Spectral Modelling of Quantum Superlattice and Application to the Mott-Peierls Simulated Transitions

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Abstract

A local perturbation theory for the spectral analysis of the Schrödinger operator with two periodic potentials whose periods are commensurable has been constructed. It has been shown that the perturbation of the periodic 1D Hamiltonian by an additional small periodic potential leads to the following spectral deformation: all gaps in the spectrum of the unperturbed periodic Hamiltonian bear shifts while any band splits by arising additional gaps into a set of smaller spectral bands. The spectral shift, the position of additional gaps and their widths have been calculated explicitly. The applications to the operational regime of a nanoelectronic device based on Mott-Peierls stimulated transition have also been discussed.

1 Introduction

In series of papers \cite{1, 2, 3, 4, 5, 6} a new type of nanoelectronic device based on the phenomenon of the stimulated Mott-Peierls transition (SMPT) has been studied in one electron and one-mode approximation. The spectral properties and the operational regimes of the device have been calculated for the ballistic electrons moving along the quantum wire (QW) treated as the conducting electrode of the device. The effect of QW-structure has been taken into account by the effective mass \( m^* \) in the Schrödinger equation

\[
-\frac{\hbar^2}{2m^*} \frac{d^2 \Psi}{dx^2} = E \Psi
\]

under assumption that normally the conducting electrode is in metallic state. When a nontrivial operating voltage has been applied to the governing electrodes distributed periodically along the QW it has been shown that the effect of the governing electrodes can been reduced to an effective periodic potential \( V_{\text{eff}} \) in the Schrödinger operator \cite{1}:

\[
-\frac{\hbar^2}{2m^*} \frac{d^2 \Psi}{dx^2} + V_{\text{eff}} \Psi \equiv H_{\text{eff}} = E \Psi.
\]

The spectrum of the operator \cite{2} consists of spectral bands separated by gaps. The device is in conducting state if the Fermi level of the conducting electrode gets into one of the
artificially created spectral bands. On the contrary, if the Fermi level gets into a gap between the spectral bands the conductivity vanishes and thus the conducting electrode is effectively transformed into the dielectric state. Summarizing what has been said one can conclude that the formation of the energy gaps in the continuous spectrum of the operator (1) and the control of the parameters of $V_{\text{eff}}$ may be considered as the physical base of a new type of nanoelectronic device.

For a more detailed analysis of spectral properties and physical characteristics (say, conductance) of the device described above deviations from the ideal behavior (one-electron, one-mode ballistic regime at zero temperature) should be considered because the effect of electron-phonon interaction, electron-electron interaction, stimulated superlattice structure of governing electrode, etc., may become important for real device. In particular, if the electron concentration is large enough, electrons may be affected by a atomic lattice structure of a QW that could change the behavior of the conductance. Also if an artificial lattice (periodic) structure could be fabricated for quantum wire then two periodic structures (atomic and artificial) could change the spectral properties of the device as well as its operational regimes.

In the present paper we study the spectral properties of the controlled QW which is described by 1D quantum Hamiltonian

$$H = -\frac{d^2}{dx^2} + q_0(x) + \delta q_1(x)$$

(3)

with the periodic potentials $q_0(x)$ and $q_1(x)$ playing the role of the atomic potential of QW in one-electron approximation ($q_0$) and the effective potential ($q_1$) generated by the periodic system of governing electrodes. Everywhere below we set $\hbar/2m = 1$ where $m$ is the electron mass and in these units the parameter $\delta$ is proportional to the ratio of $q_0$ and $q_1$ amplitudes. We assume that the periods $a$ and $b$ of $q_0$ and $q_1$ respectively are commensurable and we shall call such QW as 1D superlattice. We consider $\delta$ as a small parameter which is in agreement with strength of the atomic potential in comparison with the amplitude of the $V_{\text{eff}}$ calculated in [3]. To study the spectrum of the Hamiltonian (3) and its eigenfunctions we develop a special local perturbation theory which allows to calculate all spectral ingredients of $H$ not only for regular points but also for singular ones. The latter as it is shown in the paper coincide with the ends of spectrum of the operator $H_0$:

$$H_0 = -\frac{d^2}{dx^2} + q_0(x)$$

(4)

and with some set of points inside the bands of $H_0$. This set is described in the frame of our approach explicitly. We prove that the main spectral effect of the perturbation is the following deformation of $\sigma(H_0)$: all gaps of $H_0$ bear shifts while any spectral band of $H_0$ splits by the arising additional gaps into a number of smaller spectral bands of $H$. It is shown that spectral shifts, the locations of additional gaps and their widths can be calculated in arbitrary order of the perturbation theory explicitly. In this respect the spectral analysis presented here can be considered as the sound mathematical background for numerical calculations of real nanoelectronic devices fabricated on the basis of narrow-
gap semiconductors \[2\]. The calculations of the spectral characteristics and operational regimes for real SMPT-device will be done elsewhere.

2 The Perturbation Theory at Regular Points

We consider the perturbation of the Schrödinger operator with a periodic potential by another periodic potential with a small amplitude. So the Hamiltonian has the form

$$H = -\partial_x^2 + q_0(x) + \delta q_1(x), \; x \in \mathbb{R},$$

where \(q_0(x + a) = q_0(x)\) and \(q_1(x + b) = q_1(x)\) are two periodic functions, the parameter \(\delta\) is considered to be small. We assume that the periods \(a\) and \(b\) are commensurable, i.e. \(b/a = m/n\) where \(m\) and \(n\) are integers. Hence, the perturbed Hamiltonian \(H\) remains to be the operator with a periodic potential and \(c = bn = am\) is the common period of functions \(q_0\) and \(q_1\).

In what follows we need some well known facts \[7, 8\] from the theory of the periodic Schrödinger operators \(H_{\text{per}}\). The spectrum of such operators consists of spectral bands separated by gaps. In the general case there are infinite number of bands and gaps. If the period of the potential is \(A\) then the so-called Bloch functions of \(H_{\text{per}}\) are solutions of equation \(H_{\text{per}} \Psi = E \Psi\) which obey the quasiperiodic boundary conditions on the period \(\Psi_\pm(x + A, k) = e^{\pm ikA} \Psi_\pm(x, k)\). The quasimomentum \(k\) is linked with the energy \(E\) by the dispersion function \(E = E(k)\). Under this mapping to the \(N\)-th band of \(H_{\text{per}}\) there corresponds the Brillouin zone \([\pi(N-1)/A, \pi N/A]\) of the values of quasimomentum. To the \(N\)-th gap there corresponds the cut \([\pi N/A, \pi N/A + i \gamma_N]\) drawn on the complex plane of quasimomentum. The so-called Lyapounov function \(F(E) = \cos kA\) is the entire function of \(E\), \(|F(E)| < 1\) in bands and \(|F(E)| > 1\) in gaps. At the end of bands \(\frac{d}{dE} E(k) = 0\) and at the gap points \(E^{(N)}\) corresponding to the tops \(\pi N/A + i \gamma_N\) of cuts the relation \(\frac{d}{dE} F(E) = 0\) is valid.

We assume that the location of bands of the unperturbed operator \(H_0 = -\partial_x^2 + q_0(x)\), its Bloch functions and the dispersion relation are known. Our aim is to study the corresponding quantities for the perturbed operator \(H\) and to describe its spectrum in comparison with the spectrum of the unperturbed operator.

Let us present the Bloch solutions \(\Psi(x, p)\) of the perturbed spectral problem

$$H \Psi = E \Psi$$

in the form

$$\Psi(x, p) = e^{i(p-k)x} \Phi(x, p),$$

where \(E = E(p)\) and \(p = p(E)\) are the dispersion function and the quasimomentum corresponding to the operator \(H\), \(\lambda = \lambda(k)\) and \(k = k(\lambda)\) are the analogous objects for the unperturbed problem

$$H_0 \Psi_0 = \lambda \Psi_0, \; H_0 = -\partial_x^2 + q_0(x).$$
Due to Floquet theorem the function $e^{-ikx}\Phi(x,p)$ is the periodic one with a period $c$. Hence the function $\Phi(x,p)$ is quasiperiodic and

$$\Phi(x+c,p) = e^{ikc}\Phi(x,p).$$

To fix the Bloch solution $\Psi(x,p)$ and hence the function $\Phi(x,p)$ unambiguously we normalize it as follows

$$\Psi(0,p) = 1, \quad \Psi(c,p) = e^{ipc}.$$  \hspace{1cm} (9)

Obviously,

$$\Phi(0,p) = 1, \quad \Phi(c,p) = e^{ikc}.$$  \hspace{1cm} (8)

On use of eqs. (8) and (9) one can see that the function $\Phi(x,p)$ satisfies the equation

$$\left[-\partial_x^2 - 2i(p-k)\partial_x + (p-k)^2 + q_0(x) + \delta q_1(x) - E\right]\Phi(x,p) = 0.$$  \hspace{1cm} (10)

This equation is to be solved in the class of functions with the boundary conditions (8).

Let us seek the solution of eq. (10) in the form

$$\Phi(x,p) = \Psi_0(x,k) + \sum_{n \geq 1} \delta^n \Psi_n(x,k)$$

assuming that the perturbed quasimomentum $p$ and the dispersion function $E = E(p)$ are also expanded in series

$$p = k + \sum_{n \geq 0} \delta^n \mu_n(k)$$

and

$$E(p) = \lambda(k) + \sum_{n \geq 0} \delta^n \lambda_n(k),$$

where $k$ and $\lambda(k)$ are the quasimomentum and the dispersion function corresponding to the unperturbed problem (7).

Since the unperturbed Bloch function $\Psi_0(x,k)$ satisfies the condition $\Psi_0(x+a,k) = e^{ika}\Psi_0(x,k)$ and hence $\Psi_0(x+c,k) = e^{ikc}\Psi_0(x,k)$, in order to provide the boundary condition (8) one has to seek the correction terms under the same conditions, i.e.

$$\Psi_n(x+c,k) = e^{ikc}\Psi_n(x,k), \quad n \geq 1.$$  \hspace{1cm} (14)

The normalization conditions

$$\Psi_0(0,k) = 1, \quad \Psi_0(a,k) = e^{ika},$$

$$\Psi_n(0,k) = \Psi_n(c,k) = 0, \quad n \geq 1$$

provide the property (9) of the exact Bloch solution.

In what follows we propose a procedure of calculation of all correction terms $\Psi_n(x,k)$, $\mu_n(k)$, $\lambda_n(k)$ and define the values of unperturbed quasimomentum $k$ at which this procedure fails. The corresponding energy points $\lambda_s = \lambda(k_s)$ we shall call as singular points of perturbation series constructed here. The complement of a set of singular points on real
axis we shall call as a set of regular points. In the next Section we construct the local perturbation series which are valid at the above singular points.

The procedure of calculating the correction terms $\Psi_n(x,k)$, $\mu_n(k)$ and $\lambda_n(k)$ includes the following steps:

1. For each $n \geq 1$ we find the linear link between the terms $\lambda_n(k)$ and $\mu_n(k)$ in expansions (12) and (13). To this end we use the fact that these expansions are not independent and are linked with each other by means of equation

\[ F(E) = \cos pc \]  

where $F(E)$ is the Lyapounov function of the perturbed operator $H$.

2. For each $n \geq 1$ we find the second linear link between $\lambda_n(k)$ and $\mu_n(k)$ which is necessary to define $\lambda_n(k)$ and $\mu_n(k)$ unambiguously. This second link is obtained by examining the solvability condition of the inhomogeneous equation for $\Psi_n(x,k)$ in the class of functions with boundary conditions (14).

3. Finally we find the solution $\Psi_n(x,k)$ which satisfies the boundary conditions (14) and (16).

All technical details of the realization of the above three steps are contained in the proofs of statements formulated below.

**Proposition 1.** The Lyapounov function $F(E)$ associated with the operator $H$ in the leading order of $\delta$ can be expressed in terms of the unperturbed quasimomentum $k$ as follows

\[ F(E) = \cos pc + O(\delta) \]  

**Proof.** Let us insert the expansion (13) into the r.h.s. of the dispersion relation (17) and expand the r.h.s. in the Taylor series at the vicinity of $k$. If we restrict the Taylor series to the leading order we obtain the statement of proposition. Q.E.D.

**Remark.** It should be noted that the leading term $\cos pc$ of the Lyapounov function $F(E)$ does not coincide with the Lyapounov function $F_0(\lambda) = \cos ka$ of the unperturbed operator $H_0$. This fact has crucial consequences for the spectrum of the perturbed operator which is to be discussed below.

To formulate the next statement we need the following notations: $F(\mu)|_{\lambda=\lambda(k)} \equiv \cos kc$, $F' = \frac{d}{d\lambda} F(\lambda)$, $F^{(n)} = \frac{d^n}{d\lambda^n} F(\lambda)$, $\dot{\lambda}(k) = \frac{d}{dk} \lambda(k)$.

**Proposition 2.** The correction terms of series (13) and (12) for $E(p)$ and $p$ are linked by the recursion relations

\[ \dot{\lambda}(k)\mu_n(k) - \lambda_n(k) = T_n \{\lambda_i, \mu_i, i \leq n-1\} \]  

where $T_1 = \text{const}$ and $T_n \{\cdot, \cdot, \cdot\}, n > 1$, are some functions of $\lambda_i, \mu_i, i \leq n-1$, which can be calculated explicitly for arbitrary $n$. In particular, the first $T_n, n = 1, 2, 3,$ have the form

\[
T_1 = 0,
\]

\[
T_2(\lambda_1, \mu_1) = \frac{1}{2} \left( \frac{F''}{F'} \lambda_1^2 + \frac{F}{F'} \mu_1^2 \right),
\]

\[
T_2(\lambda_1, \mu_1, \lambda_2, \mu_2) = \frac{\dot{\lambda}(k) \mu_1^3}{6} + \frac{F''}{F'} \lambda_1 \lambda_2 + \frac{F'''}{6F'} \lambda_1^3 + \frac{F}{F'} \mu_1 \mu_2 c^2.
\]
Proof. To obtain the above relations one has to insert expansions (13) and (12) for $E$ and $p$ into the dispersion relation (17), to expand the l.h.s into the Taylor series at the vicinity of $\lambda$, to expand the r.h.s. into the Taylor series at the vicinity of $k$ and to equate coefficients at each power of $\delta$. Finally one has to take into account that in the leading order $F(E) = F(\lambda)$. Q.E.D.

The $n$-th relation in (18) gives one linear link between two quantities $\lambda_n(k)$ and $\mu_n(k)$. To define them unambiguously one needs the second link between them. To obtain it let us consider the solvability condition of the equation defining the $n$-th correction term $\Psi_n(x,k)$ of the Bloch function. To write down this equation let us insert the expansions (11), (12) and (13) into the exact equation (10) and equate the terms at each power of $\delta$.

As the result one obtains the set of equations

$$
\left[-\partial_x^2 + q_0(x) - \lambda(k)\right] \Psi_n(x,k) = R_n(x,k),
$$

where the inhomogeneous term $R_n(x,k)$ can be expressed in terms of functions $\Psi_i(x,k)$ at $i \leq n - 1$, $\lambda_i(k)$ and $\mu_i$ at $i \leq n$ and the potential $q_1(x)$. For instance, the first two terms have the form

$$
R_1(x,k) = [\lambda_1(k) - q_1(x) + 2i\mu_1(k)\partial_x] \Psi_0(x,k),
$$

$$
R_2(x,k) = [\lambda_1(k) - q_1(x) + 2i\mu_1(k)\partial_x] \Psi_1(x,k) + 
+ \left[\lambda_2(k) - \mu_1^2(k) + 2i\mu_2(k)\partial_x\right] \Psi_0(x,k)
$$

Equation (19) is to be solved in the class of functions with quasiperiodic boundary conditions

$$
\Psi_n(x + c, k) = e^{ikc} \Psi_n(x, k).
$$

According to the Fredholm theorem the solvability conditions of eq. (19) is the orthogonality of the r.h.s. of (19) to the solutions of the corresponding homogeneous equation

$$
\left[-\partial_x^2 + q_0(x) - \lambda(k)\right] \Psi_n^{(0)}(x,k) = 0
$$

with the same boundary conditions (20). It is obvious that the unique solution of eq. (19) satisfying the boundary conditions (20) is given by the Bloch function $\Psi_0(x,k)$. Thus the solvability conditions have the form

$$
\langle R_n, \Psi_0 \rangle \equiv \int_0^c R_n(x,k) \bar{\Psi}_0(x,k) dx = 0.
$$

The $n$-th solvability condition from (22) gives the second linear link between $\lambda_n(k)$ and $\mu_n(k)$.

Before writing down it explicitly let us note that the solvability conditions of equations similar to (19) has been used in [9, 10] for constructing the quasiclassical series in the problem of the adiabatic perturbation of the periodic potential. In the present paper we construct the perturbational series, however the specific character of perturbation leads to
the necessity of using the technical tools which are more appropriate for the quasiclassical approach.

Turn back to the link between \( \lambda_n(k) \) and \( \mu_n(k) \) and introduce the following functions of \( k \):

\[
N_n(k) = \int_0^c \Psi_n(x,k)\bar{\Psi}_0(x,k)dx, \quad \beta_n(k) = \int_0^c q_1(x)\Psi_n(x,k)\bar{\Psi}_0(x,k)dx, \\
v_n(k) = -i \int_0^c \Psi'_n(x,k)\bar{\Psi}_0(x,k)dx.
\]

The constructions described above can be summarized in the following

**Proposition 3.** The links between \( \lambda_n(k) \) and \( \mu_n(k) \) have the form

\[
\lambda_n(k)N_0(k) - 2v_0(k)\mu_n(k) = \hat{T}_n\{\lambda_i, \mu_i, N_i(k), v_i(k) \mid i \leq n-1, \beta_{n-1}(k)\}.
\]

where \( \hat{T}_n \) are some nonlinear functions of its arguments which can be calculated explicitly for arbitrary \( n \). In particular, the first two functions have the form

\[
\hat{T}_1 = \beta_0(k), \\
\hat{T}_2 = \beta_1(k) + \mu_1^2N_0 - \lambda_1N_1 + 2\mu_1v_1.
\]

**Remark.** To calculate \( \hat{T}_n \) for arbitrary \( n \) one has to insert \( R_n(x,k) \) which are known explicitly into the solvability condition (22).

Eqs. (18) and (23) give the \( 2 \times 2 \) linear system for the functions \( \lambda_n(k) \) and \( \mu_n(k) \). By solving this system one obtains the following formulae.

**Lemma 1.** The correction terms of expansions (12) and (13) for the quasi momentum \( p \) and dispersion function \( E(p) \) have the form

\[
\lambda_n(k) = \frac{\hat{T}_n\lambda(k) + 2v_0(k)T_n}{\lambda(k)N_0(k) - 2v_0(k)},
\]

\[
\mu_n(k) = \frac{\hat{T}_n + N_0(k)T_n}{\lambda(k)N_0(k) - 2v_0(k)}.
\]

Here \( T_n \) and \( \hat{T}_n \) are described in propositions 1 and 2 respectively.

Finally one has to find the correction terms in the series (11) by solving the boundary value problem (19), (20). Its solution can be represented as the linear combination of a general solution of (21) and a particular solution of (19). Thus

\[
\Psi_n(x,k) = B_n(k)\Psi_0(x,k) - \bar{\Psi}_0(x,k)\int_{x_n}^x \Psi_0^{-2}dx'\int_{x_n}^{x'} R_n\bar{\Psi}_0dx''
\]

where \( B_n(k), x_n \) and \( x'_n \) are some constants w.r.t. \( x \). These constants can be defined unambiguously by means of quasiperiodic boundary conditions (20) and the normalization
or outside the bands of the unperturbed operator $H$ points are compensated by the factor $\dot{\lambda}$. One needs to analyze the properties of correction terms corresponding real values of quasimomentum $k$. As it has been said already we call the corresponding points $\lambda_s(k)$ as the singular points.

**LEMMA 2.** There are two sets of singular points. One of them $\{E^0_i\}_{i \geq 1}$ coincides with the ends of bands of the unperturbed operator $H_0$. The singular points $\{\varepsilon^0_{IN}\}$ of another set are located inside bands of $H_0$. If the ratio of the perturbed potential period to the unperturbed potential period is $m \equiv c/a$ then inside the $N$-th band there are $(m - 1)$ singular points distributed in such a way that the corresponding values of quasimomentum divide the Brillouin zone by $m$ equal segments, so

$$
\varepsilon^0_{lN} = \lambda \left( \frac{\pi lN}{ma} \right), \quad l = 1, \ldots, m - 1.
$$

**Proof.** Firstly let us show that at the ends of bands of the unperturbed operator $H_0$ the function $v_0(k)$ vanishes: $v_0(k_N) = 0$, $(k_N = \pi N/a)$. Indeed at the ends of bands the Bloch functions $\Psi_0(x, k)$ and $\Psi_0(x, k)$ coincide: $\Psi_0 = \Psi_0$. Hence

$$
v_0 = -i \int_0^c \Psi_0' \Psi_0 dx = -i \int_0^c \Psi_0' \Psi_0 dx = -\frac{i}{2} \left[ e^{2i\pi lm} \Psi_0^2(0, k_l) - \Psi_0^2(0, k_l) \right] = 0.
$$

As it has been mentioned already at the ends of bands $\dot{\lambda}(k_l) = 0$. Hence the denominator of fractions $\{24\}, \{25\}$ vanishes at the ends of bands and the perturbation series $\{11\}, \{12\}$ and $\{13\}$ are not valid at these points.

The second set of singular points is generated by the singularities of $T_n$ which can be shown to be the same as of $T_2$ given by (20) and hence are defined by the equation $F'(\lambda) \equiv \frac{d}{d\lambda} F(\lambda) = 0$. Since $F(\lambda) = \cos kc$ one has that $F'(\lambda) = - \sin kc \frac{dk}{d\lambda}$. and hence $F'(\lambda) = 0$ if $\sin kc = 0$ or $dk/d\lambda = 0$. In the first case $k = k_{lN} = \pi lN/ma$, $l = 1, \ldots, m, N \in \mathbf{Z}$. However if $l = m$ the quasimomentum $k_{mN}$ corresponds to the end of band of the unperturbed operator $H_0$ and the zero of $\sin k_{mNC}$ is compensated by the zero of $\lambda(k_{mN})$. So we have to consider only $k_{lN}$ with $l = 1, \ldots, m - 1$. These points divide each Brillouin zone by $m$ equal segments. The corresponding energy points $\varepsilon^0_{IN} = \lambda(k_{lN})$, $l = 1, \ldots, m - 1$, are located inside the $N$-th band.

The points where $dk/d\lambda = 0$ lie inside gaps. However the singularities of $T_n$ at these points are compensated by the factor $\dot{\lambda}(k)$ entering the fractions $\{24\}$ and $\{25\}$, Q.E.D.

To complete the study of expansions $\{11\}, \{12\}$ and $\{13\}$ outside the singular points one needs to analyze the properties of correction terms $\lambda_n(k)$ and $\mu_n(k)$ when $k$ is inside or outside the bands of the unperturbed operator $H_0$. Remind that to the bands there correspond real values of quasimomentum $k$, while in gaps quasimomentum has nontrivial imaginary part: $k = \pi N/a + i\gamma$ ($N$ is the gap number).

**LEMMA 3.** At real $k$ ($k \neq \pi N/a, N = 1, 2, \ldots$) the corrections terms $\lambda_n(k)$ and $\mu_n(k)$ are real. If $k = \pi N/a + i\gamma$ the correction terms $\lambda_n(k)$ of the dispersion function are real while the correction terms $\mu_n(k)$ of quasimomentum are pure imaginary.
Remark. The statement of lemma means that outside the singular points the spectral bands and gaps of the unperturbed operator $H_0$ are stable under the perturbation. It means that if some point $\hat{\lambda}$ ($\hat{\lambda} \neq \varepsilon_i^0$, $\lambda \neq E_i^0$) belongs to the band (gap) of $H_0$ the shifted point $\hat{E} = \hat{\lambda} + O(\delta)$ should also belong to the band (gap) of the perturbed operator $H$. Indeed, if $k$ is real then $\mu_n(k)$ are also real and the perturbed quasimomentum $p$ given by expansion (12) is also real. If $k = \pi N/a + i \gamma$ then $\mu_n(k)$ are pure imaginary and $p = \pi N/a + i (\gamma + O(\delta))$. Hence the corresponding spectral point $E(p)$ belongs to the gap of $H$. It should be noted that the number of this gap is equal to $mN$ since the width of the Brillouin zone of the perturbed operator is $\pi/e \equiv \pi/ma$.

Proof. Here we prove the statement of lemma for $n = 1$. For $n \geq 2$ the statement can be proven analogously. Remind that

$$\hat{\lambda} = \frac{\beta_0(k) \dot{\lambda}(k)}{\lambda(k) N_0(k) - 2 v_0(k)}, \quad \dot{\lambda}(k) = \frac{\beta_0(k)}{\lambda(k) N_0(k) - 2 v_0(k)}.$$ 

To prove lemma we show: 1) that at real $k$ the quantities $\dot{\lambda}(k)$, $\beta_0(k)$, $N_0(k)$ and $v_0(k)$ are real; 2) if $k = \pi N/a + i \gamma$ the functions $N_0(k)$ and $\beta_0(k)$ are real while the functions $\dot{\lambda}(k)$ and $v_0(k)$ are pure imaginary.

Since $\cos ka = F_0(\lambda)$ where $F_0(\lambda)$ is the Lyapounov functions of the unperturbed operator $H_0$, one has

$$\dot{\lambda} = \frac{d}{d\lambda} \lambda(k) = - \frac{a \sin ka}{F'_0(\lambda)}, \quad F'_0(\lambda) = \frac{d}{d\lambda} F_0(\lambda).$$

Since the function $F'_0(\lambda)$ is always real at $\lambda \in \mathbb{R}$, the function $\sin ka$ is real at real $k$ and $\sin(N \pi + i \gamma a) = (-1)^N i \sinh \gamma a$ is pure imaginary at $k = \pi N/a + i \gamma$, then $\dot{\lambda}(k)$ is real inside bands and is pure imaginary inside gaps.

The fact that functions $N_0(k)$ and $\beta_0(k)$ are always real directly follows from their definitions. Inside gaps ($k = \pi N/a + i \gamma$) the Bloch functions are real. Therefore the function

$$v_0(k) = -i \int_0^c \Psi'_0(x,k) \bar{\Psi}_0(x,k) dx$$

is pure imaginary. At real $k$

$$\bar{v}_0(k) = i \int_0^c \bar{\Psi}'_0(x,k) \Psi_0(x,k) dx = i \bar{\Psi}'_0 \Psi_0|_0^c - i \int_0^c \Psi'_0 \bar{\Psi}_0 dx =$$

$$= -i \int_0^c \Psi'_0 \bar{\Psi}_0 dx \equiv v_0(k),$$

so the function $v_0(k)$ is real. Q.E.D.
3 Local perturbation series at singular points

In this Section we construct the local perturbation series at singular points and by the study of their properties prove two basic statements. To formulate the first statement we need the following notations. Let \( m = c/a \) be the ratio of the perturbed potential period to the unperturbed potential one. We introduce the points \( k_{lN} = \pi lN/ma \), \( l = 1, ..., m - 1 \), where \( N \) is arbitrary integer. According to lemma 2 the points \( \varepsilon_{lN}^0 = \lambda(k_{lN}) \) are singular.

Let us introduce the functions

\[
\phi_0(x) = \frac{1}{2} \left[ \Psi_0(x, k_{lN}) + \bar{\Psi}_0(x, k_{lN}) \right] \\
\hat{\phi}_0(x) = \frac{1}{2i} \left[ \Psi_0(x, k_{lN}) - \bar{\Psi}_0(x, k_{lN}) \right],
\]

where \( \Psi_0(x, k) \) is the Bloch function of the unperturbed operator \( H_0 \) fixed by the conditions \( (15) \). Consider the quantities \( \varepsilon_{lN} \) and \( p_{lN} \) given up to the second order of \( \delta \) as follows

\[
\varepsilon_{lN} = \varepsilon_{lN}^0 + \delta \varepsilon_{lN}^1 + O(\delta^2) \\
p_{lN} = k_{lN} + i\delta \beta_{lN}^1 + O(\delta^2)
\]

Here

\[
\varepsilon_{lN}^1 = \frac{\int_0^c q_1(x) \phi_0^2(x) dx}{\int_0^c \phi_0^2(x) dx}
\]

and

\[
\beta_{lN}^1 = -\frac{\varepsilon_{lN}^1 \int_0^c \phi_0(x) \hat{\phi}_0(x) dx + \int_0^c q_1(x) \phi_0(x) \hat{\phi}_0(x) dx}{2 \int_0^c \phi_0^2(x) dx}.
\]

Under these notations the following statement is valid.

**Theorem 1.** At the singular points \( \varepsilon_{lN}^0, l = 1, ..., m - 1 \) the \( N \)-th spectral band of the unperturbed operator \( H_0 \) is splitted under the perturbation \( \delta q_1(x) \) into \( m \) bands. The separating gaps are concentrated around the points \( \varepsilon_{lN} \) given by \( (30) \). The quasimomenta \( p_{lN} \) corresponding to these points are complex and are described by \( (31) \). The width of the \( lN \)-th gap in the leading order of \( \delta \) is

\[
\Delta_{lN} \sim 2\delta |\beta_{lN}^1| + O(\delta^2)
\]

with \( \beta_{lN}^1 \) given by eq. \( (33) \).

**Proof.** To proof the statement we construct the local perturbation series at the singular point \( \varepsilon_{lN}^0 \). Denote by \( \varepsilon_{lN} \) the point obtained from \( \varepsilon_{lN}^0 \) under the perturbation \( \delta q_1(x) \). Let us seek this point in the form

\[
\varepsilon_{lN} = \varepsilon_{lN}^0 + \sum_{n \geq 1} \delta^n \varepsilon_{lN}^n.
\]
The corresponding value of quasimomentum \( p \) we denote by \( p_{lN} \) and also seek in the form of series

\[
p_{lN} = k_{lN} + \sum_{n \geq 1} \delta^n \mu_{lN}^n,
\]

(36)

where \( k_{lN} = \pi lN/ma \) and \( \epsilon_{lN}^0 = \lambda(k_{lN}) \).

According to eq. (8) the function \( \Phi(x, p) \) related with the Bloch function \( \Psi(x, p) \) by eq. (6) at the point \( p = p_{lN} \) has the property

\[
\Phi(x + c, p_{lN}) = e^{ik_{lN} c} \Phi(x, p_{lN}) = (-1)^lN \Phi(x, p_{lN}).
\]

(37)

Thus \( \Phi(x) \equiv \Phi(x, p_{lN}) \) is periodic or antiperiodic function. Let us seek it in the form

\[
\Phi(x) = \varphi_0(x) + \sum_{n \geq 1} \delta^n \varphi_n(x),
\]

(38)

where the function \( \varphi_0(x) \) is given by (28). Note that due to (15) the leading term \( \varphi_0(x) \) is periodic or antiperiodic, i.e. \( \varphi_0(x + c) = (-1)^lN \varphi_0(x) \). To provide the property (37) the correction terms \( \varphi_n(x) \) are to be sought in a class of functions with the same boundary condition: \( \varphi_n(x + c) = (-1)^lN \varphi_n(x) \).

After inserting the Bloch function \( \Psi(x, p_{lN}) = \exp\{i(p_{lN} - k_{lN}) x\} \Phi(x) \) into equation (10) with \( E = \epsilon_{lN} \) one obtains for \( \Phi(x) \) the following equation

\[
\left[-\partial_x^2 - 2i(p_{lN} - k_{lN}) \partial_x + (p_{lN} - k_{lN})^2 + q_0(x) + \delta q_1(x) - \epsilon_{lN}\right] \Phi(x) = 0.
\]

Now we insert the expansions (35), (36), (38) into the last equation and equate terms at equal powers of \( \delta \). In the leading order of \( \delta \) one obtains identity

\[
\left[-\partial_x^2 + q_0(x) - \epsilon_{lN}\right] \varphi_0(x) = 0.
\]

In the first order one has the equation

\[
\left[-\partial_x^2 + q_0(x) + \epsilon_{lN}\right] \varphi_1(x) = \left[\epsilon_{lN}^1 - q_1(x) + 2i\mu_{lN}^1 \partial_x\right] \varphi_0(x) \equiv R_1(x).
\]

Following the discussions of Sec.2 one concludes that the condition of solvability of this equation in a class of periodic (antiperiodic) functions is the orthogonality of \( R_1(x) \) to periodic (antiperiodic) solutions of the corresponding homogeneous equation. Since there are two such solutions (say, for example, \( \varphi_0(x) \) and \( \hat{\varphi}_0(x) \) given by (28) and (29) respectively) one has two solvability conditions

\[
\int_0^c R_1(x) \varphi_0(x) \, dx = 0, \quad \int_0^c R_1(x) \hat{\varphi}_0(x) \, dx = 0,
\]

where the fact that \( \varphi_0 \) and \( \hat{\varphi}_0 \) are real is taken into account. Since \( \int_0^c \hat{\varphi}_0(x) \varphi_0(x) \, dx = 0 \), the first condition allows to define \( \epsilon_{lN}^1 \) and yields relation (32). The second condition leads to the relation \( \mu_{lN}^1 = i\beta_{lN}^1 \) with \( \beta_{lN}^1 \) defined by (33).
Now one knows the r.h.s. $R_1(x)$ explicitly and can easily find the periodic (antiperiodic) solution $\varphi_1(x)$. Then the whole procedure can be repeated. Namely, one can write down the equation in the second order of $\delta$ (equation for $\varphi_2(x)$) and find the correction terms $\varepsilon_{1N}^2$ and $p_{1N}^2$ from two solvability conditions

$$\int_0^c R_2(x)\varphi_0(x)dx = 0,$$

$$\int_0^c R_2(x)\varphi_0(x)dx = 0.$$

The described procedure allows to define the correction terms in expansions (35), (36), (38) of arbitrary order. However this is out the scope of the present paper.

Since the width of the Brillouin zone for the perturbed operator is $\pi/c = \pi/ma$ then according to the general theory of periodic operators the complex quasimomentum $p_{1N} = \pi lN/ma + i\delta_{1N} + O(\delta^2)$ corresponds to the real energy $\varepsilon_{1N} = E(p_{1N})$ which lies in the $lN$-th gap of $H$.

To calculate the width of gaps appeared under the perturbation let us calculate the Lyapunov function $F(E)$ of the perturbed operator at the point $E = \varepsilon_{1N}$:

$$F(\varepsilon_{1N}) = \cos(k_{1N} + i\delta_{1N} + O(\delta^2)) = (-1)^{lN} \cosh(\delta |\beta_{1N}| + O(\delta^2)) =$$

$$= (-1)^{lN} \left( 1 + \frac{\delta^2 |\beta_{1N}|}{2} + O(\delta^4) \right).$$

Now let us expand the Lyapunov function in the vicinity of $\varepsilon_{1N}$ in the Taylor series $F(E) = F(\varepsilon_{1N}) + \frac{F''(\varepsilon_{1N})}{2}(E - \varepsilon_{1N})^2 + O((E - \varepsilon_{1N})^3)$ and set $E = E_{1N}^\pm$ where $E_{1N}^\pm$ are the ends of the gap. Here we used the fact that $F'(\varepsilon_{1N}) = 0$. Since the number of the considered gap is $lN$ one has

$$F(E_{1N}^\pm) = (-1)^{lN}, \quad F''(\varepsilon_{1N}) = (-1)^{lN+1} |F''(\varepsilon_{1N})|,$$

and hence the width of the $lN$-th gap in the leading order of $\delta$ is

$$\Delta_{1N} \equiv (E_{1N}^+ - \varepsilon_{1N}) - (E_{1N}^- - \varepsilon_{1N}) \sim 2\delta |\beta_{1N}|.$$ 

Q.E.D.

Now it remains to consider the singular points which coincide with ends of bands (gaps) of the unperturbed operator. Let us denote by $E_{1N}^{(0)} = \lambda(\pi N/a + 0)$ and $E_{1N}^{(0)} = \lambda(\pi N/a - 0)$ the right and left ends of the $N$-th gap in the spectrum of the unperturbed operator $H_0$. The following statement is valid.

**Lemma 4.** Under the perturbation $\delta q_1(x)$ the ends of the $N$-th gap of the unperturbed operator are shifted as follows

$$E_{1N}^\pm = E_{1N}^{(0)} + \delta E_{1N}^{(1)} + O(\delta^2)$$

where

$$E_{1N}^{(1)} = \frac{\int_0^c q_1(x)\Psi_0^2(x)dx}{\int_0^c \Psi_0^2(x)dx}$$

(39)
and \( \Psi_0(x) \equiv \Psi_0(x, \pi N/a \pm 0) \) is the Bloch function \( \Psi_0(x, k) \) of \( H_0 \) taken at the ends of the \( N \)-th gap.

**Proof.** To obtain the expansion (39) let us insert the series

\[
E_{lN \pm} = E_{N \pm}^{(0)} + \sum_{n \geq 1} \delta^n E_{N \pm}^{(n)}, \quad \Psi(x) = \Psi_0(x) + \sum_{n \geq 1} \delta^n \psi_n(x) \tag{41}
\]

into equation (10) considered at \( E = E_{lN \pm} \) where \( E_{lN \pm} \) are the boundary points of the perturbed operator spectrum. Here \( \Psi(x) \) is the Bloch function of \( H \) at the point \( E_{lN \pm} \).

In the leading order of \( \delta \) one obtains the identity

\[
\left[ -\partial_x^2 + q_0(x) - E_{N \pm}^{(0)} \right] \psi_0(x) = 0.
\]

The first order term has the form

\[
\left[ -\partial_x^2 + q_0(x) - E_{N \pm}^{(0)} \right] \psi_1(x) = E_{N \pm}^{(1)} \psi_0(x) - q_1(x) \psi_0(x) \equiv R_1. \tag{42}
\]

Since the functions \( \Psi(x) \) and \( \psi_0(x) \) are periodic (antiperiodic) with the period \( c \), one has to find the correction terms \( \Psi_n(x) \) in the same class. The solvability condition of equation (42) in such class of functions is the orthogonality of \( R_2 \) to periodic (antiperiodic) solutions of homogeneous equation. Since at the boundary points of spectrum \( \Psi_0(x, k) = \bar{\Psi}_0(x, k) \), the function \( \Psi_0(x) \) is the single periodic (antiperiodic) solution and the solvability condition has the form \( \int_0^c R_2(x) \Psi_0(x) dx = 0 \). It yields the first correction term \( E_{N \pm}^{(1)} \) in the form (10).

Obviously the above described procedure can be repeated again and allows to define all terms \( E_{n \pm}^{(l)} \) in expansion (41). Q.E.D.

It is convenient to combine the statements of theorem 1 and lemma 4 in the following form.

**Theorem 2.** Let \( c/a = m \in \mathbb{N} \) be the ratio of the perturbed operator \( H \) period to the unperturbed operator \( H_0 \) one. Then the gaps in the spectrum of \( H \) can be divided into two sets: the "old" gaps with numbers \( mN \), \( N = 1, 2, ..., \) which are just shifted gaps of the unperturbed operator \( H_0 \) with the shifts given by eqs. (39), (40); and "new" gaps with numbers \( lN, l = 1, 2, ..., m-1 \), \( (N = 1, 2, ...) \) which arise under perturbation. These new gaps are located inside the \( N \)-th band of the unperturbed operator, are concentrated around the points \( \varepsilon_{lN} \) given by eq. (30) and have the widths described by eq. (33).

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