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Asymptotic Behavior of Energy Band Associated with a Negative Energy Level

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The mathematical foundation of the tight binding approximation is given. If λ_0 is a negative energy level of a real potential q, then there exists an energy band for a one-dimensional chain with period $2T$ of the same atoms which lies near λ_0. We study this band when T tends to infinity.

KEY WORDS: Tight binding approximation; negative energy level; one-dimensional chain; energy band.

INTRODUCTION

I discuss the energy band in a one-dimensional chain of identical atoms with well-localized atomic states. This problem is usually studied in the framework of the tight binding method[1,3]: a Bloch function is approximated by a linear combination of atomic orbitals (LCAO method), and with the help of this Bloch function the corresponding energy band can be calculated. The tight binding method is expected to give reliable results only for bands generated by well-localized atomic states. The main criticism of the method lies in the difficulty of testing its convergence. On the other hand, if the states are not well-localized, the energy band equation is quite difficult to evaluate due to the presence of three-center integrals. A common, but not always valid, approximation is to neglect these integrals altogether (two-center approximation). If the two-center approximation is adopted, then for a one-dimensional chain one can get the band formula [see Eq. (2.3)]. In Eq. (2.3) the integral shows the "crystal field integral" and the next term coincides with the "interaction

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integral" (ref. 3, p. 104). The parameter d in Eq. (2.3) can be writen as $2\cos 2Tm$, where m is a Bloch wave number or a quasimomentum. In this paper I give the mathematical foundation of Eq. (2.3) if a potential function satisfies Eq. (1.2). It should be noted that Eq. (2.3) is not true in the general case (ref. 3, pp. 107–108).

1. ONE ATOM

First we consider the one-dimensional Schrödinger equation

$$-y''(x)+q(x)\,y(x)=\lambda y(x), \qquad -\infty<x<+\infty \tag{1.1}$$

for a real potential $q(x)$ that

$$\int_{-\infty}^{+\infty}|q|\,dx<\infty \qquad \text{and} \qquad \lim_{T\to+\infty} T\int_{|x|\geqslant T}|q|\,dx=0 \tag{1.2}$$

The spectrum $\sigma_1(q)\subset\mathbb{R}^1$ of this atom consists of a finite number[2] of negative energy levels and the half-axis $[0,+\infty)$. Let $\lambda_0<0$ be an eigenvalue and let $\theta(x)$ be a solution of Eq. (1.1) with $\lambda=\lambda_0$ such that $\int_{-\infty}^{+\infty}\theta^2\,dx=1$, i.e., θ is a normalized eigenfunction. Let $\varphi(x)$ be another solution of Eq. (1.1) with $\lambda=\lambda_0$ such that the Wronskian $\theta\varphi'-\theta'\varphi=1$; then for some constants $C_{\theta,\varphi}>0$ and $C_\pm\neq0$ we have

$$|\theta(x)|\leqslant C_\theta e^{-k|x|}, \qquad |\varphi(x)|\leqslant C_\varphi e^{k|x|}, \qquad -\infty<x<+\infty \tag{1.3}$$

$$C_\pm=\lim_{x\to\pm\infty}\theta(x)\,e^{k|x|}=\mp\lim_{x\to\pm\infty}\theta'(x)\,e^{k|x|}/k \tag{1.4}$$

$$(2C_\pm)^{-1}=\pm\lim_{x\to\pm\infty}k\varphi(x)\,e^{-k|x|}=\lim_{x\to\pm\infty}\varphi'(x)e^{-k|x|} \tag{1.5}$$

Here $k=(-\lambda_0)^{1/2}$.

For later use we *ill need the following combination of two functions* $f(x)$ and $g(x)$:

$$[f,g](x)\stackrel{\text{def}}{=}f(x)\,g'(-x)-f'(x)\,g(-x) \tag{1.6}$$

Then for the solutions θ and φ of (1.1) using (1.4)–(1.5) we will establish the following asymptotic formulas ($|x|\to+\infty$):

$$a(x)=[\varphi,\varphi](x)=(2C_+C_-k)^{-1}\,e^{2k|x|}[1+o(1)] \tag{1.7}$$

$$b(x)=[\theta,\varphi](x)=o(1) \tag{1.8}$$

$$c(x)=[\theta,\theta](x)=2C_+C_-ke^{-2k|x|}[1+o(1)] \tag{1.9}$$

2. INFINITE CHAIN OF ATOMS

For some $T>0$, using the potential $q(x)$, we consider the periodic potential $\tilde{q}(x, T)$ [in shortened form, $\tilde{q}(x)$ or $\tilde{q}$] with period $2T$ defined by

$$\tilde{q}(x, T)=\sum_{n=-\infty}^{+\infty} q(x+2Tn) \tag{2.1}$$

We now consider the Schrödinger equation

$$-y''(x)+\tilde{q}(x, T)\, y(x)=\lambda y(x), \qquad -\infty<x<+\infty \tag{2.2}$$

The spectrum $\sigma_\infty(T, q)\subset \mathbb{R}^1$ of this chain consists of intervals (allowed energy bands) a finite number of which belong to the half-axis $(-\infty, 0)$ (ref. 7, p. 290). Pavlov and Smirnov[6] have proved that if $xq(x)\in L^1(\mathbb{R}^1)$, then there is an allowed energy band which lies near the eigenvalue $\lambda_0=-k^2$ $(k>0)$ of the potential $q(x)$ and its width $\Delta(k, T)$ is of order e^{-2TK} when $T\to +\infty$. It was found Kirsch *et al.*[5] that if $q(x)\, e^{2a|x|}\in L^1(\mathbb{R}^1)$, then

$$\lim_{T\to +\infty} \Delta(k, T)\, e^{2Tk}=8k[|dt^{-1}(ik)/dz|]^{-1}$$

Here $t(z)$ is the transmission coefficient for the operator $1=-d^2/dx^2+q$ and $-a^2<\inf(\text{spectrum } 1)$. In this paper we shall prove the following asymptotic formulas for the nearest band. There is a constant t such that for every $T>t$ and for every $d\in[-2, 2]$ the number $\lambda(d, T)$ which is given by

$$\lambda(d, T)=\lambda_0+\int_{-T}^{T} (\tilde{q}-q)\, \theta^2\, dx-2dkC_+C_-e^{-2Tk}+\varepsilon(d, T) \tag{2.3}$$

belongs to the nearest band. Here $\varepsilon(d, T)$ is a "small" function. If $d=\pm 2$, we obtain the limits of this band and

$$\lim_{T\to +\infty} \Delta(k, T)\, e^{2TK}=8k\,|C_+C_-|$$

Remark. It would be interesting to find the direct proof of the identity $[|dt^{-1}(ik)/dz|]^{-1}=|C_+C_-|$.

3. THE BAND STRUCTURE EQUATION

To find the spectrum σ_∞, we first need two linearly independent solutions $\tilde{\varphi}(x)$ and $\tilde{\theta}(x)$ of Eq. (2.2) with Wronskian $\tilde{\theta}\tilde{\varphi}'-\tilde{\theta}'\tilde{\varphi}=1$. If we put

$$F(\lambda, T)=[\tilde{\theta}, \tilde{\varphi}](T)+[\tilde{\theta}, \tilde{\varphi}](-T) \tag{3.1}$$

then (ref. 4, p. 64)

$$\sigma_\infty(T, q) = \{\lambda \in \mathbb{R}^1 : |F(\lambda, T)| \leqslant 2\} \tag{3.2}$$

Therefore the band limits are defined by

$$F(\lambda, T) = \pm 2 \tag{3.3}$$

We shall consider (3.3) only near λ_0.

4. CONSTRUCTION OF $\tilde{\varphi}$ AND $\tilde{\theta}$

We construct $\tilde{\varphi}(x)$ and $\tilde{\theta}(x)$ using the method of variation of constants. Putting $\kappa = \lambda - \lambda_0$,

$$v(x, T) = \tilde{q}(x, T) - q(x), \qquad w(x, \kappa, T) = v(x, T) - \kappa \tag{4.1}$$

we can write the Schrödinger equation (2.2) as

$$-y'' + (q - \lambda_0)\, y = -wg \tag{4.2}$$

(a) The functions φ and θ are solutions of (4.2), with the right-hand side being zero. Therefore we put

$$\tilde{\varphi}(x) = \alpha(x)[\varphi(x) + \gamma(x)\,\theta(x)] \tag{4.3}$$

Here $\alpha(x)$ and $\gamma(x)$ are such that $\alpha(0) = 1$, $\gamma(0) = 0$, and

$$\alpha'(x)\varphi(x) + [\alpha(x)\gamma(x)]'\,\theta(x) = 0 \tag{4.4}$$

As a consequence of (4.4), we have $\tilde{\varphi}(0) = \varphi(0)$, $\tilde{\varphi}'(0) = \varphi'(0)$, and the function $\tilde{\varphi}(x)$ will be the solution of (4.2) if and only if the functions $\alpha(x)$ and $\gamma(x)$ are the solutions of the following system of nonlinear differential equations:

$$\begin{aligned} \alpha' &= \alpha w \theta(\varphi + \gamma\theta), \qquad & \alpha(0) &= 1 \\ \gamma' &= -w(\varphi + \gamma\theta)^2, \qquad & \gamma(0) &= 0 \end{aligned} \tag{4.5}$$

Here we have used (4.4) and the identity $\theta\varphi' - \theta'\varphi = 1$.

The system (4.5) is equivalent to the system of nonlinear Volterra integral equations

$$\begin{aligned} \alpha(x) &= \exp \int_0^x w\theta(\varphi + \gamma\theta)\, d\xi \\ \gamma(x) &= -\int_0^x w(\varphi + \gamma\theta)^2\, d\xi \end{aligned} \tag{4.6}$$

As will be shown later, in fact we have to find only $\gamma(x)$ and then to calculate $\alpha(x)$.

(b) Furthermore, we shall need to construct the solution $\tilde{\theta}(x)$ of (4.2) such that the Wronskian $\tilde{\theta}\tilde{\varphi}' - \tilde{\theta}'\tilde{\varphi} = 1$. In order to do so, we put $\tilde{\theta}(x) = \alpha^{-1}(x)\,\theta(x) + \alpha_1(x)\,\tilde{\varphi}(x)$ with $(\alpha^{-1})'\,\theta + \alpha_1'\tilde{\varphi} = 0$ and $\alpha_1(0) = 0$. Thus $\tilde{\theta}' = \alpha^{-1}\theta' + \alpha_1\varphi'$ and the Wronskian relation $\tilde{\theta}\tilde{\gamma}' - \tilde{\theta}'\tilde{\varphi} = 1$ holds since $\theta(x)\,\tilde{\varphi}'(x) - \theta'(x)\,\tilde{\varphi}(x) \equiv \alpha(x)$. The function $\tilde{\theta}(x)$ will be a solution of (4.2) if and only if

$$\alpha_1(x) = \int_0^x w\theta^2\alpha^{-2}\,d\xi \tag{4.7}$$

Indeed, $\theta(x)$ is the solution of (1.1) with $\lambda = \lambda_0$ and $\tilde{\varphi}(x)$ is that of (4.2). Therefore, substituting $\tilde{\theta}$ into (4.2), we get the system

$$\begin{aligned} &(\alpha^{-1})'\,\theta + \alpha_1'\,\tilde{\varphi} = 0 \\ &(\alpha^{-1})'\,\theta' + \alpha_1'\,\tilde{\varphi}' = w\theta/\alpha, \qquad \alpha_1(0) = 0 \end{aligned} \tag{4.8}$$

and since $\theta\tilde{\varphi}' - \theta'\tilde{\varphi} \equiv \alpha$, this yields (4.7).

For later use we remark that the functions α, γ, and α_1 depend on x, κ, T, and $\lambda_0 = -k^2$.

5. THE PRINCIPAL EQUATION

Now inserting $\tilde{\theta}$ and $\tilde{\varphi}$ into (3.1) and using the abbreviations (1.7)–(1.9), we obtain

$$\begin{aligned} F(\kappa - k^2, T) = {} & [\alpha_1(T) - \alpha_1(-T)]\,\alpha(T)\,\alpha(-T)\{a(T) \\ & \gamma(T)\,b(T) - \gamma(-T)\,b(-T) + \gamma(T)\,\gamma(-T)\,c(T)\} \\ & + \{b(T)\,\alpha(-T)/\alpha(T) + c(T)\,\gamma(-T)\,\alpha(-T)/\alpha(T) \\ & + b(-T)\,\alpha(T)/\alpha(-T) + c(-T)\,\gamma(T)\,\alpha(T)/\alpha(-T)\} \end{aligned} \tag{5.1}$$

Let

$$G = \alpha_-\alpha_+(a + \gamma_+b_+ + \gamma_-b_- + \gamma_+\gamma_-c) \tag{5.2}$$

$$H = (b_+ + \gamma_-c)\,\alpha_-/\alpha_+ - (b_- + \gamma_+c)\,\alpha_+/\alpha_- \tag{5.3}$$

with $\alpha_\pm = \alpha(\pm T)$, $\gamma_\pm = \gamma(\pm T)$, $a = a(T)$, $b_\pm = \pm b(\pm T)$, and $c = c(T)$.

The functions H and G depend on κ, T, and k. So from (5.1) we find

$$F(\kappa - k^2, T) = G\int_{-T}^{T} (v - \kappa)\,\theta^2\alpha^{-2}\,dx + H \tag{5.4}$$

Hence for every $d \in [-2, 2]$ the band structure equation $F = d$ can be rewritten in the form

$$\kappa = \left[\int_{-T}^{T} v\theta^2\alpha^{-2}\,dx + (H-d)/G\right]\left(\int_{-T}^{T}\theta^2\alpha^{-2}\,dx\right)^{-1} \tag{5.5}$$

For the sake of simplicity, we write (5.5) as

$$\kappa = f(\kappa)$$

Thus, we have established the principal equation for κ. We remark that the function f depends also on d, T, and k. As will be shown later, $\alpha \to 1$, $H \to 0$, $G^{-1} = 2kC_+C_-[1 + o(1)]\exp(-2kT)$ when $T \to +\infty$ and $\kappa \to 0$. Therefore it is clear that the asymptotic formula (2.3) should be valid. Equation (5.1) was found by the author and L. K. Lapshin.

6. ESTIMATES OF THE FUNCTIONS $\gamma(x)$ AND $\alpha(x)$

Let

$$p(T) = \int_{|x| \geqslant T} |q|\,dx + \exp(-2kT) \tag{6.1}$$

It follows from (1.2) and (4.1) that

$$p(T) = \int_{-T}^{T} |v|\,dx + e^{-2kT} \qquad \text{and} \qquad \lim_{T \to +\infty} Tp(T) = 0 \tag{6.2}$$

Using the function $p(T)$, we shall get the required estimates.

To formulate the problem precisely, we make the following assumption concerning κ: For some positive constant C_κ and for every T

$$|\kappa| \leqslant C_\kappa\, p(T) \tag{6.3}$$

According to (4.6), we will need to study the nonlinar Volterra equation

$$\gamma(x) = \int_0^x [\kappa - v(\xi)][\varphi(\xi) + \gamma(\xi)\,\theta(\xi)]^2\,d\xi \tag{6.4}$$

The solution of this equation behaves asymptotically for $|x| \gg 1$ as $\exp(2k\,|x|)$.

Therefore we introduce the new function

$$Z(x) = \gamma(x)\exp(-2k\,|x|) \tag{6.5}$$

which satisfies the equation

$$Z(x)=\int_0^x e^{2k(|\xi|-|x|)}[\kappa-v(\xi)][\varphi_0(\xi)+Z(\xi)\,\theta_0(\xi)]^2\,d\xi \tag{6.6}$$

with $\varphi_0(x)=\varphi(x)\exp(-k\,|x|)$, and $\theta_0(x)=\theta(x)\exp(k\,|x|)$. The function $Z(x)$ will therefore be a bounded function on $[-T, T]$ uniformly with respect to T.

For the proof we shall use the principle of contractive mappings on the space of continuous functions $C[-T, T]$ with the norm

$$\|Z\|=\max_{[-T,T]}|Z(x)| \tag{6.7}$$

Let A be an operator on the right-hand side of (6.6), i.e.,

$$AZ(x)=\int_0^x e^{2k(|\xi|-|x|)}(\kappa-v)(\varphi_0+Z\theta_0)^2\,d\xi \tag{6.8}$$

The operator A maps the closed unit ball

$$B_1(T)=\{Z\in C[-T, T]\colon \|Z\|\leqslant 1\}$$

into itself for sufficiently small T^{-1} and κ. Indeed, the estimates (1.3) give

$$|\theta_0(x)|\leqslant C_\theta, \qquad |\varphi_0(x)|\leqslant C_\varphi, \qquad -\infty<x<+\infty \tag{6.9}$$

Hence if $Z\in B_1$ and $x\in[-T, T]$, we obtain

$$\begin{aligned}|AZ(x)|&\leqslant\left(\int_{-|x|}^{|x|}|v|\,d\xi+2\,|\kappa|\int_0^{|x|}e^{-2kt}\,dt\right)(C_\varphi+C_\theta)^2\\&=\left[\int_{-|x|}^{|x|}|v|\,d\xi+|\kappa|\,(1-e^{-2k|x|})/k\right](C_\varphi+C_\theta)^2\end{aligned} \tag{6.10}$$

By the assumption (6.3)

$$\|AZ\|\leqslant(1+C_\kappa/k)(C_\varphi+C_\theta)^2\,p(T) \tag{6.11}$$

Therefore, by (6.2), there is $T_0>0$ such that for every $T>T_0$

$$\|AZ\|\leqslant 1 \tag{6.12}$$

if $Z\in B_1$.

On the other hand, A is a contractive operator on B_1. To see this, let Z_1, $Z_2\in B_1$. Then, as above,

$$\|AZ_1-AZ_2\|\leqslant 2(1+C_\kappa/k)\,C_\theta(C_\varphi+C_\theta)\,p(T)\,\|Z_1-Z_2\| \tag{6.13}$$

Hence we may set T_0 such that for every $T > T_0$

$$\|AZ_1 - AZ_2\| \leqslant \|Z_1 - Z_2\|/2 \tag{6.14}$$

if $Z_1, Z_2 \in B_1$.

Finally, if T_0 is such that

$$p(T) \leqslant [4(1 + C_\kappa/k)(C_\varphi + C_\theta)^2]^{-1} \tag{6.15}$$

then we have both (6.12) and (6.14) on B_1. Hence, for every $T > T_0$ and for every $\kappa \in [-C_\kappa\, p(T), C_\kappa\, p(T)]$ there exists one and only one solution $Z(x)$ of (6.6) on the interval $|x| \leqslant T$ satisfying the condition $\|Z\| \leqslant 1$. Hence, if $x \in [-T, T]$, then

$$|\gamma(x)| \leqslant \|Z\|\, e^{2k|x|} = \|AZ\|\, e^{2k|x|} \leqslant C_\gamma\, p(T)\, e^{2k|x|} \tag{6.16}$$

with $C_\gamma = (1 + C_\kappa/k)(C_\varphi + C_\theta)^2$.

For later use we will need an estimate of the derivative $\partial\gamma/\partial\kappa$ of the function γ with respect to the parameter κ. Since $\partial\gamma/\partial\kappa = \partial Z/\partial\kappa \exp(2k\,|x|)$, putting $u = \partial Z/\partial\kappa$, we shall consider the identity

$$u(x) = \int_0^x e^{2k(|\xi| - |x|)}(\varphi_0 + Z\theta_0)^2\, d\xi$$

$$+ 2\int_0^x e^{2k(|\xi| - |x|)}(\kappa - v)(\varphi_0 + Z\theta_0)\,\theta_0 u\, d\xi \tag{6.17}$$

For the sake of simplicity, we write (6.17) as

$$u(x) = g(x) + Vu(x) \tag{6.17$'$}$$

Since $\|g\| \leqslant (C_\varphi + C_\theta)^2/k$ and since the inequality

$$\|V\| \leqslant 2(1 + C_\kappa/k)\, C_\theta(C_\varphi + C_\theta)\, p(T) \leqslant 1/2 \tag{6.18}$$

holds by (6.15), we can find $U(x)$ from (6.17) by using the Neumann series for the solution of the linear integral equation. Therefore

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

Hence

$$\left|\frac{\partial\gamma}{\partial\kappa}(x)\right| \leqslant C'_\gamma e^{2k|x|}$$

with $C'_\gamma = 2(C_\varphi + C_\theta)^2/k$. Accordingly, we have the following results.

Lemma 6.1. Let C_κ be a positive constant. There exists a positive number T_0 such that for every $T \geqslant T_0$ and for every $\kappa \in [-C_\kappa p(T), C_\kappa p(T)]$ there is one and only one solution $\gamma(x)$ of Eq. (6.4) such that on the interval $|x| \leqslant T$

$$|\gamma(x)| \leqslant C_\gamma p(T) \exp(2k\,|x|) \tag{6.16'}$$

$$|\partial\gamma(x)/\partial\kappa| \leqslant C'_\gamma \exp(2k\,|x|) \tag{6.19}$$

with the constants $C_\gamma = (1 + C_\kappa/k)(C_\varphi + C_\theta)^2$ and $C'_\gamma = 2(C_\varphi + C_\theta)^2/k$.

Note that we may choose T_0 such that for every $T \geqslant T_0$

$$\int_{|x| \geqslant T} |q|\,dx + e^{-2kT} \leqslant [4(1 + C_\kappa/k)(C_\varphi + C_\theta)^2]^{-1} \tag{6.20}$$

Hence one can solve (6.4) by the method of successive approximations. Hence from (4.6) we obtain

$$\ln\alpha(x) = \int_0^x [v(\xi) - \kappa]\,\theta(\xi)[\varphi(\xi) + \gamma(\xi)\,\theta(\xi)]\,d\xi \tag{6.21}$$

We will need estimates of the function $\ln\alpha(x)$ and its derivative $\partial\ln\alpha/\partial\kappa$.

Lemma 6.2. Let C_κ, C_α, and C'_α be positive constants such that $C_\alpha > C_\kappa C_\theta C_\varphi$ and $C'_\alpha > C_\theta C_\kappa$. Let T_0 be a positive number as in Lemma 6.1. There exists a number $T_1 \geqslant T_0$ such that for every $\kappa \in [-C_\kappa p(T), C_\kappa p(T)]$ we have the estimates

$$\|\ln\alpha\| \leqslant C_\alpha T p(T) \qquad \text{and} \qquad \|\partial\ln\alpha/\partial\kappa\| \leqslant C'_\alpha T \tag{6.22}$$

Proof. The proof is identical to the one for Lemma 6.1. Let $T \geqslant T_0$. By (1.3), (6.3), and (6.16'), we have

$$\|\ln\alpha\| \leqslant \left(\int_{-T}^{T} |v|\,dx + |\kappa|\,T\right) C_\theta$$

$$[C_\varphi + C_\gamma C_\theta\,p(T)] \leqslant T_p(T)(T^{-1} + C_\kappa)\,C_\theta[C_\varphi + C_\gamma C_\theta\,p(T)]$$

Hence there is $T_1 \geqslant T_0$ such that

$$C_\kappa C_\theta C_\varphi < (T^{-1} + C_\kappa)\,C_\theta[C_\varphi + C_\gamma C_\theta\,p(T)] \leqslant C_\alpha$$

and $\|\ln\alpha\| \leqslant C_\alpha T_p(T)$ as $T \geqslant T_1$.

Similarly, by (6.19) and the definition (6.21), we have

$$\left\|\frac{\partial\ln\alpha}{\partial\kappa}\right\| \leqslant \left\|\int_0^x \theta(\varphi + \gamma\theta)\,d\xi\right\| + \left\|\int_0^x (v - \kappa)\,\theta^2\,\frac{\partial\gamma}{\partial\kappa}\,d\xi\right\|$$

$$\leqslant C_\theta[C_\varphi + C_\gamma C_\theta\,p(T)]\,T + (T^{-1} + C_\kappa)\,C_\theta^2 C'_\gamma T p(T) \leqslant C'_\alpha T$$

when T_1 is such that for every $T \geqslant T_1$

$$C_\theta C_\varphi < C_\theta [C_\varphi + C_\gamma C_\theta p(T)] + (T^{-1} + C_\kappa)\, C_\theta^2 C'_\gamma p(T) \leqslant C'_\alpha$$

Remark. We can set, for instance, $C_\alpha = C_\kappa C_\theta C_\varphi + 1$ and $C'_\alpha = C_\theta C_\kappa + 1$.

7. ESTIMATES OF THE FUNCTIONS *H* AND *G*

It should be noted first that the functions $G(\kappa)$ and $H(\kappa)$ depend on T.

Lemma 7.1. Let C_κ, C_g be positive constants and $C_g > 2k\, |C_+ C_-|$. Let T_1 be as in Lemma 6.2. There is a positive number $T_2 \geqslant T_1$ such that for every $T \geqslant T_2$ we have

$$|G(\kappa, T)| \geqslant C_g^{-1} \exp(2kT) \tag{7.1}$$

as $|\kappa| \leqslant C_\kappa p(T)$. Furthermore, if T tends to the infinity, then

$$1/G(\kappa, T) = 2kC_+ C_- [1 + o(1)] \exp(-2kT) \tag{7.2}$$

uniformly with respect to $\kappa \in [-C_\kappa p(T), C_\kappa p(T)]$.

Proof. By (5.2), using the estimates (1.7)–(1.9), (6.16′), and (6.22), we obtain

$$\begin{aligned} |G(\kappa, T)| \geqslant {} & [(2k\, |C_+ C_-|)^{-1} - \varepsilon_1(T) - 2C_\gamma p(T)\, \varepsilon_2(T) \\ & - C_\gamma^2 2k\, |C_+ C_-|\, p(T)^2\, \varepsilon_3(T)] \exp[2kT - 2C_\alpha T p(T)] \end{aligned}$$

with $0 < \varepsilon_j(T) = o(1)$ as $T \to +\infty$. This inequality yields (7.1). Finally, combining (5.2) and (1.7) as above, we obtain (7.2). QED

Lemma 7.2. The function $H(\kappa, T)$ is $o(1)$ uniformly with respect to $\kappa \in [-C_\kappa p(T), C_\kappa p(T)]$ as $T \to +\infty$.

Proof. By (5.3) and (1.8)–(1.9), we have

$$|H(\kappa, T)| \leqslant 2[\varepsilon(T) + C_\gamma p(T)] \exp[2C_\alpha T_p(T)] = o(1)$$

Lemma 7.3. Uniformly with respect to $\kappa \in [-C_\kappa p(T), C_\kappa p(T)]$, we have

$$\left(\int_{-T}^{T} \theta^2 \alpha^{-2}\, dx \right)^{-1} = 1 + o(1) \tag{7.3}$$

as $T \to +\infty$.

Proof. By (6.22) and the normalization condition, we obtain

$$\int_{-T}^{T} \theta^2 \, dx \, e^{-\varepsilon(T)} \leqslant \int_{-T}^{T} \theta^2 \alpha^{-2} \, dx \leqslant e^{\varepsilon(T)}$$

where $\varepsilon(T) = 2C_\alpha T_p(T)$ is a small function. Hence, the formula (7.3) holds. QED

8. EXISTENCE PROOF FOR THE ENERGY BAND

Theorem 8.1. Let C_κ and d_0 be positive constants and $C_\kappa > \max(C_\theta^2, 2k \, |C_+ C_-| \, d_0)$. There exists a positive number t_0 such that for every $T \geqslant t_0$ and for every $d \in [-d_0, d_0]$, Eq. (5.5) has one and only one solution such that $|\kappa| \leqslant C_\kappa p(T)$.

Proof. The equation $\kappa = f(\kappa)$ can be solved by the method of successive approximations. First we will need to prove that if $|\kappa| \leqslant C_\kappa p(T)$, then

$$|f(\kappa)| \leqslant C_\kappa p(T) \tag{8.1}$$

Indeed, using Lemmas 7.1–7.3, we obtain

$$\begin{aligned}
|f(\kappa)| &\leqslant \left[C_\theta^2 \int_{-T}^{T} |v| \, dx[1 + o(1)] + (|H| + d_0)/G \right] [1 + o(1)] \\
&= C_0^2 \int_{-T}^{T} |v| \, dx + 2k \, |C_+ C_-| \, d_0 e^{-2kT} + o[\rho(T)] \\
&\leqslant \max(C_\theta^2, 2k \, |C_+ C_-| \, d_0) \, \rho(T) + o[\rho(T)] \leqslant C_\kappa \rho(T)
\end{aligned}$$

where T is a sufficiently great number.

On the other hand, we shall prove that there is t_0 such that for every $T \geqslant t_0$ and $|\kappa| \leqslant C_\kappa \rho(T)$ we have the estimate

$$|f'(\kappa)| \leqslant 1/2 \tag{8.2}$$

Putting $f(\kappa) = f_1(\kappa) f_2(\kappa)$ with $f_2(\kappa) = (\int_{-T}^{T} \theta^2 \alpha^{-2} \, dx)^{-1}$, we obtain $f_1 = O(p(T))$ and $f_2 = 1 + o(1)$ as $T \to +\infty$. To estimate the derivates, we shall use Lemmas 6.1 and 6.2. Hence $H'(\kappa) = o(T)$,

$$\begin{aligned}
G'(\kappa) &= O[T \exp(2kT)] \\
|f_1'(\kappa)| &\leqslant 2C_\theta^2 C_\alpha' T \int_{-T}^{T} |v| \, dx + |H'/G| + (|H| + d_0) \, |G'/G^2| \\
&= O[Tp(T)] + o[Te^{-2kT}) + O(Te^{-2kT}) = O[Tp(T)]
\end{aligned} \tag{8.3}$$

and

$$|f_2'(\kappa)| \leqslant 2f_2(\kappa)\,\|\partial \ln \alpha/\partial\kappa\| = O(T) \tag{8.4}$$

as $T \to +\infty$. This gives

$$|f'(\kappa)| = O[T_p(T)] \tag{8.5}$$

Therefore there is a positive number t_0 such that for every $T \geqslant t_0$ and $|\kappa| \leqslant C_\kappa p(T)$ the estimate (8.2) is valid.

According to (8.1) and (8.2), Eq. (5.5) can now be solved by the method of successive approximations. QED

Let $d_0 \geqslant 2$, $C > \max(C_0^2, 2k\,|C_+C_-|\,d_0)$ and let $\kappa(d, T)$ ($|d| \leqslant d_0$) be the solution of Eq. (5.5) such that $|\kappa(d, T)| \leqslant Cp(T)$ for T large. We know [Eq. (3.2)] that $\lambda(d, T) = \lambda_0 + \kappa(d, T) \in \sigma_\infty(T, q)$, if $d \in [-2, 2]$ and $\lambda(d, T) \notin \sigma_\infty(T, q)$ when $|d| > 2$. Therefore the interval $\{\lambda(d, T)\colon -2 \leqslant d \leqslant 2\}$ coincides with the energy band which lies near λ_0.

9. ASYMPTOTIC FORMULAS FOR THE BAND

We shall now prove the asymptotic formulas for the band.

Theorem 9.1. Fix a function $q(x)$ obeying (1.2) and let $\tilde{q}(x, T)$ be given by (2.1). Suppose that $\lambda_0 = -k^2 < 0$ and that $\theta(x) \in L^2(-\infty, +\infty)$ is a normalized solution of the Schrödinger equation

$$-y''(x) + q(x)\,y(x) = \lambda_0\,y(x)$$

Let C_0, $C_\pm$ be given by (1.3), (1.4). If $C > \max(C_0^2, 4k\,|C_+C_-|)$ and $\kappa(d, T)$ is a solution of Eq. (5.5) with $d \in [-2, 2]$ such that $|\kappa(d, T)| \leqslant Cp(T)$ for T large, where $p(T)$ is given by (6.1), then:

1. $\lambda(d, T) = \lambda_0 + \kappa(d, T) \in \sigma_\infty(T, q), \quad d \in [-2, 2]$
2. $\lambda(\pm 2, T)$ are the edges of the band
3. $\lambda(d, T) = \lambda_0 + \int_{-T}^{T} [\tilde{q}(x, T) - q(x)]\,\theta^2(x)\,dx$
$$-2kdC_+C_-\exp(-2Tk) + \varepsilon(d, T) \tag{9.1}$$

where $\varepsilon(d, T) = o[p(T)]$ uniformly with respect to $d \in [-2, 2]$ as $T \to +\infty$; and

4. $\lim_{T \to +\infty} |\lambda(2, T) - \lambda(-2, T)|\exp(2Tk) = 8k\,|C_+C_-|$

Proof. According to Theorem 8.1, there exists a constant t such that for every $T > t$ and for every $d \in [-2, 2]$, Eq. (5.5) has one and only one solution $\kappa(d, T) \in [-Cp(T), Cp(T)]$ and by (3.1)–(3.3), $\lambda(d, T) \in \sigma_\infty(T, q)$ iff $d \in [-2, 2]$. This implies parts 1 and 2 of the theorem.

Inserting $\kappa(d, T)$ into (5.5), we obtain

$$\kappa(d, T)=\left\{\int_{-T}^{T}[\tilde{q}(x, T)-q(x)]\,\theta^2(x)\,\alpha^{-2}(x, d, T)\,dx + [H(d, T)-d]/G(d, T)\right\}\left[\int_{-T}^{T}\theta^2(x)\,\alpha^{-2}(x, d, T)\,dx\right]^{-1} \tag{9.2}$$

By Lemmas 7.1–7.3 we can rewrite (9.2) in the form

$$\begin{aligned}\kappa(d, T)&=\left\{\int_{-T}^{T}[\tilde{q}(x, T)-q(x)]\,\theta^2(x)\,dx[1+o(1)] + [o(1)-d]\,2kC_+C_-[1+o(1)]\exp(-2Tk)\right\}[1+o(1)]\\ &=\int_{-T}^{T}[\tilde{q}(x, T)-q(x)]\,\theta^2(x)\,dx-2dkC_+C_-\exp(-2Tk)+o[p(T)]\end{aligned}$$

uniformly with respect to $d\in[-2, 2]$ as $T\to+\infty$. Therefore we have part 3. To prove part 4, we shall consider the derivative $\partial\kappa/\partial d$. Since $\kappa(d, T)\equiv f(\kappa(d, T), d)$,

$$\frac{\partial\kappa}{\partial d}=\frac{\partial f}{\partial\kappa}\frac{\partial\kappa}{\partial d}+\frac{\partial f}{\partial d}$$

Next, note that $\partial f/\partial\kappa=O[Tp(T)]$ [see Eq. (8.5)] and by Lemmas 7.1, 7.3 that

$$\frac{\partial f}{\partial d}=-\left(G\int_{-T}^{T}\theta^2\alpha^{-2}\,dx\right)^{-1}=-2kC_+C_-\exp(-2Tk)[1+o(1)]$$

as $T\to+\infty$. Thus, since $Tp(T)=o(1)$, we have that $\partial\kappa/\partial d=-2kC_+C_-\exp(-2Tk)[1+o(1)]$ uniformly with respect to $d\in[-2, 2]$, which yields 4.

QED

10. THE DIRAC COMB

To illustrate the technique above, we shall consider the Dirac comb. Let $\delta(x)$ be the Dirac function and $q(x)=-2\alpha\delta(x)$, $\alpha>0$. Then the negative eigenvalue if $\lambda_0=-\alpha^2$ with normalized eigenfunction $\theta(x)=\sqrt{\alpha}\exp(-\alpha\,|x|)$. Therefore $\beta=\alpha$ and by (9.1) we obtain

$$\lim_{T\to+\infty}[\lambda(-2, T)-\lambda(2, T)]\exp(2\alpha T)=8\alpha^2 \tag{10.1}$$

where $\lambda(\pm 2, T)$ are the limits of the negative allowed energy band of the potential function $\tilde{q}(x)=-2\alpha\sum_{n=-\infty}^{+\infty}\delta(x+2nT)$. In this case the negative band is determined by the following equation (ref. 4, p. 65):

$$|k\cosh 2kT-\alpha\sinh 2kT|\leqslant k \tag{10.2}$$

It is easy to check that (10.2) yields (10.1) when $k=\alpha+o(1)$ as $T\to+\infty$.

Finally, we remark that for every $\kappa < \alpha^2$ the functions $\varphi(x)$, $\tilde{\varphi}(x)$, $\alpha(x)$, and $\gamma(x)$ are given on the interval $|x| \leqslant T$ by $\varphi(x) = \alpha^{-3/2} \sinh \alpha x$, $\tilde{\varphi}(x) = (\beta \sqrt{a})^{-1} \sinh \beta x$,

$$\alpha(x) = \beta^{-1}(\beta \cosh \beta x + \alpha \sinh \beta |x|) \exp(-\alpha |x|) \tag{10.3}$$

$$\gamma(x) = \frac{\alpha \sinh \beta x \cosh \alpha x - \beta \sinh \alpha x \cosh \beta x}{\alpha^2(\beta \cosh \beta x + \alpha \sinh \beta |x|)} \tag{10.4}$$

with $\beta = (\alpha^2 - \kappa)^{1/2}$.

Indeed, the function φ is a solution of (1.1) and Wronskian $\theta\varphi' - \varphi\theta' = 1$; on the other hand, $v(x) \equiv 0$ and the function $\tilde{\varphi}(x)$ is a solution of (2.2) with $\lambda = -\beta^2 = -\alpha^2 + \kappa$ such that $\tilde{\varphi}(0) = \varphi(0) = 0$ and $\tilde{\varphi}'(0) = \varphi'(0) = \alpha^{-1/2}$. Finally, we can find the functions $\alpha(x)$ and $\gamma(x)$ as the solutions of the following system of equations:

$$\alpha\varphi + \alpha\gamma\theta = \tilde{\varphi}$$

$$\alpha\varphi' + \alpha\gamma\theta' = \tilde{\varphi}'$$

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