(n)=\lambda y(n), \qquad n\in\mathbf{Z} \tag{2.2}$$

The spectrum $\sigma(Q)\subset\mathbf{R}$ of this chain consists of at most $2N$ closed intervals (allowed energy bands).

It is known[8] that

$$\sigma(Q)=\{\lambda\in\mathbf{R}^1\ |F(\lambda,N)|\leqslant 2\} \tag{2.3}$$

where $F(\lambda, N)$ is the discriminant of Eq. (2.2). Hence the band limits are defined by

$$F(\lambda, N)=\pm 2$$

Let θ_N and φ_N be two linearly independent solutions of Eq. (2.2) with $W[\theta_N, \varphi_N]\equiv 1$. Then, using the abbreviation (1.8), we obtain[3]

$$F(\lambda,N)=[\theta_N,\varphi_N](N)+[\theta_N,\varphi_N](-N) \tag{2.4}$$

Now our problem is to choose functions $\varphi_N(n)$ and $\theta_N(n)$.

3. CONSTRUCTION OF $\varphi_N(n)$ AND $\theta_N(n)$

We construct $\varphi_N(n)$ and $\theta_N(n)$ using the method of variation of constants. Putting

$$\kappa=\lambda-\lambda_0, \quad v(n,N)=Q(n,N)-q(n), \quad w(n,\kappa,N)=v(n,N)-\kappa \tag{3.1}$$

we can write the Schrödinger equation (2.2) as

$$-y(n+1)-y(n-1)+[q(n)-\lambda_0]\,y(n)=-w(n,\kappa,N)\,y(n) \tag{3.2}$$

Note that the functions $\varphi(n)$ and $\theta(n)$ are solutions of (3.2), with the right-hand side being zero. Hence we can put

$$\varphi_N(n)=\alpha(n)[\varphi(n)+\gamma(n)\,\theta(n)] \tag{3.3}$$

where $\alpha(n)$ and $\gamma(n)$ satisfy the conditions $\alpha(0)=1$, $\gamma(0)=0$, and

$$[\alpha(n+1)-\alpha(n)]\,\varphi(n+1)+[\alpha(n+1)\,\gamma(n+1)-\alpha(n)\,\gamma(n)]\,\theta(n+1)=0 \tag{3.4}$$

Then, from (3.4) we have $\varphi_N(0)=\varphi(0)$, $\varphi_N(1)=\varphi(1)$. Furthermore, the function $\varphi_N(n)$ will be the solution of Eq. (3.2) if and only if the functions $\alpha(n)$ and $\gamma(n)$ satisfy the following system of nonlinear recurrence equations

$$\alpha(n+1)-\alpha(n)=\alpha(n+1)\,w(n+1)\,\theta(n+1)\times[\varphi(n+1)+\gamma(n+1)\,\theta(n+1)] \tag{3.5}$$

$$\gamma(n+1)-\gamma(n)=-w(n+1)[\varphi(n+1)+\gamma(n+1)\,\theta(n+1)]^2 \tag{3.6}$$

Here we have used the relations (3.4) and (1.4).

Furthermore, we shall need to construct the solution $\theta_N(n)$ of Eq. (3.2) so that the Wronskian $W[\theta_N, \varphi_N]\equiv 1$. To do so we put

$$\theta_N(n)=\alpha^{-1}(n)\,\theta(n)+\beta(n)\,\varphi_N(n) \tag{3.7}$$

where the function $\beta(n)$ is such that $\beta(0)=0$ and

$$[\alpha^{-1}(n+1)-\alpha^{-1}(n)]\,\theta(n+1)+[\beta(n+1)-\beta(n)]\,\varphi_N(n+1)=0 \tag{3.8}$$

By (3.8) we have $\theta_N(n+1)=\alpha^{-1}(n)\,\theta(n+1)+\beta(n)\,\varphi_N(n+1)$. Thus, as a consequence of this fact and the identity $\theta(n)\,\varphi_N(n+1)-\theta(n+1)\,\varphi_N(n)\equiv\alpha(n)$, the Wronskian of the functions θ_N and φ_N is equal to one. Moreover, $\theta_N(0)=\theta(0)$, $\theta_N(1)=\theta(1)$, and the function $\theta_N(n)$ will be the solution of Eq. (3.2) if and only if the function $\beta(n)$ satisfies the following recurrence relation:

$$\beta(n+1)-\beta(n)=w(n+1)\,\theta^2(n+1)\,\alpha^{-1}(n)\,\alpha^{-1}(n+1) \tag{3.9}$$

Note that the functions α, γ, and β depend on n, κ, N, and λ_0.

4. THE PRINCIPAL EQUATION

Now inserting formulas (3.3) for $\varphi_N(n)$ and (3.7) for $\theta_N(n)$ into (2.4) and using the abbreviations (1.9)–(1.11), we obtain

$$\begin{aligned}F(\kappa+\lambda_0, N)=&[\beta(N)-\beta(-N)]\,\alpha(N)\,\alpha(-N)[\alpha(N)+\gamma(N)\,b(N)\\&-\gamma(-N)\,b(-N)+\gamma(N)\,\gamma(-N)\,c(N)]+[b(N)\\&+c(N)\,\gamma(-N)]\,\alpha(-N)/\alpha(N)+[b(-N)\\&+c(-N)\,\gamma(N)]\,\alpha(N)/\alpha(-N)\end{aligned} \tag{4.1}$$

Let

$$G=\alpha_-\alpha_+(a+\gamma_+b_++\gamma_-b_-+\gamma_-\gamma_+c) \tag{4.2}$$

$$H=(b_++\gamma_-c)\,\alpha_-/\alpha_+-(b_-+\gamma_+c)\,\alpha_+/\alpha_- \tag{4.3}$$

with $\alpha_\pm = \alpha(\pm N)$, $\gamma_\pm = \gamma(\pm N)$, $a = a(N)$, $b_\pm = \pm b(\pm N)$, and $c = c(N)$. Taking into account (3.9), we can rewrite Eq. (4.1) in the following form:

$$F(\kappa + \lambda_0, N) = G \sum_{k \in Y(N)} [v(k) - \kappa]\, \theta^2(k)\, \alpha^{-1}(k)\, \alpha^{-1}(k-1) + H$$

Note that the functions G and H depend on κ, N, and $\xi = \xi(\lambda_0)$.

According to (2.3), for every $d \in [-2, 2]$ the equation $F(\lambda, N) = d$ defines the spectrum $\lambda(d; N) \in \sigma(Q)$. We write this equation in the form

$$\kappa = \left[\sum_{k \in Y(N)} v(k)\, \theta^2(k)\, \alpha^{-1}(k)\, \alpha^{-1}(k-1) + (H - d)\, G^{-1} \right] \times \left[\sum_{k \in Y(N)} \theta^2(k)\, \alpha^{-1}(k)\, \alpha^{-1}(k-1) \right]^{-1} \tag{4.4}$$

or, in shortened form, $\kappa = f(\kappa)$. It is worthwhile noting that the function $f(\kappa)$ depends also on d, N, and $\xi = \xi(\lambda_0)$.

The main goal of our paper is to investigate the asymptotic behavior of the solution $\kappa(d; N) = \lambda(d; N) - \lambda_0$ of Eq. (4.4) which tends to zero as $N \to +\infty$.

5. ASYMPTOTIC FORMULAS FOR $\alpha(n)$ AND $\gamma(n)$

Let us define a decreasing function $r(N)$ as

$$r(N) = \sup_{t \geqslant N} \sum_{n \in Y(t)} |v(n, t)|\, \xi^{-2|n|} + \xi^{-2N}, \qquad N > 0 \tag{5.1}$$

Note that the definition of the function $p(N)$ can be rewritten in the following form:

$$p(N) = \sum_{n \in Y(N)} \sum_{k \neq 0} |q(n + 2kn)| + \xi^{-2N}, \qquad N > 0$$

Therefore, for every $N > 0$

$$p(N) \geqslant \sum_{n \in Y(N)} |v(n, N)| + \xi^{-2N} \geqslant r(N)$$

Using these two functions, we will get all required estimates.

We will study the spectrum $\sigma(Q)$ near λ_0. Hence, as follows from the perturbation theory, we can suppose that

$$|\kappa| \leqslant C_\kappa r(N) \tag{5.2}$$

for some fixed positive constant C_κ.

The condition (5.2) defines the interval $I = I(N) = [-C_\kappa r(N), C_\kappa r(N)] \subset \mathbf{R}$ on which we will investigate the equation $\kappa = f(\kappa)$.

In this paper we shall write $\partial/\partial\kappa$ as ∂_κ.

Lemma 5.1. Let C_κ be a positive constant. There exists a positive number N_0 such that for every $N \geqslant N_0$ and for every $\kappa \in I(N)$ there is one and only one solution $\gamma(n)$ of Eq. (3.6) such that on the interval $n \in Y(N)$ we have estimates

$$|\gamma(n)| \leqslant C_\gamma\, p(N)\, \xi^{2|n|} \qquad \text{and} \qquad |\partial_\kappa \gamma(n)| \leqslant C'_\gamma \xi^{2|n|} \tag{5.3}$$

where C_γ and C'_γ are some constants. We can set, for instance,

$$C_\gamma = (1 + C_\kappa)(C_\varphi + C_\theta)^2/(1 - \xi^{-2}) \quad \text{and} \quad C'_\gamma = 2(C_\varphi + C_\theta)^2/(1 - \xi^{-2})$$

Proof. We need to study Eq. (3.6). The solution γ of this equation behaves asymptotically for n large enough as $\xi^{2|n|}$. Introduce the new function z

$$z(n) = \gamma(n)\, \xi^{-2|n|}, \qquad n \in \mathbf{Z} \tag{5.4}$$

Putting (5.4) in (3.6), we get

$$z(n) = \begin{cases} \xi^{-2} z(n-1) - w(n)[\varphi_0(n) + z(n)\,\theta_0(n)]^2, & n > 0 \\ \xi^{-2}\{z(n+1) + w(n+1)[\varphi_0(n+1) \\ \qquad + z(n+1)\,\theta_0(n+1)]^2\}, & n \leqslant 0 \end{cases} \tag{5.5}$$

with $\varphi_0(n) = \varphi(n)\, \xi^{-|n|}$ and $\theta_0(n) = \theta(n)\, \xi^{|n|}$. We will now show that the function $z(n)$ is a bounded function on $Y(N)$ uniformly with respect to N.

For the proof we will use the contraction mapping principle on the space of bounded functions $c(Y(N))$ with the norm

$$\|z\|_N = \max_{n \in Y(N)} |z(n)|, \qquad z \in c(Y(N))$$

Let A be an operator on the right-hand side of (5.5), i.e.,

$$(Az)(n) = \begin{cases} \xi^{-2} z(n-1) - w(n)[\varphi_0(n) + z(n)\,\theta_0(n)]^2, & n > 0 \\ \xi^{-2}\{z(n+1) + w(n+1)[\varphi_0(n+1) \\ \qquad + z(n+1)\,\theta_0(n+1)]^2\}, & n \leqslant 0 \end{cases}$$

The operator A maps the closed unit ball

$$B_1(N) = \{z \in c(Y(N)) \colon \|z\|_N \leqslant 1\}$$

into itself for sufficiently small N^{-1} and κ. Indeed, the estimates (1.6) give $|\theta_0(n)| \leqslant C_\theta$, $|\varphi_0(n)| \leqslant C_\varphi$, $n \in \mathbf{Z}$.

Hence for $z \in B_1(N)$ we obtain

$$\|Az(n)\|_N \leqslant \xi^{-2} + (C_\kappa + 1)(C_\varphi + C_\theta)^2\, p(N)$$

Therefore, there is a number $N_0 > 0$ such that for every $N > N_0$

$$\|Az\|_N \leqslant 1 \tag{5.6}$$

if $z \in B_1(N)$. On the other hand, A is a contractive operator on B_1. To see this, suppose $z_1, z_2 \in B_1(N)$. Then, as above,

$$\|Az_1 - Az_2\|_N \leqslant [\xi^{-2} + 2(C_\kappa + 1)(C_\varphi + C_\theta)^2\, p(N)]\, \|z_1 - z_2\|_N$$

Hence we can set N_0 such that for every $N > N_0$

$$\|Az_1 - Az_2\|_N \leqslant \|z_1 - z_2\|_N/2 \tag{5.7}$$

if $z_1, z_2 \in B_1(N)$. Finally, if N_0 is such that

$$p(N) \leqslant \delta[4\xi(C_\kappa + 1)(C_\varphi + C_\theta)^2]^{-1} \tag{5.8}$$

then we have both (5.6) and (5.7) on $B_1(N)$. Hence for every $N > N_0$ and for every $\kappa \in I(N)$ there exists one and only one solution $z \in c(Y(N))$ of Eq. (5.5) satisfying the condition $\|z\|_N \leqslant 1$.

Therefore, if $n \in Y(N)$, then

$$|\gamma(n)| \leqslant \|z\|_N\, \xi^{2|n|} \leqslant \|Az\|_N\, \xi^{2|n|} \leqslant C_\gamma\, p(N)\, \xi^{2|n|}$$

with $C_\gamma = (1 + C_\kappa)(C_\varphi + C_\theta)^2/(1 - \xi^{-2})$.

For further use we will need an estimate of the derivative $\partial_\kappa \gamma$ of the function γ with respect to the parameter κ. Since $\partial_\kappa \gamma(n) = \xi^{2|n|}\partial_\kappa z(n)$, putting $u(n) = \partial_\kappa z(n)$, we shall consider the identity with $n > 0$ (the case with $n \leqslant 0$ is analogous)

$$\begin{aligned} u(n) = {} & [\varphi_0(n) + z(n)\, \theta_0(n)]^2 \\ & + \{\xi^{-2}u(n-1) - 2w(n)[\varphi_0(n) + z(n)\, \theta_0(n)]^2\, \theta_0(n)\, u(n)\} \end{aligned} \tag{5.9}$$

For the sake of simplicity, we write (5.9) as

$$u(n) = g(n) + (Vu)(n)$$

Since $\|g\|_N \leqslant (C_\varphi + C_\theta)^2/(1 - \xi^{-2})$ and since the inequalities

$$\|V\| \leqslant \xi^{-2} + 2(C_\kappa + 1)(C_\varphi + C_\theta)^2\, p(N) \leqslant (1 + \xi^{-2})/2 < 1$$

hold by (5.8), we can estimate the function u,

$$\|u\|_N \leqslant (1 - \|V\|)^{-1} \|g\|_N \leqslant 2(C_\varphi + C_\theta)^2/(1 - \xi^{-2})$$

Hence

$$|\partial_\kappa \gamma(n)| \leqslant C'_\gamma \xi^{2|n|} \qquad \text{with} \quad C'_\gamma = 2(C_\varphi + C_\theta)^2/(1 - \xi^{-2})$$

Note that we may choose N_0 such that for every $N \geqslant N_0$ the function $p(N)$ satisfies (5.8). Hence one can solve (5.5) by the method of successive approximations. QED

Lemma 5.2. Let C_κ be a positive constant. There exists a positive number N_1 such that for every $N \geqslant N_1$ and for every $\kappa \in I(N)$ when $n \in Y(N)$ we have the estimates

$$|\ln \alpha(n)| \leqslant C_\alpha(r(N)\,|n| + p(N)) \qquad \text{and} \qquad |\partial_\kappa \ln \alpha(n)| \leqslant C'_\alpha\,|n| \tag{5.10}$$

where C_α and C'_α are some constants. We can set, for instance,

$$C_\alpha = C_\varphi C_\theta (C_\kappa + 1) \qquad \text{and} \qquad C'_\alpha = C_\varphi C_\theta + 1$$

Proof. According to (3.7), we will need to study the following recurrence relation:

$$\alpha(n) = \alpha(n+1)[1 - w(n+1)\,\psi(n+1)]$$

with $\psi(n) \equiv \theta(n)[\varphi(n) + \gamma(n)\,\theta(n)]$. In order to estimate the function $\alpha(n)$ we rewrite the relation for α in expanded form

$$\ln \alpha(n) = -\text{sign}(n) \sum_{k \in J(n)} \ln[1 - w(k)\,\psi(k)]$$

where $J(n)$ is defined in Section 1 and

$$\text{sign}(n) \equiv \begin{cases} 1, & n > 0 \\ -1, & n \leqslant 0 \end{cases} \tag{5.11}$$

Since $\|w(n, \kappa, N)\,\psi(n)\|_N \to 0$ as $N \to +\infty$ we can express the logarithm function as a power series in $w(k)\,\psi(k)$. Then we get

$$\|\ln \alpha(n)\|_N \leqslant C_\alpha[Nr(N) + p(N)]$$

with $C_\alpha \geqslant C_\theta(C_\kappa + 1/N)[C_\varphi + C_\gamma C_\theta p(N)]$. By analogy we can find an estimate for $\partial_\kappa \ln \alpha(n)$ from

$$\partial_\kappa \ln \alpha(n) = \text{sign}(n) \sum_{k \in J(n)} [1 - w(k)\,\psi(k)]^{-1} [w(k)\,\partial_\kappa \psi(k) + \psi(k)\,\partial_\kappa w(k)]$$

Since $w(k)\,\partial_\kappa \psi(k) + \psi(k)\,\partial_\kappa w(k)$ is a bounded function, we immediately obtain the required estimate. QED

From (3.6) and (3.5), taking into account the estimates for the functions $\alpha(n)$ and $\gamma(n)$, as a consequence of Lemmas 5.1 and 5.2, we obtain the following:

Consequence. Uniformly with respect to $\kappa \in I(N)$ and $n \in Y(N)$ we have

$$\gamma(n) = \text{sign}(n) \sum_{k \in J(n)} [\kappa - v(k, N)]\, \varphi^2(k) + \xi^{2|n|} O(p^2(N))$$

$$\ln \alpha(n) = -\kappa\, \text{sign}(n) \sum_{k \in J(n)} \theta(k)\, \varphi(k) + O(p(N)[1 + |n|\, r(N)])$$

as $N \to +\infty$.

6. ASYMPTOTIC FORMULAS FOR THE FUNCTIONS *G* AND *H*

In this section we will investigate the asymptotic behavior of functions G and H.

Lemma 6.1. Let C_α and C'_α be as in Lemma 5.2. Let C_κ, C_g, and C'_g be positive constants and $C_g > \delta\,|C_+ C_-|$, $C'_g > 2C'_\alpha(\delta\,|C_+ C_-|)^{-1}$. Then:

(a) There is a positive number N_2 such that for every $N \geqslant N_2$ and for every $\kappa \in I(N)$ we have

$$\begin{aligned} |G(\kappa, N)|^{-1} &\leqslant C_g \xi^{-2N} \exp[2C_\alpha N r(N)] \\ |\partial_\kappa G(\kappa, N)| &\leqslant C'_g N \xi^{2N} \exp[2C_\alpha N r(N)] \end{aligned} \tag{6.1}$$

(b) Uniformly with respect to $\kappa \in I(N)$ we have

$$G^{-1}(\kappa, N) = \delta C_+ C_- [1 + O(p(N/2))]\, \xi^{-2N}$$
$$\times \exp\left[\kappa \left(\sum_{n \in J(N)} - \sum_{n \in J(-N)} \right) \theta(n)\, \varphi(n) + O(N p(N)\, r(N))\right]$$

as N tends to the infinity.

Proof. (a) To get the required estimate for the function $G(\kappa, N)$ we will evaluate all terms on the right-hand side of Eq. (4.2), which defines the function $G(\kappa, N)$. Now we will use Lemmas 5.1 and 5.2 and asymptotic formulas (1.9)–(1.11). Let $N \geqslant \max\{N_0, N_1\}$ and $\kappa \in I(N)$. Therefore

$$|\alpha_+ \alpha_-| \geqslant \exp\{-2C_\alpha[r(N)\, N + p(N)]\} \qquad \text{and} \qquad |\gamma_\pm| \leqslant C_\gamma\, p(N)\, \xi^{2N}$$

Furthermore, $a=\xi^{2N}[\varepsilon_1+(\delta C_+C_-)^{-1}]$, $b_\pm=\varepsilon_2$, and $c=\xi^{-2N}(\varepsilon_3+\delta C_+C_-)$, where ε_j are independent of κ and $\varepsilon_j=o(1)$ as $N\to+\infty$, $j=1,2,3$. Hence

$$|G(\kappa,N)|\geqslant[(\delta\,|C_+C_-|)^{-1}-|\varepsilon_1|-2\,|\varepsilon_3|\,C_\gamma\,p(N)$$
$$-C_\gamma^2\,p^2(N)(\delta\,|C_+C_-|+|\varepsilon_3|)]$$
$$\times\xi^{2N}\exp\{-2C_\alpha[r(N)\,N+p(N)]\}$$

Since $p(N)$ and ε_j, $j=1,2,3$, tend to zero with $N\to+\infty$, there is a number $N_2\geqslant\max\{N_0,N_1\}$ such that for every $N\geqslant N_2$ and for every $\kappa\in I(N)$ the required inequality holds:

$$|G(\kappa,N)|\geqslant C_g^{-1}\xi^{2N}\exp[-2C_\alpha r(N)\,N]$$

The estimate for the derivative $\partial_\kappa G$ is obtained analogously from its explicit expression

$$\partial_\kappa G=[\partial_\kappa(\alpha_+\alpha_-)](a+b_+\gamma_++b_-\gamma_-+\gamma_+\gamma_-c)$$
$$+\alpha_+\alpha_-[b_+\partial_\kappa\gamma+b_-\partial_\kappa\gamma+c\partial_\kappa(\gamma_+\gamma_-)]$$

Here we suppose that the positive number N_2 was chosen so that for every $N\geqslant N_2$ estimates for G and $\partial_\kappa G$ would both be true.

(b) To get the asymptotic formula for G it is enough to find the asymptotic behavior of the main term $\alpha_+\alpha_-a$. Substituting the results (1.9) and (5.5) into (4.2), we obtain the required asymptotic formula. QED

Lemma 6.2. Let C_α be as in Lemma 5.2. For some positive constant C_κ there are positive numbers N_3, C_h, and C_h' such that for every $N\geqslant N_3$ and for every $\kappa\in I(N)$ the following estimates are true:

$$\begin{aligned}|H(\kappa,N)|&\leqslant C_h\,p(N/2)\exp[2C_\alpha r(N)\,N]\\|\partial_\kappa H(\kappa,N)|&\leqslant C_h'[1+Np(N/2)]\exp[2C_\alpha r(N)\,N]\end{aligned}\tag{6.2}$$

Proof. By (4.3), using the asymptotic formulas (1.9)–(1.11) and Lemmas 5.1 and 5.2, we obtain

$$|H(\kappa,N)|\leqslant2\{O(p(N/2))+\delta\,|C_+C_-|\,C_\gamma\,p(N)[1+O(p(N))]\}$$
$$\times\exp[2C_\alpha r(N)\,N]$$

It leads to the required estimate for H.

The estimate of the derivative $\partial_\kappa H$ is done analogously. Here it is helpful to take into account the identity $\partial_\kappa(\alpha^{\pm1})=\pm\alpha^{\pm1}\partial_\kappa\ln\alpha$. QED.

Now, let us prove an additional asymptotic formula.

Lemma 6.3. Uniformly with respect to $\kappa \in I(N)$ we have

$$\left[\sum_{n \in Y(N)} \theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1)\right]^{-1} = 1 + O(p(N)) \tag{6.3}$$

as $N \to +\infty$.

Proof. We will use the following formula, which is a discrete analog of the formula of integration by parts:

$$\sum_{n=L}^{M} [a(n) - a(n-1)]\, b(n) = a(M)\, b(M+1) - a(L-1)\, b(L) - \sum_{n=L}^{M} a(n)[b(n+1) - b(n)] \tag{6.4}$$

To prove this lemma we will take

$$a(n) = -\sum_{m=n+1}^{N} \theta^2(m), \qquad b(n) = \alpha^{-1}(n)\,\alpha^{-1}(n-1), \qquad L = 1, \quad M = N$$

This leads to

$$\sum_{n=1}^{N} \theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1) = \alpha^{-1}(1) \sum_{n=1}^{N} \theta^2(n) + \sum_{n=1}^{N} \alpha^{-1}(n)[\alpha^{-1}(n+1) - \alpha^{-1}(n-1)] \sum_{m=n+1}^{N} \theta^2(m)$$

Therefore

$$\left|\sum_{n=1}^{N} \theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1) - \sum_{n=1}^{\infty} \theta^2(n)\right| \leqslant \sum_{n=N+1}^{\infty} \theta^2(n) + |w(1)\,\psi(1)| \sum_{n=1}^{N} \theta^2(n) + \sum_{n=1}^{N} \alpha^{-2}(n)\,|1 - w(n+1)\,\psi(n+1) - [1 - w(n)\,\psi(n)]^{-1}| \times \sum_{m=n+1}^{N} \theta^2(m) = O(p(N))$$

where $\psi(n)$ is as in the proof of the Lemma 5.2.

Here we have taken into account that because of (1.5) the following estimate is true: $|a(n)| \leqslant (C_\theta^2/\delta)\,\xi^{-2n}$ for $n \in Y(N)$. The part of the series with $n \leqslant 0$ is calculated analogously. Hence, by the last results and the normalization condition, we obtain

$$\sum_{n \in Y(N)} \theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1) = 1 + O(p(N)) \quad \text{QED}$$

Lemma 6.4. Let $v(n) = v(n, N)$ be defined by (3.1). Then uniformly with respect to $\kappa \in I(N)$ we have

$$\sum_{n \in Y(N)} v(n)\,\theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1) = \sum_{n \in Y(N)} v(n)\,\theta^2(n) + O(p(N)\,r(N))$$

as $N \to +\infty$.

Proof. The proof is identical to the one for Lemma 6.3. We will use Eq. (6.4) with

$$a(n) = -\sum_{m=n+1}^{N} v(m)\,\theta^2(m), \quad b(n) = \alpha^{-1}(n)\,\alpha^{-1}(n-1), \quad L = 1, \quad M = N$$

Note that now $|a(n)| \leqslant (C_\theta^2/\delta)\,p(N)\,\xi^{-2n}$ with $n \in Y(N)$. Therefore

$$\begin{aligned}
&\left|\sum_{n=1}^{N} v(n)\,\theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1) - \sum_{n=1}^{N} v(n)\,\theta^2(n)\right| \\
&\quad \leqslant |w(1)\,\psi(1)| \sum_{n=1}^{N} |v(n)|\,\theta^2(n) \\
&\qquad + \sum_{n=1}^{N} \alpha^{-2}(n)\,|1 - w(n+1)\,\psi(n+1) \\
&\qquad - [1 - w(n)\,\psi(n)]^{-1}| \sum_{m=n+1}^{N} |v(m)|\,\theta^2(m) \\
&\quad = O(p(N)\,r(N))
\end{aligned}$$

We have used here that

$$\sum_{n=1}^{N} |v(n)|\,\xi^{-2n}\alpha^{-2}(n) = \sum_{n=1}^{N} |v(n)|\,\xi^{-2n} + O(p(N)\,r(N))$$

The part of the series with $n \leqslant 0$ is calculated analogously. Finally, combining the last results, we obtain the required formula. QED.

7. EXISTENCE PROOF FOR THE ENERGY BAND

The following theorem is true.

Theorem 7.1. Let C_κ and d_0 be positive constants such that $C_\kappa > \max\{C_\theta^2, \delta\,|C_+C_-|\,d_0\}$ if $r(N)\,N \to 0$ with $N \to +\infty$, and $C_\kappa > C_\theta^2$ in the opposite case. There exists a positive number n_0 such that for every $N \geqslant n_0$ and for every $d \in [-d_0, d_0]$, Eq. (4.4) has one and only one solution $\kappa = \kappa(d; N)$ such that $\kappa \in I(N)$.

Proof. The equation $\kappa = f(\kappa)$ can be solved by the method of successive approximations. Using results of the last section, we obtain

$$|f(\kappa)| \leqslant \left\{ \sum_{n \in Y(N)} |v(n)|\, \theta^2(n)[1 + o(1)] + (d_0 + |H|)/|G| \right\} [1 + o(1)]$$

$$\leqslant \sum_{n \in Y(N)} |v(n)|\, \theta^2(n) + o(r(N)) + \{d_0 + C_h\, p(N/2) \exp[2C_\alpha r(N)\, N]\}$$
$$\times \delta\, |C_+C_-|[1 + o(1)]\, \xi^{-2N} \exp[2C_\alpha r(N)\, N] \tag{7.1}$$

If $r(N)\,N \to 0$ with $N \to +\infty$, then for large N

$$|f(\kappa)| \leqslant \sum_{n \in Y(N)} |v(n)|\, \theta^2(n) + \delta\, |C_+C_-|\, d_0 \xi^{-2N} + o(r(N))$$
$$\leqslant C_\kappa r(N) \tag{7.2}$$

In the opposite case, i.e., if $r(N)\,N$ does not tend to zero, then for every sufficiently large N we have the obvious inequality

$$\xi^{-2} \exp[4C_\alpha r(N)] < \xi^{-1} \tag{7.3}$$

Hence, since $\xi^{-N} = o(r(N))$ we obtain

$$|f(\kappa)| \leqslant \sum_{n \in Y(N)} |v(n)|\, \theta^2(n) + o(r(N))$$
$$\leqslant C_\theta^2 r(N)[1 + o(1)] \leqslant C_\kappa r(N) \tag{7.4}$$

Thus, there exists a positive number n_0 such that for every $N \geqslant n_0$ the function $f(\kappa)$ maps the interval $I(N)$ into itself.

On the other hand, we will prove that we can choose n_0 such that for every $N \geqslant n_0$ and for every $\kappa \in I(N)$ the mapping $f(\kappa)$ satisfies the contraction condition

$$|f'(\kappa)| < 1/2 \tag{7.5}$$

Putting $f(\kappa)=f_1(\kappa)\, f_2(\kappa)$ with

$$f_2(\kappa)=\left[\sum_{n\in Y(N)} \theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1)\right]^{-1}$$

we obtain at $N\to +\infty$

$$f_1(\kappa)=O(r(N)), \qquad f_2(\kappa)=1+O(p(N)) \tag{7.6}$$

To estimate the derivatives, we will use the results of the last section. By the definition of the function f_1 we have

$$|f_1'(\kappa)|\leqslant 2 \sum_{n\in Y(N)} |v(n)|\,\theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1)\,|\partial_\kappa \ln \alpha(n)|$$
$$+\,|\partial_\kappa H|\cdot|G|^{-1}+(|H|+d_0)\,|\partial_\kappa G|\cdot|G|^{-2}$$

It is easily verified that, according to (7.3), uniformly with respect to $\kappa\in I(N)$ and for every $n\in Y(N)$ we get

$$\theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1)\,|\partial_\kappa \ln \alpha(n)|\leqslant C_\theta^2 C_\alpha'(2\ln \xi)^{-1}$$

Hence

$$|f_1'(\kappa)|\leqslant C_\theta^2 C_\alpha'(\ln \xi)^{-1}\, p(N)+C_h'[Np(N/2)+1]\; C_g \xi^{-2N}\exp[4C_\alpha r(N)\,N]$$
$$+\,C_h p(N/2)\,\xi^{-2N}\exp[8C_\alpha r(N)\,N]+d_0 C_g \xi^{-2N}\exp[2C_\alpha r(N)\,N]$$

where N is a sufficiently large number. Thus, we obtain

$$|f_1'(\kappa)|=o(1) \qquad \text{as} \quad N\to +\infty \tag{7.7}$$

Analogously for sufficiently large N we have the estimate of f_2'

$$|f_2'(\kappa)|\leqslant 2f_2^2(\kappa) \sum_{n\in Y(N)} \theta^2(n)\,\alpha^{-1}(n)\,\alpha^{-1}(n-1)\,|\partial_\kappa \ln \alpha(n)|$$
$$\leqslant 2C_\theta^2 C_\alpha' \sum_{n\in Y(N)} |n|\,\xi^{-2|n|}\exp[2C_\alpha\,|n|\,r(N)+2C_\alpha\, p(N)]$$
$$\leqslant 3C_\theta^2 C_\alpha'(\ln \xi)^{-1}$$

Thus, we obtain

$$|f_2'(\kappa)|=O(1) \qquad \text{as} \quad N\to +\infty \tag{7.8}$$

Combining (7.6)–(7.8), we conclude that there is a positive number n_0 such that for every $N\geqslant n_0$ and for every $\kappa\in I(N)$ the estimate (7.5) is valid.

According to (7.2), (7.4), and (7.5), Eq. (4.4) can now be solved by the method of successive approximations. QED

Because of (2.3) we have the following consequence of Theorem 7.1.

Consequence 7.2. Let $d_0 \geqslant 2$, $C > \max\{C_\theta^2, \delta\,|C_+ C_-|\, d_0\}$, and let $\kappa(d; N)$ (here $|d| \leqslant d_0$) be a solution of Eq. (4.4) such that $|\kappa(d; N)| \leqslant Cr(N)$ for N large. According to (3.1), we know that $\lambda(d; N) = \lambda_0 + \kappa(d; N)$. Then $\lambda(d; N) \in \sigma(Q)$ if $d \in [-2, 2]$ and $\lambda(d; N) \notin \sigma(Q)$ when $|d| > 2$. Therefore the interval $\{\lambda(d; N)\colon -2 \leqslant d \leqslant 2\}$ coincides with the energy band, which lies near λ_0.

8. ASYMPTOTIC FORMULAS FOR THE ENERGY BAND

We shall now prove asymptotic formulas for the band.

Theorem 8.1. Suppose $q(n)$ is a function from $l^1(\mathbf{Z})$. Let N be a positive number and let $Q(x, N)$ be given by (2.1). Suppose that $\lambda_0 \notin [-2, 2]$ is an eigenvalue and that $\theta(n) \in l^2(\mathbf{Z})$ is a normalized eigenfunction of the Schrödinger equation (1.1) with $\lambda = \lambda_0$. Let the function $\varphi(x)$ be another solution of Eq. (1.1) with $\lambda = \lambda_0$ obeying the condition (1.4). Let $\xi > 1$, $\xi = [|\lambda_0| + (\lambda_0^2 - 4)^{1/2}]/2$, and $\delta = (\lambda_0^2 - 4)^{1/2}$, and positive constants C_θ as in (1.5) and $C_\pm$ as in Lemma 1.1. Let the functions $p(N)$, $r(N)$, and $\operatorname{sign}(n)$ be given by (1.6), (5.1), and (5.11), respectively. Put

$$s(N) \equiv s(q, \lambda_0; N) \equiv \sum_{n=-N+1}^{N} [Q(n, N) - q(n)]\, \theta^2(n) \tag{8.1}$$

If $C > \max\{C_\theta^2, 2\delta\,|C_+ C_-|\}$ and $\kappa(d; N)$ is a solution of (4.4) with $d \in [-2, 2]$ such that $|\kappa(d; N)| \leqslant Cr(N)$ for N large, then:

1. $\lambda(d; N) = \lambda_0 + \kappa(d; N) \in \sigma(Q)$ with $d \in [-2, 2]$.

2. $\lambda(\pm 2; N)$ are the edges of the band and $|\lambda(2; N) - \lambda(-2; N)| \equiv \Delta(N)\, \xi^{2N}$ is the width of the band.

3. The following asymptotic formula for the shift of the band relative to λ_0 holds:

$$\lambda(0; N) = \lambda_0 + s(N) + \varepsilon_1(N) \tag{8.2}$$

where $\varepsilon_1(N) = o(r(N))$ as $N \to +\infty$.

4. The following formulas for the bandwidth $\Delta(N)\, \xi^{2N}$ hold

(a) In the general case

$$\ln \Delta(N) = s(N) \sum_{k=-N+1}^{N} \operatorname{sign}(k)\, \theta(k)\, \varphi(k) + \varepsilon_2(d; N) \tag{8.3}$$

where $\varepsilon_2(d; N) = O(1 + p(N)\, r(N)\, N)$ uniformly with respect to $d \in [-2, 2]$ as $N \to +\infty$.

(b) For a potential function $q(x)$ such that $p(N)\, r(N)\, N \to 0$ as $N \to +\infty$

$$\Delta(N) = 4\delta\, |C_+ C_-|\, [1 + \varepsilon_3(d; N)] \times \exp\left[s(N) \sum_{k=-N+1}^{N} \operatorname{sign}(k)\, \theta(k)\, \varphi(k) \right] \tag{8.4}$$

where $\varepsilon_3(d; N) = o(1)$ uniformly with respect to $d \in [-2, 2]$ as $N \to +\infty$.

(c) For a potential function $q(x)$ such that $r(N)\, N$ is a bounded quantity for every N

$$\Delta(N) = 4\delta\, |C_+ C_-| \exp[2Ns(N)/\delta] + \varepsilon_4(d; N) \tag{8.5}$$

where $\varepsilon_4(d; N) = o(1)$ uniformly with respect to $d \in [-2, 2]$ as $N \to +\infty$.

(d) For a potential function $q(x)$ such that $r(N)\, N \to 0$ as $N \to +\infty$

$$\Delta(N) = 4\delta\, |C_+ C_-| + \varepsilon_5(d; N) \tag{8.6}$$

where $\varepsilon_5(d; N) = o(1)$ uniformly with respect to $d \in [-2, 2]$ as $N \to +\infty$.

Proof. According to Theorem 7.1, there exists a positive number such that for every $N \geqslant n_0$ and for every $d \in [-2, 2]$, Eq. (4.4) has one and only one solution $\kappa(d; N) \in [-Cr(N), Cr(N)]$ and from Consequence 7.2 we have $\lambda(d; N) \in \sigma(Q)$ iff $d \in [-2, 2]$. Points $\lambda(\pm 2; N)$ correspond to edges of the band. This implies parts 1 and 2 of Theorem 8.1.

Substituting $\kappa(d; N)$ into (4.4), we obtain the following identity with respect to variables d and N:

$$\kappa(d; N) = \left\{ \sum_{n=-N+1}^{N} [Q(n, N) - q(n)]\, \theta^2(n)\, \alpha^{-1}(n, d, N)\, \alpha^{-1}(n-1, d, N) + [-d + H(d; N)]\, G^{-1}(d; N) \right\} \times \left[\sum_{n=-N+1}^{N} \theta^2(n)\, \alpha^{-1}(n, d, N)\, \alpha^{-1}(n-1, d, N) \right]^{-1} \tag{8.7}$$

According to Lemmas 6.1–6.4, we can rewrite (8.7) in the form

$$\kappa(d;N)=\Big(s(N)+O(p(N)\,r(N))+\{-d+O(p(N/2))$$
$$\times\exp[2C_\alpha r(N)\,N]\}\,\delta C_+C_-\xi^{-2N}$$
$$\times\exp\left[s(N)\sum_{n=-N+1}^{N}\operatorname{sign}(n)\,\theta(n)\,\varphi(n)+O(p(N)\,r(N)\,N)\right]\Big)$$
$$\times[1+O(p(N))]$$

uniformly with respect to $d\in[-2,2]$ as $N\to+\infty$. Then, putting $d=0$, we get (8.2) and part 3 of Theorem 8.1.

Now we will prove formulas (8.3)–(8.6) for the width of the band. Let us consider the derivative $\partial_d\kappa$. Since $\kappa(d;N)\equiv f(\kappa(d;N),d)$,

$$\partial_d\kappa=(\partial_\kappa f)\,\partial_d\kappa+\partial_d f \tag{8.8}$$

Next, note that $\partial_\kappa f=o(1)$ uniformly with respect to $d\in[-2,2]$ as $N\to+\infty$ (see proof of Theorem 7.1) and by Lemmas 6.1 and 6.3 we obtain

$$\partial_d f=-\left[G\sum_{n=-N+1}^{N}\theta^2(n)\,\alpha^{-1}(n,d,N)\,\alpha^{-1}(n-1,d,N)\right]^{-1}$$
$$=-\delta C_+C_-\xi^{-2N}\exp\left[s(N)\sum_{n=-N+1}^{N}\operatorname{sign}(n)\,\theta(n)\,\varphi(n)\right.$$
$$\left.+O(p(N)\,r(N)\,N)\right][1+o(1)]$$

as $N\to+\infty$. Thus, by (8.8) we have

$$\partial_d\kappa=-\delta C_+C_-\xi^{-2N}\exp\left[s(N)\sum_{n=-N+1}^{N}\operatorname{sign}(n)\,\theta(n)\,\varphi(n)\right.$$
$$\left.+O(p(N)\,r(N)\,N)\right][1+o(1)]$$

This leads to (8.3)–(8.6) under conditions 4(a)–4(d), respectively. Moreover in case 4(c) we have used the last fact of Lemma 1.1. Thus, Theorem 8.1 is proved completely.

Remark. We should notice that the sets $\sigma(q)$ and $\sigma(Q)$ are independent of an arbitrary potential shear, i.e., these sets do not change with substitution of $q(n+m)$ for $q(n)$ in Eqs. (1.1) and (2.2). At the same time, the formulas (8.2)–(8.6) are not invariant under this substitution. However, we can remove this defect by the choice of the reference point for every particular potential function.

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