The Integrated Density of States for 1D Nanostructures at Zero Bias Limit

L.A.Dmitrieva

Department of Mathematical and Computational Physics, St.Petersburg State University, 198504 St.Petersburg, Russia
E-mail: mila@JK1454.spb.edu

Abstract

By methods of quasiclassical asymptotics the behaviour of the integrated density of states for 1D periodic nanostructures at the zero bias limit is studied. It is shown that the density of states at the zero bias limit has no regular limit while the integrated density of states has. The rigorous proof of this phenomenon given in the paper is based on a novel approach for the quasiclassical asymptotics on the spectrum of the Stark-Wannier operators. A connection of this phenomenon with the zero bias limits of the current through the nanostructures and their conductivity is briefly discussed.

1 Introduction

Some experimental works with tunneling devices have observed an increasing conductivity near zero bias [1]. This "zero-bias anomaly" has been explained in a number of papers by different physical phenomena [2, 3, 4]. Some of these explanations are based on the electron density of states and its behaviour near zero bias. In the present paper we study the behaviour of the density of states and integrated density of states at zero bias and show that the first one has no regular limit while the latter has.

Because the current through the device and, in turn, the conductivity are defined through the integral from the density of states and some smooth function, it means that we should look for a "weak limit" of the density of states. We proof rigorously that the integrated density of states tends to an appropriate limit as the strength of the applied electric field goes to zero. This prove is the main novelty of the paper.
The main mathematical objects in our constructions are the spectral projections kernels of the operator
\[ H = -\frac{d^2}{dx^2} + p(x) - \varepsilon x, \]
which describes 1D periodic structure embedded in an external electric field with the strength \( \varepsilon > 0 \) \(^1\). The function \( p \) is assumed to be a periodic one. The operator \( H \) has been an object of the intensive investigations (see [14, 15, 16, 17, 18, 19] and references therein). However to our best knowledge the behaviour of spectral projections and of the integrated density of states which is expressed in their terms have not been considered as \( \varepsilon \to 0 \).

In papers [16, 17, 18] there has been performed the quasiclassical study of the equation \( Hg = Eg \). These results have been used in [14, 15] for the solution of a number of spectral problems related to the operator \( H \). For instance, there has been studied the behaviour of the residues of the analytical continuation of the resolvent kernel of \( H \) and proved that in an appropriate sense the ladders of resonances are concentrated \( \varepsilon \to 0 \) on the spectral band of the operator \( H_0 \). However the methods used in the above papers do not allow to study the behaviour of the operator \( H \) characteristics on the spectrum which fills the whole axis. In the present paper we overcome the difficulties related to the asymptotics constructions at real energies and hence provide the mathematical basis for studying the integrated density of states and the conductivity near the zero bias limit.

One of the advantages of the approach proposed in the present paper is that we explicitly take into account in the leading order of \( \varepsilon \) the tunneling probabilities through spectral gaps for the device embedded into the electric field. These probabilities are known [17, 18, 19] to be exponentially small w.r.t. to \( \varepsilon \) however they strongly influence the behaviour of the integrated density of states.

## 2 Preliminaries

In this section we recall some facts concerning the one-dimension Schrödinger operator
\[ H_0 = -\frac{d^2}{dx^2} + p(x) \]
with a periodic potential \( p(x + a) = p(x) \) and the Hamiltonian \( H \) given by (1).

The spectrum of \( H_0 \) in \( L_2(\mathbb{R}) \) consists of bands \([\lambda_{2l-2}, \lambda_{2l-1}]\) separated by gaps \((\lambda_{2l}, \lambda_{2l-1})\) [11]. In the present paper we assume that the number of gaps in the spectrum is finite, i.e. \( l = 1, 2, \ldots, N \). Let us note that the class of the \( N \)-gap potentials has been described completely [12] in connection with the algebraic-

\(^1\)It might be the 1D periodic nanostructure generated by the stimulated Mott-Peierls transition on quantum wire (see [6-10] ) with the bias applied
geometrical integration of the Korteweg-de Vries equation. However in the present paper we do not need the knowledge of the explicit form of these potentials but only make use of the fact that number of gaps is finite.

The integrated density of states for the operator $H_0$ is given by the formula \[5\]:

$$N(\lambda) = \frac{1}{a} \int_0^a e(x, x, \lambda) dx,$$

(2)

where $e(x, y, \lambda)$ is the spectral function of $H_0$:

$$e(x, y, \lambda) = \sum_{j=1}^m e_j(x, y)$$

if $\lambda$ belongs to the $m+1$-gap $(\lambda_{2m}, \lambda_{2m+1})$ and

$$e(x, y, \lambda) = \sum_{j=1}^m e_j(x, y) + \frac{1}{\pi} \int_{\lambda_{2m}}^\lambda \frac{\Re[\psi(x, \lambda)\overline{\psi(y, \lambda)}]}{\dot{\lambda}(k)} d\lambda$$

if $\lambda$ belongs to the $(m+1)$-th band $[\lambda_{2m}, \lambda_{2m+1}]$. Here $e_j(x, y)$ is the kernel of the spectral projection of $H_0$ on the $j$-th band $\Delta_j = [\lambda_{2j-2}, \lambda_{2j-1}]$:

$$e_j(x, y) = \frac{1}{\pi} \int_{\Delta_j} \frac{\Re[\psi(x, \lambda)\overline{\psi(y, \lambda)}]}{\dot{\lambda}(k)} d\lambda.$$  \hspace{1cm} (3)

The Bloch functions $\psi(x, \lambda)$ here are assumed to be normalized by the condition

$$\frac{1}{a} \int_0^a \psi(x, \lambda)\overline{\psi(y, \lambda)} dx = 1.$$  \hspace{1cm} (4)

By $\dot{\lambda}(k)$ we denote $\frac{d}{dk} \lambda(k)$ where $\lambda(k)$ is the dispersion function which give the dependence of the spectral parameter $\lambda$ on quasimomentum $k$ [13]. Recall that the Bloch function $\psi(x, \lambda)$ is a quasiperiodic one and $\psi(x + a, \lambda) = e^{ikx} \psi(x, \lambda)$.

Thus the integrated density of states for the operator $H_0$ is nondecreasing function which equals 0 at $\lambda < \inf \sigma(H_0) = \lambda_0$ and is constant on each gap $\Delta_j = (\lambda_{2j-1}, \lambda_{2j})$. It is known that

$$N(\lambda) = \frac{k(\lambda)}{\pi}$$

where $\tilde{k}(\lambda) = \Re k(\lambda)$ and $k(\lambda)$ is the global quasimomentum introduced in [13]. The quasimomentum $k(\lambda)$ is real in bands and has nontrivial imaginary part inside gaps.
We introduce the integrated density of states for the operator $H$ given by (1) as follows

$$N_\varepsilon(E) = \frac{1}{a} \int_0^a e_\varepsilon(x, x, E) dx$$

(5)

where $e_\varepsilon(x, y, E)$ is the corresponding spectral function. In [14, 15] it has been shown that $e_\varepsilon(x, y, E)$ has the form

$$e_\varepsilon(x, y, E) = \frac{1}{2\pi} \int_{-\infty}^E \frac{g(x, E')g(y, E')}{|M(E)|^2} dE'.$$

(6)

Here $g(x, E)$ is a solution of equation $Hg = Eg$ which satisfies the condition $g \to 0$ as $x \to -\infty$. Let us normalize it by the asymptotic relation

$$g(x, E) \sim \frac{c}{\sqrt{E + \varepsilon x}} e^{-\frac{1}{2} \sqrt{|E + \varepsilon x|^3}}$$

(7)

where the real constant $c$ will be fixed later. The function $M(E)$ is the so-called Jost function and is defined by the equation

$$M(E) = \frac{W[g, f]}{W[f, f]}.$$

(8)

Here $W[g, f] \equiv gf' - g'f$ and $f(x, E)$ is the solution of the same equation having the oscillating behaviour as $x \to +\infty$ and normalized by the asymptotic relation

$$f(x, E) \sim \frac{1}{\sqrt{2\sqrt{E + \varepsilon x}}} e^{\frac{1}{2} \sqrt{|E + \varepsilon x|^3}}.$$

From equations (6) and (8) it is clear that $e_\varepsilon(x, y, \lambda)$ does not depend on the choice of the constant $c$ in (7). However it is convenient to fix the normalization of the Jost function $M(E)$ unambiguously. Since we shall study the behaviour of $N_\varepsilon(E)$ end hence of $e_\varepsilon(x, x, E)$ as $\varepsilon \to 0$ it is enough to fix the constant $c$ in the leading order of $\varepsilon$. Let us set

$$c = \exp \left[-\frac{1}{\varepsilon} \left( \int_{-\infty}^{\lambda_0} |k(\lambda)| d\lambda - \int_{-\infty}^0 \sqrt{-\lambda} d\lambda \right) - \int_{-\infty}^{\lambda_0} \Phi(\lambda) d\lambda \right] (1 + O(\varepsilon))$$

(9)

where

$$\Phi(\lambda) = \frac{1}{a} \langle \partial_\lambda \phi(x, \lambda), \phi(x, \lambda) \rangle,$$

(10)

$\phi(x, \lambda)$ is the periodic part of the Bloch function $\psi$ normalized by the condition (4) and $\langle \cdot, \cdot \rangle$ is the standard inner product in $L_2(0, a)$. Since $|k(\lambda)| \sim \sqrt{\lambda}$ as $|\lambda| \to \infty$, the difference of integrals in (9) converges.

To study the behaviour of the integrated density of states for Bloch electrons in electric field (5) at the limit of vanishing strength $\varepsilon$ we have to study the asymptotics of the spectral density $|M(E)|^{-2}$ and of the solution $g(x, E)$ at real values of $E$. 


3 An asymptotic behaviour of the spectral density.

In [14, 15] there has been obtained the asymptotic formula for $M(E)$ which allowed to study the structure of roots of $M(E)$ in the lower half-plane (resonances) and to estimate their imaginary parts. However the formulae obtained can not be effectively used to study the behaviour of the spectral density $|M(E)|^{-2}$ as $\varepsilon \to 0$ on the spectrum and hence the behaviour of the integrated density of states (5).

As it has been mentioned in Introduction in the present paper we propose a novel method of analysis of the Jost function. The advantage of the asymptotic formulae obtained below is that although we study the spectral density only in the leading order of $\varepsilon$ we artificially preserve a number of terms which are exponentially small with respect to $\varepsilon$. However it is these terms which allow us to effectively study the behaviour of the integrated density of states as $\varepsilon \to 0$.

In the case of $N$-gap potential the Jost function $M(E)$ is described in the leading order of $\varepsilon$ as follows

$$M(E) = e^{ix} F_N(E)[1 + O(\varepsilon)].$$

(11)

The function $F_N(E)$ is given by the matrix product

$$
\begin{pmatrix}
F_N \\
F_N
\end{pmatrix} = X_N \ldots X_1 \begin{pmatrix}
F_0 \\
F_0
\end{pmatrix},
$$

(12)

where $F_0 = -i$ and $\xi$ is some phase factor.

The matrices

$$X_l(E) = \begin{pmatrix}
\alpha_l & \beta_l \\
\bar{\beta}_l & \bar{\alpha}_l
\end{pmatrix},$$

(13)

$l = 1, \ldots, N$, have the entries

$$\alpha_l = -i P_l^{-1/2} e^{i(\omega - \omega_l)},$$

(14)

$$\beta_l = -i \sqrt{P_l^{-1}} - 1 e^{-i(\omega - \omega_l)}.$$  

(15)

Here

$$\omega = \frac{E\pi}{\varepsilon a}$$

(16)

is the rescaled energy and $\omega_l$ is the constant:

$$\omega_l = \int_{\pi(l-1)/a}^{\pi l/a} \left( \frac{1}{\varepsilon} \lambda(k) + \Phi(k) \right) dk,$$

(17)
where $\Phi(k)dk \equiv \Phi(\lambda)d\lambda$ with $\Phi(\lambda)$ given by (10). The integration in (17) is performed over the $l$-th Brillouin zone \( \left[ \frac{\pi(l-1)}{a}, \frac{\pi l}{a} \right] \) which corresponds to the $l$-th spectral band $\Delta_l$ under the mapping $k(\lambda)$.

The constant $P_l$ is given as follows

$$P_l = e^{-2\pi\mu_l} \tag{18}$$

with

$$\mu_l = \frac{1}{\varepsilon} \int_{\Delta_l} |\Im k(\lambda)| d\lambda. \tag{19}$$

Here $\Delta_l = (\lambda_{2l-1}, \lambda_{2l})$ is the $l$-th gap in the spectrum of $H_0$. It should be noted that $P_l$ is the probability of transmission of an electron under the influence of applied electric field from the conducting band $\Delta_l$ to the band $\Delta_{l+1}$ (see [16, 17, 19] and references therein).

The phase factor $\xi$ in (11) also can be described explicitly. However we do not need its knowledge since to study the integrated density of states $N\varepsilon(E)$ (5) we need $|M(E)|$ only.

In what follows we show how to simplify the matrix product (12). Let us introduce the parameter

$$\sigma_l = \frac{1}{4} \ln(1-P_l)^{-1} \tag{20}$$

On the basis of (18) and (19) one sees that

$$\sigma_l \sim \frac{1}{4} e^{-2\pi\mu_l} \to 0 \quad \text{as} \quad \varepsilon \to 0 \tag{21}$$

Thus the quantity $\sigma_l$ can be considered as an additional parameter of the problem which is exponentially small in $\varepsilon$. Let

$$\sigma = \max_l \{\sigma_l\}.$$ 

Then the following statement is valid.

**Proposition 1.** Let the function $F_l(E)$ be defined by the matrix product (12). Then in the leading order of $\sigma$

$$\frac{F_l(E)}{F_l(E)} = -1 + O(\sigma) \tag{22}$$

This estimate is uniform w. r. t. $E \in \mathbb{R}$.

**Proof.** This statement can be proved by the mathematical induction method. For $l = 1$ one has

$$\frac{F_1(E)}{F_1(E)} = \frac{e^{-2\sigma - i(\omega - \omega_1)} - e^{i(\omega - \omega_1)}}{e^{i(\omega - \omega_1)-2\sigma} - e^{-i(\omega - \omega_1)}} = \frac{1 - e^{2i(\omega - \omega_1)} + O(\sigma)}{e^{2i(\omega - \omega_1)} + O(\sigma)} = -1 + O(\sigma).$$
Here we used the fact that $F_0 = -i$ and in the second equality we expanded $e^{-2\sigma}$ into the Taylor series as $\sigma \to 0$.

Now suppose that the statement is valid for $l - 1$. Since $(F_l, \overline{F_l})_T = X_l(F_{l-1}, \overline{F_{l-1}})_T$ one has that

$$F_l = i \left(1 - e^{-4\sigma_l}\right)^{-1/2} \left[ e^{i(\omega_1 - 2\sigma_l)} F_{l-1} + e^{-i(\omega_1 - 2\sigma_l)} \overline{F_{l-1}} \right].$$

Hence

$$\frac{F_l}{\overline{F_l}} = \frac{F_l}{-\overline{F_l}} \left( \frac{e^{-2\sigma_l} F_{l-1} + e^{2i(\omega_1 - \omega_l)}}{e^{2i(\omega_1 - \omega_l)} F_{l-1} F_{l-1} + 1} \right).$$

(24)

Now expanding $e^{-2\sigma_l}$ as $\sigma_l \to 0$ and using the induction supposition we obtain (22). $\Box$

On use of this proposition one can obtain the asymptotics of $F_l$ as $\sigma \to 0$.

**Lemma 1.** On the real axis $E$ the functions $F_l, l = 1, \ldots, N$, in the leading order of $\sigma$ are given as follows

$$F_l(E) = e^{i\tilde{\phi}_l(E)} \prod_{j=1}^l \left(1 - e^{-4\sigma_j}\right)^{-1/2} \left( e^{2i(\omega_1 - 2\sigma_j)} - 1 \right) [1 + O(\sigma)],$$

(25)

where

$$\tilde{\phi}_l(E) = -\pi l / 2 - \sum_{j=1}^l (\omega - \omega_1).$$

(26)

**Proof.** Take out from square brackets in (23) the multiplier $F_{l-1}$, and then use the recursion procedure. This yields:

$$F_l = (i)^l \prod_{j=1}^l \left(1 - e^{-4\sigma_j}\right)^{-1/2} \prod_{j=1}^l \left[ e^{i(\omega_1 - 2\sigma_j)} \left( \frac{F_{j-1}}{F_{j-1}} \right) + e^{-i(\omega_1 - \omega_j)} \right].$$

Now the statement of the lemma is obtained easily on use of the asymptotic relation (22) for the ratio $(F_{j-1}/F_{j-1})$. $\Box$

Taking now the absolute value of the r.h.s. of (25) one easily obtains $|F_N|$. To write down it in a compact form let us introduce the function

$$\delta(\omega, \omega', \sigma) = \frac{\tanh \sigma}{\sin^2 (\omega - \omega') + \tanh^2 \sigma \cos^2 (\omega - \omega')}$$

and the functions

$$\delta_j(E) \equiv \delta(E \pi \varepsilon / a, \omega_j, \sigma_j), \quad j = 1, \ldots, N$$

(28)

(recall that $\omega_j$ and $\sigma_j$ are given by (17) and (20) respectively). Then

$$\frac{1}{|F_N(E)|^2} = \prod_{l=0}^N \delta_l(E)(1 + O(\sigma)).$$

(29)
Now on use of the asymptotics (11) one obtains the main statement of this section.

**Theorem 1.** In the leading order of $\varepsilon$ the spectral density $|M(E)|^{-2}$ is given as follows

\[ \frac{1}{|M(E)|^2} = \prod_{j=1}^{N} \delta_j(E)(1 + O(\varepsilon)), \quad (30) \]

where the functions $\delta_j$ are defined by (28).

4 Weak limit of the spectral density.

The asymptotic formula (30) obtained in the previous section allows to prove that the spectral density $|M(E)|^{-2}$ in a weak sense as $\varepsilon \to 0$ tends to unit. This important fact will be essentially used in the study of the integrated density of states (5).

**Theorem 2.** Let $\Delta E$ be an interval of the real axis $E$ and $f(E)$ be an arbitrary smooth function defined on it. Then

\[ \lim_{\varepsilon \to 0} \int_{\Delta E} \frac{f(E)dE}{|M(E)|^2} = \int_{\Delta E} f(E)dE. \quad (31) \]

On use of the asymptotic relation (30) it is enough to show that

\[ \lim_{\varepsilon \to 0} \int_{\Delta E} \left( \prod_{j=1}^{N} \delta_j(E) \right) f(E) = \int_{\Delta E} f(E)dE. \quad (32) \]

Will shall prove the latter fact by several steps.

**Proposition 2.** Let $\Delta \omega_n = [\omega' + \pi n - \pi/2, \omega' + \pi n - \pi/2]$, $\omega'$ be the fixed point, $n$ be an arbitrary integer and $f(\omega)$ be a smooth function on $\Delta \omega_n$. Let $\delta(\omega, \omega', \sigma)$ be defined by (27). Then

\[ \lim_{\sigma \to 0} \frac{1}{\pi} \int_{\Delta \omega_n} \delta(\omega, \omega', \sigma)f(\omega)d\omega = f(\omega' + \pi n) \quad (33) \]

**Proof.** Make the change of variables

\[ z = \tan(\omega - \omega' - \pi n) \]

and denote

\[ \hat{\sigma} = \tanh \sigma, \quad \hat{f}(z) = f(z + \omega' + \pi n) \]

Then

\[ \lim_{\sigma \to 0} \frac{1}{\pi} \int_{\Delta \omega_n} \delta(\omega, \omega', \sigma)f(\omega)d\omega = \lim_{\sigma \to 0} \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\hat{\sigma}\hat{f}(z)}{\sigma^2 + z^2}dz. \]
Due to the fact that $\hat{\sigma}/(\hat{\sigma}^2 + z^2)$ as $\sigma \to 0$ is the $\delta$-type sequence the r.h.s. of the latter equals $\hat{f}(0) = f(\omega' + \pi n)$. □

Lemma 2. Let $\Delta E$ be an real interval, $f(E)$ be a smooth function and $\delta_j(E)$ is given by (28). Then

$$\lim_{\varepsilon \to 0} \int_{\Delta E} \delta_j(E) f(E) dE = \int f(E) dE. \quad (34)$$

Proof. On use of the definition of $\delta_j$ one has

$$\int_{\Delta E} \delta_j(E) f(E) dE = \frac{\varepsilon a}{\pi} \int_{\Delta \omega} \delta(\omega, \omega_j, \sigma_j) \tilde{f}(\omega) d\omega, \quad (35)$$

where

$$\Delta \omega = \frac{\pi \Delta E}{\varepsilon a} \quad \text{and} \quad \tilde{f}(\omega) = f\left(\frac{\varepsilon a \omega}{\pi}\right).$$

Let us split the interval $\Delta E$ on subintervals which have the length $\varepsilon a$ and the middle points

$$E_j^{(n)} = \frac{\varepsilon a}{\pi} \omega_j + \varepsilon an = \frac{a}{\pi} \int_{\Delta j} [\lambda(k) + \varepsilon \Phi(k)] dk + \varepsilon an$$

(here $n \in \mathbb{Z}$ is such that $E_j^{(n)} \in \Delta E$). Under this procedure the interval $\Delta \omega = \frac{\varepsilon a \Delta E}{\pi}$ is splitted into subintervals $\Delta \omega_n^{(j)} = [\omega_j + \pi n - \pi/2, \omega_j + \pi n - \pi/2]$ where $\omega_j$ is given by (17). Thus the integral in the r. h. s. of (35) can be presented as the sum of integrals over $\Delta \omega_n^{(j)}$. According to proposition 2 each of them as $\sigma_j \to 0$ tends to $\pi \tilde{f}(\omega_j + \pi n) \equiv \pi f(E_j + \varepsilon an)$. Thus the r. h. s. of (35) takes the form

$$\varepsilon a \sum_n f(E_j + \varepsilon an)$$

where summation is performed over such $n$ that $E_j^{(n)} = E_j + \varepsilon an \in \Delta E$. Obviously as $\varepsilon \to 0$ this sum gives the integral in the r. h. s. of (34). □

The statement of lemma 2 differs from that we need to prove, namely equation (32), by the change of the single multiplier $\delta_j(E)$ by their product. In this connection we have to prove that in appropriate sense for some $j$

$$\prod_{l=0}^N \delta_l(E) \sim \delta_j(E) \quad \text{as} \quad \varepsilon \to 0 \quad (36)$$

Due to the singular behaviour of $\delta_j(E)$ as $\varepsilon \to 0$ the direct analytic proof of (36) meets serious difficulties. Therefore we shall use the relation (29), take into account that the function $F_N(E)$ is defined by the matrix product (12) and perform more detailed analysis of the latter.

Together with functions $F_N(E)$ let consider the functions $F_N^{(l)}(E)$ which we define as follows

$$\left( \begin{array}{c} F_N \\ F_N^{(l)} \\ \end{array} \right) = X_N \cdots X_l \left( \begin{array}{c} F_{l-1} \\ F_{l-1}^{(l)} \\ \end{array} \right) = \frac{i}{2} F_{l-1} - \frac{i}{2} F_{l-1}^{(l)}$$
On use of (14),(15) one has that
\[ \det X_l = 1. \]

Hence
\[ F_N F_N^{(l)} - F_N F_N^{(l)} = -i |F_{l-1}|^2 \]
and therefore
\[ \left| \frac{F_{l-1}}{F_N} \right|^2 = -2 \Im \left( \frac{F_N^{(l)}}{F_N} \right). \tag{37} \]

Now one can easily obtain the asymptotic formula for \( F_N^{(l)} (E) \). To this end repeat the proof of lemma 1 taking into account the additional multiplier \( -\frac{i}{2} \) in definition of \( F_N^{(l)} (E) \). The result is the following statement.

**Proposition 3.** In the leading order of \( \sigma \) the functions \( F_N^{(l)} (E) \) have the form
\[
F_N^{(l)} (E) = i e^{\hat{\phi}_N (E)} \prod_{j=1}^N \left( 1 - e^{-4\sigma_j} \right)^{-1/2} \left( e^{2i(\omega - \omega_j)} - 2\sigma_l + 1 \right) \star \] 
\[
\prod_{j=1}^N \left( e^{2i(\omega - \omega_j)} - 2\sigma_l - 1 \right) \left[ 1 + O(\sigma) \right].
\]

Compare now the obtained formula for \( F_N^{(l)} \) with the equation (25) for \( F_N \). Obviously
\[
\frac{F_N^{(l)}}{F_N} = i \left( e^{2i(\omega - \omega_l)} - 2\sigma_l + 1 \right) \left( e^{2i(\omega - \omega_l)} - 2\sigma_l - 1 \right) \left[ 1 + O(\sigma) \right]
\]
Inserting this representation into (37) and performing simple calculations one obtains the following statement.

**Lemma 3.** On the real axis \( E \) in the leading order of \( \sigma \)
\[
\left| \frac{F_{l-1}(E)}{F_N(E)} \right|^2 = \delta_l(E)(1 + O(\sigma)) \tag{38}
\]
when \( \delta_l(E) \) is given by (28).

The estimate (36) is just the simple consequence of (38). Indeed, set \( l = 1 \) and note that \( F_0 = -i \). Then
\[
\prod_{j=1}^N \delta_j(E) \left[ 1 + O(\sigma) \right] = \left| \frac{1}{F_N(E)} \right|^2 = \delta_1(E) \left[ 1 + O(\sigma) \right] \tag{39}
\]
Here the first equality is due to (29) and the second follows from (38).

Now the statement of the theorem formulated in the beginning of the present section is the direct consequence of lemma 2 and the relation (39).
5 Nonuniform asymptotics of the solution \( g(x, E) \)

In this short section we essentially use the results of the paper [14]. However we need this section since the nonuniform w. r. t. \( E \) asymptotics of solution \( g(x, E) \) combined with the behaviour of \( M(E) \) studied in the previous section define the asymptotic behaviour of the integrated density of states (5).

Quasiclassical analysis of equation \( Hf = Ef \) performed in [14, 15, 16, 17, 18] leads to an important link between the dispersion function \( \lambda(k) \) of the operator \( H_0 \) and the variable \( E + \varepsilon x \) which naturally arises in the asymptotics of \( g(x, E) \) given by (7) as \( x \to -\infty \). This the link has form

\[
\lambda(k) = E + \varepsilon x \tag{40}
\]

and is valid for all \( x \). At any fixed \( x \) this link can be considered as identification between the real axis \( E \) and the spectral axis \( \lambda \) of the operator \( H_0 \). Let us denote by

\[
\Delta_l(\varepsilon) = [\lambda_{2l-2} - \varepsilon x, \lambda_{2l-1} - \varepsilon x] \tag{41}
\]

the shifted \( l \)-th band of \( H_0 \) By

\[
\overline{\Delta_l}(\varepsilon) = (\lambda_{2l-2} - \varepsilon x, \lambda_{2l-1} - \varepsilon x) \tag{42}
\]

we denote the shifted \( l \)-th gap.

As \( \varepsilon \to 0 \) the asymptotics of \( g(x, E) \) turns out to be essentially different at \( E \in \Delta_l(\varepsilon) \) and at \( E \in \overline{\Delta_l}(\varepsilon) \). Inside the shifted bands \( \Delta_l(\varepsilon) \)

\[
g(x, E) = (A_l(E)f_l(x, E) + \bar{A}_l\overline{f_l(x, E)})[1 + O(\varepsilon)]. \tag{43}
\]

Here

\[
A_l(E) = e^{i\eta}F_{l-1}(E) \tag{44}
\]

and

\[
f_l(x, E) = (\lambda(k))^{-1/2} \exp \left[ \int_{E + \varepsilon x}^{E+e x} \left( -\frac{i}{\varepsilon}k(\lambda) + \Phi(\lambda) \right) d\lambda \right] \phi(x, \lambda) \tag{45}
\]

The phase factor \( \eta \) in (44) can be written down explicitly but we do not need it below. The function \( \phi(x, \lambda) \) in (45) is a periodic part of the Bloch solution \( \psi(x, \lambda) \) normalized by the condition (4). The variables \( k \) and \( \lambda \) depend on \( (E + \varepsilon x) \) according to the relation (40) and \( \Phi(\lambda) \) is given by (10).

Remark. The asymptotics (43) is valid outside the \( \varepsilon^{1/3} \)-vicinity of the shifted edges \( \lambda_l - \varepsilon x \) [14, 16]. In the vicinity of these points one has to use the local asymptotics [18].
In the shifted gaps $\Delta_l(\varepsilon)$ outside the $\varepsilon^{1/3}$-vicinity of the shifted edges $\lambda_l - \varepsilon x$ the solution $g$ has the form
\[
g(x, E) = (H_l(E)h_l^-(x, E) + G_l(E)h_l^+(x, E))[1 + O(\varepsilon)]
\] (46)

The coefficients $H_l(E)$ and $G_l(E)$ are related with coefficients $A_l, \bar{A}_l$ as follows
\[
H_l = \frac{1}{2} \left[ e^{i\pi/4} e^{i(\omega - \omega_l)} A_l + e^{-i\pi/4} e^{-i(\omega - \omega_l)} \bar{A}_l \right]
\] (47)
\[
G_l = \left[ e^{-i\pi/4} e^{i(\omega - \omega_l)} A_l + e^{i\pi/4} e^{-i(\omega - \omega_l)} \bar{A}_l \right]
\] (48)

Recall that $\omega$ and $\omega_l$ are given by (16) and (17) respectively.

The functions $h_l^\pm(x, E)$ have the form
\[
h_l^\pm(x, E) = |\hat{\lambda}(k)|^{-1/2} \exp \left[ \pm \int_{\lambda_{2l-1}}^{E+\varepsilon x} \left( \frac{1}{\varepsilon} |\Im \lambda(k)| + \Phi(\lambda) d\lambda \right) \phi_\pm(x, \lambda) \right]
\] (49)

The function $h^+$ exponentially increases and $h^-$ exponentially decreases as $\varepsilon \to 0$ inside the interval $\Delta_l(\varepsilon)$.

6 The asymptotics of spectral projections kernels.

Let us denote by $e_\varepsilon(x, y, \Delta E)$ the kernel of the spectral projection of the operator $H$ on the interval $\Delta E$. Due to (6) it has the form
\[
e_\varepsilon(x, y, \Delta E) = \frac{1}{2\pi} \int_{\Delta E} \frac{g(x, E)g(y, E)}{|M(E)|^2}
\] (50)

**Theorem 3.** Let $\Delta'_l(\varepsilon) \subset \Delta_l(\varepsilon)$ be a subinterval of the shifted $l$-th band $\Delta_l(\varepsilon)$ such that it does not contain the $\varepsilon^{2/3}$-vicinity of the edges and $\Delta'_l(\varepsilon) \to \Delta_l$ as $\varepsilon \to 0$ where $\Delta_l$ is the $l$-th band of $H_0$. Then at bounded $|x|, |y|$\[
\lim_{\varepsilon \to 0} e_\varepsilon(x, y, \Delta'_l(\varepsilon)) = e_l(x, y)
\]

where $e_l(x, y)$ is the kernel of the spectral projection of the operator $H_0$ on the $l$-th band $\Delta_l \equiv \Delta_l(0)$.

**Proof.** Let us rewrite (45) in the form
\[
f_l(x, E) = (\hat{\lambda}(k))^{-1/2} \psi(x, \lambda) e^{iS(x, E, \varepsilon)}
\] (51)

where
\[
S(x, E, \varepsilon) = \frac{1}{\varepsilon}(E + \lambda_{2l-2})k - \int_{\pi(l-1)}^{K} \left( \frac{1}{\varepsilon} \lambda(k) + \Im \Phi(k) \right) dk.
\]
Since $k$ depends on $(E + \varepsilon x)$ accordingly to (40) then on the basis of (43), (51) one has that at $E \in \Delta_l(\varepsilon)
abla$

$$g(x, E)g(y, E) = (T_1 + T_2)(1 + O(\varepsilon))$$  \hspace{0.5cm} (52)

where

$$T_1 = \frac{2\Re[\psi(x, \lambda)\overline{\psi(y, \lambda)}]}{\lambda(k)}|A_l(E)|^2$$  \hspace{0.5cm} (53)

$$T_2 = 2\lambda^{-1}\Re\left[\psi(x, \lambda)\psi(y, \lambda)e^{2iS(x, E, \varepsilon)}A_l^2(E)\right].$$  \hspace{0.5cm} (54)

Consider the contribution of each term in (52) into the kernel $e_\varepsilon(x, y, \Delta_l(\varepsilon))$ given by (6). Taking into account that $|A_l| = |F_{l-1}|, |M| = |F_N|$ and using the statement of Lemma 3, namely the estimate (38), one obtains

$$\frac{1}{2\pi} \int_{\Delta_l(\varepsilon)} \frac{T_1(x, E)}{|M(E)|^2}dE = \frac{1}{\pi} \int_{\Delta_l(\varepsilon)} \frac{\Re[\psi(x, \lambda)\overline{\psi(y, \lambda)}]}{\lambda(k)}\delta_l(E)[1 + O(\varepsilon)]dE$$  \hspace{0.5cm} (55)

Make use of (34) and note that $\Delta_l(\varepsilon) \to \Delta_l$ and $E \to \lambda$ as $\varepsilon \to 0$. Then it is obvious that the limit of r. h. s. of (55) is exactly the kernel of spectral projection $e_l(x, y)$ of $H_0$ on the $l$-th band given by (3). Consequently the statement of the theorem is valid if

$$\frac{1}{2\pi} \int_{\Delta_l(\varepsilon)} \frac{T_2(x, E)}{|M(E)|^2}dE \to 0 \hspace{0.5cm} \varepsilon \to 0.$$  \hspace{0.5cm} (56)

However this fact is quite obvious due to the rapid oscillations of the phase factor $\exp [iS(x, E, \varepsilon)]$ as $\varepsilon \to 0$. \hspace{0.5cm} $\square$

**Theorem 4.** Let $\Delta_l'(\varepsilon) \subset \overline{\Delta_l(\varepsilon)}$ be a subinterval of the shifted $l$-th gap $\Delta_l(\varepsilon)$ given by (42) such that it does not contain the $\varepsilon^2/3$-vicinity of the edges and $\Delta_l'(\varepsilon) \to \overline{\Delta_l}$ as $\varepsilon \to 0$ where $\overline{\Delta_l}$ is the $l$-th gap of $H_0$. Then at bounded $|x|, |y|$ and bounded $|\Delta_l(\varepsilon)|$

$$\lim_{\varepsilon \to 0} e_\varepsilon(x, y, \Delta_l'(\varepsilon)) = 0.$$  \hspace{0.5cm} (57)

**Proof.** At $E \in \overline{\Delta_l(\varepsilon)}$ the solution $g(x, E)$ is given by (46). For the sake of simplicity let us assume that $x = y$ (note that in studying the integrated density of states we need namely this case). Then

$$g^2(x, E) = (G_l^2(h_l^+)^2 + 2H_lG_lh_l^+h_l^- + H_l^2(h_l^-)^2)[1 + O(\varepsilon)]$$  \hspace{0.5cm} (58)

Let us subsequently consider the contribution to $e_\varepsilon(x, x, \Delta_l')$ of each term in (58). On use of (50) and (56) the contribution of the first term can be written as

$$\int_{\Delta_l'(\varepsilon)} \frac{G_l^2(E)h_l^+(x, E)^2}{|M(E)|^2} = (-i(I_1 - \bar{I}_1) + I_2)[1 + O(\varepsilon)]$$
where
\[ I_1 = \int_{\Delta_1(\varepsilon)} e^{2i(\omega - \omega_I)} e^{2\gamma(x, E, \varepsilon)} \frac{F_{l-1}^2(E)}{|F_N(E)|^2} q(x, E, \varepsilon) dE \]
and
\[ I_2 = \int_{\Delta_2(\varepsilon)} e^{2\gamma(x, E, \varepsilon)} \frac{|F_{l-1}(E)|^2}{|F_N(E)|^2} q(x, E, \varepsilon) dE \]

Here
\[ \gamma(x, E, \varepsilon) = \frac{1}{\varepsilon} \int_{\lambda_{2l-1}}^{E_{+\varepsilon}} |\Re(k(\lambda))| d\lambda > 0 \]
and
\[ q(x, E, \varepsilon) = \frac{\phi^2(x, k)}{|\lambda(k)|} \exp \left[ 2 \int_{\lambda_{2l-1}}^{E_{+\varepsilon}} \Phi(\lambda) d\lambda \right]. \]

Now make simple estimates of \( I_2 \). Recall that
\[ \left| \frac{F_{l-1}(E)}{F_N(E)} \right|^2 = -\delta_I(E)(1 + O(\sigma)). \] (57)

Then notice that at \( E \in \Delta_l(\varepsilon) \):
\[ \gamma(x, E, \varepsilon) \leq \frac{1}{\varepsilon} \int_{\lambda_{2l-1}}^{\lambda_{2l}} |\Re(k(\lambda))| d\lambda \equiv \pi \mu_l \]
end hence
\[ e^{2\gamma(x, E, \varepsilon)} \leq e^{2\pi \mu_l} \equiv \frac{1}{1 - e^{-4\sigma_l}} \] (58)

Inserting (57), (58) into the expression for \( I_2 \) one obtains
\[ |I_2| \leq Q \int_{\Delta_l(\varepsilon)} \frac{\delta_I(E)}{(1 - e^{-4\sigma_I})} dE = \]
\[ Q \int_{\Delta_l(\varepsilon)} \frac{\tanh \sigma_I}{(1 - e^{-4\sigma_I})} \frac{1}{\sin^2(\omega - \omega_I) + \tanh^2 \sigma_I \cos(\omega - \omega_I)} dE, \]
where \( Q \geq |q(x, E, \varepsilon)| \). Expanding the latter expression in powers of \( \sigma_I \) as \( \sigma_I \to 0 \) one gets
\[ I_2 \leq \frac{Q}{4} \int_{\Delta_l(\varepsilon)} \frac{dE}{\sin^2(\omega - \omega_I)} (1 + O(\sigma_I)) = \]
\[ \frac{\varepsilon aQ}{4\pi} \left[ \cotg \left( \frac{\lambda_2 \pi}{\varepsilon a} - \omega l \right) - \cotg \left( \frac{\lambda_2 - 1 \pi}{\varepsilon a} - \omega l \right) \right] (1 + O(\varepsilon)) \]

Thus

\[ I_2 \to 0 \quad \text{as} \quad \varepsilon \to 0. \]

The integral \( I_1 \) also vanishes as \( \varepsilon \to 0 \). Indeed, due to the chain of estimates

\[ \frac{F_i^2}{|M|^2} = \frac{F_i}{F_N} (1 + O(\varepsilon)) = - \frac{F_i}{F_N} (1 + O(\varepsilon)) = - \delta_i(E)(1 + O(\varepsilon)) \]

it differs from the integral \( I_2 \) by the presence of the rapidly oscillating factor. Thus we have shown that the contribution of the first term in (56) into the kernel \( e_\varepsilon(x, x, E) \) vanishes as \( \varepsilon \to 0 \).

Consider briefly the contribution of the second term in (56). Notice that

\[ H_l G_l = \frac{1}{2} \left( e^{2i(\omega - \omega_l)} A^2_l + e^{-2i(\omega - \omega_l)} A^2_l \right) \]

and hence

\[ \int_{\Delta_l(\varepsilon)} \frac{H_l G_l h^+_l h^-_l}{|M(E)|^2} \to 0 \]

because each term in this integral contains the rapidly oscillating factor which causes the vanishing of the limits as \( \varepsilon \to 0 \).

Finally, the contribution of the third term in (56) into spectral projections on \( \Delta_l(\varepsilon) \) also tends to 0. It becomes quite clear if one compare this term with the first one. Instead of exponentially growing factor \( e^{2\gamma(x, E, \varepsilon)} \) the third term exponentially decreases as \( e^{-2\gamma(x, E, \varepsilon)} \). Since we have proved that contribution of the first term vanishes the vanishing of the third one becomes obvious.

### 7 Density of States and Integrated Density of States

Along with the integrated density of states (5) one can consider the density if states

\[ n_\varepsilon(E) = \frac{dN_\varepsilon(E)}{dE}. \]

In our case it has the form

\[ n_\varepsilon(E) = \frac{1}{a} \int_0^a \beta(x, E)dx, \]

where

\[ \beta(x, E) = \frac{1}{2\pi |M(E)|^2} g^2(x, E). \]
The density of states has no regular limit as \( \varepsilon \to 0 \). Indeed as it has been shown in Sec. 4 the spectral density \( |M(E)|^{-2} \) is a sort of periodic \( \delta \)-type sequence and its limit is defined only in a weak sense (31). The product \( g^2(x, E) \) due to (52), (54) also has no regular limit.

However the limit of the integrated density of states (5) as \( \varepsilon \to 0 \) is well defined. This is the direct consequence of the results of the previous section. Indeed if \( E \in \Delta^\prime_{m+1}(\varepsilon) \) (for the notations see theorem 3) the integral (6) at \( y = x \) can be presented in the form

\[
e(\varepsilon, x, E) = \sum_{j=1}^{m} \int_{\Delta_j(\varepsilon)} \beta(x, E) dE + \sum_{j=0}^{m} \int_{\Delta_j(\varepsilon)} \beta(x, E) dE + \\
\int_{E_{2m}^\varepsilon}^{E} \beta(x, E) dE + \sum_{j=0}^{2m} \int_{\Delta_j(\varepsilon)} \beta(x, E) dE.
\] (59)

Here \( \Delta_j(\varepsilon) \) and \( \overline{\Delta_j(\varepsilon)} \) are subintervals of shifted bands and gaps described in theorems 3 and 4 respectively. By \( V_j^\varepsilon \) we denote the \( \varepsilon^{2/3} \)-vicinity of the points \( \lambda_j - \varepsilon x \) and \( E_{2m}^\varepsilon > \lambda_{2m} - \varepsilon x \in V_j^\varepsilon \).

As it follows from theorem 3 at the zero bias limit

\[
\sum_{j=1}^{m} \int_{\Delta_j(\varepsilon)} \beta(x, E) dE \to \sum_{j=1}^{m} e_j(x, x),
\] (60)

where \( e_j(x, x) \) is given by (3) and

\[
\int_{E_{2m}^\varepsilon}^{E} \beta(x, E) dE \to \int_{\lambda_{2m}}^{\lambda} \left| \frac{\Re[\psi(x, \lambda)\psi(y, \lambda)]}{\lambda(k)} \right| d\lambda.
\] (61)

The consequences of theorem 4 is the limit

\[
\sum_{j=0}^{m} \int_{\Delta_j(\varepsilon)} \beta(x, E) dE \to 0.
\] (62)

One also can prove that

\[
\int_{V_j^\varepsilon} \beta(x, E) dE \to 0.
\] (63)

To this end one needs a more detailed analysis of the behaviour of \( \beta(x, E) \) in the \( \varepsilon^{2/3} \)-vicinity of the shifted edges \( \lambda_j - \varepsilon x \). This can be done explicitly, however it is out the scope of the present paper.
Finally inserting the limits (60) (61) (62) (63) into (59) one obtains that at zero bias limit

\[ e_\varepsilon(x, x, E) \rightarrow \sum_{j=1}^{m} e_j(x, x) + \frac{1}{\pi} \int_{\lambda_{2m}}^{\lambda} \frac{\Re[\psi(x, \lambda)\overline{\psi(x, \lambda)}]}{\lambda(k)} d\lambda \equiv e(x, x, \lambda). \quad (64) \]

Here \( E \) belongs to the \( m + 1 \)-th shifted band.

Analogously one can prove that if \( E \) belongs to the shifted \( m + 1 \)-th gap at the zero bias limit

\[ e_\varepsilon(x, x, E) \rightarrow \sum_{j=1}^{m} e_j(x, x) \quad (65) \]

Since all the limits proved above are valid for arbitrary \( x \), one can integrate them w.r.t. \( x \) within arbitrary finite interval, say \([0, a]\)

Thus we came to the following statement.

**Theorem 5** In the zero bias limit \( \varepsilon \rightarrow 0 \): \( E = \lambda \) and

\[ N_\varepsilon(E) \rightarrow N(\lambda). \]

Here the integrated density of states \( N_\varepsilon(E) \) is given by (5) and \( N(\lambda) \) is defined by (2).

**References**

[1] L.Y.L.Shen, J.M.Rowell, Phys.Rev. **165** (1968) 566

[2] C.B.Duke, *Tunneling in Solids*, Suppl.10, Solid State Phys. (Eds.F.Seitz, D.Turnbull) Academic, N.Y., 1969

[3] J.A.Appelbaum, Phys.Rev **154** (1967) 633

[4] N.C.Kluksdahl, A.M.Kriman, D.K.Ferry, Phys.Rev. **B39** (1989) 7720

[5] G.V.Rosenblum, M.Z.Solomyak, M.A.Shubin, *Spectral Theory of Differential Operators*, in Modern Topics of Mathematics, **64**, VINITI, Moscow, 1989

[6] B.S.Pavlov, G.P.Miroshnichenko, Patent Application 5032981/25 (0113431)(Russia) from 12.03.1992

[7] I.Antoniou, B.S.Pavlov, A.Yafyasov,*Quantum Electronic Devices Based on Metal-Dielectric Transition in Low-Dimensional Quantum Structures*, in: "Combinatorics, Complexity, Logic, Proceedings of DMTCS’96 (Eds. D.S.Bridges, C.Calude, J.Gibbons, S.Reeves, I.Witten) Springer-Verlag, Singapore, 1996, 90-104
[8] A.M.Yafyasov, V.B. Bogevolnov, T.V. Rudakova, *Physical Principles of Construction of Quantum Electronic Devices Based on Metal-Dielectric Transition. Quantum Interferential Electronic Transistor (QIET)*, Preprint IPRT # 99-95, 1995, St.Petersburg

[9] L.A.Dmitrieva, Yu.A.Kuperin, G.E.Rudin, *Mathematical Models and Numerical Simulations for Quantum Interferential Device Based on Metal-Dielectric Transition*, Preprint IPRT # 170-01, 2001, St.Petersburg

[10] L.A.Dmitrieva, Yu.A.Kuperin, G.E.Rudin, *Numerical Study of Finite SPMT Operational Regimes*, Preprint IPRT # 171-01, 2001, St.Petersburg

[11] E.C.Titchmarsh, *Expansion in eigenfunctions connected with differential operators of second order*, v.2, IL, Moscow, 1961

[12] B.A.Dubrovin, V.A.Matveev and S.P.Novikov, *Russian Math.Surveys* 31(1976) 55

[13] N.E.Firsova, Zap.Nauchn.Sem.Leningrad.Otdel.Mat.Inst. Steklov.(LOMI) 51 (1975) 183

[14] B.S.Buslaev, L.A.Dmitrieva, *Leningrad Math.J.* 1(1990) 287

[15] B.S.Buslaev, L.A.Dmitrieva, *Bloch Electrons in an External Electric Field*, in: *Schrödinger Operators: Standard and Non-Standard* (Eds. P.Seba, P.Exner), World Scientific, Singapore, 1989, p.103

[16] B.S.Buslaev, L.A.Dmitrieva, Thoer.Math.Phys. 73 (1987) 430

[17] B.S.Buslaev, *Russian Math.Surveys* 42 (1987) 97

[18] B.S.Buslaev, *Theor.Math.Phys.* 58 (1984) 223

[19] V.Grecchi, A.Sacchetti, *Lifetime of the Wannier-Stark resonances and perturbation theory*, preprint, math-ph 97-211, 1997