LANDAUER FORMULA AND FORMING OF SPECTRAL BANDS

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Summary

The transmission coefficients through a single potential barrier is compared with one corresponding to a finite periodic chain of N potential barriers or wells. It is proved, that even for small periodic potentials the exponential decreasing of the transmission coefficient for growing N takes place in lacunas of the corresponding periodic operator on the whole real line. Using the Landauer formula we express the conductivity of the corresponding onedimensional conductor in terms of the transmission coefficient.

1. Introduction Due to the tunnel effect the quantum particle can pass a potential barrier even if the height of it is greater than the particle's energy. But the transmission coefficient depends exponentially on the product of the hight and the width of the barrier. Consider a quantum particle in a one dimensional conductor described by the Schrödinger equation

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

with the step-wise potential which is the multiple of the indicator $\chi_{(0,L)}(x)$ of the finite interval $(0, L)$

$$q_0(x) = H\chi_{(0,L)}(x).$$

Then the corresponding transmission coefficient for scattered waves in the energy range $k^2 = \lambda \leq H$ is given by the formula

$$T(k) = \frac{4ik\sqrt{H^2 - k^2}}{\sqrt{H^2 - k^2} + ik} \times \frac{1}{e^{\sqrt{H^2-k^2}L} - e^{-\sqrt{H^2-k^2}L}},$$

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and thus is exponentially decreasing when $\sqrt{H^2-k^2}L$ tends to infinity. It means, that the corresponding conductance for electron's current is given by the Landauer formula, see [1], which involves the transmission coefficient T:

$$\frac{e^2}{\hbar}\frac{|T|^2}{1-|T|^2} \approx \frac{e^2}{\hbar}\frac{1}{H^2}e^{-2\sqrt{H^2-k^2}L}.$$

It decreases exponentially for any fixed energy k^2 with growing the "mass" HL of the barrier. This formula was deduced for the case when electron - phonon and Colomb scattering are absent.

If the potential barrier hight H measured from the vacuum level is formed by the electrostatic potential, then the question arises, if the field is strong enough, so that all conductivity electrons with the energy close to Fermi level (see [5]) k_0^2 are reflected. It terms of the asymptotics of the solutions of the relevant homogeneous Schrödinger equation it means, that the corresponding transmission coefficient T must be close to zero on some interval of energies centered at k_0^2 (then the reflection coefficient $|R| = \sqrt{1-|T|^2}$ is close to one). For simple rectangular barrier discussed above this impies, that all electrons with the energies less than k_0^2 will be reflected by the same barrier as well.

But in real conductors only electrons with energies close to Fermi level might participate in the conductivity process. This induces more special question concerning the most "economical" form of the barrier which, being created by the *minimal* electric field, would nevertheless reflect all conductivity electrons with energies close to the Fermi level k_0^2 *only* . If it would be achieved due to some special form of the electric field, then it would suffice to block the conductivity totally, since at sufficiently low temperatures all conductivity electrons have energies close to Fermi level. We call the corresponding process *selective reflection*, and the conductance (resistance) calculated on the base of T using Landauer formula will be called *selective* conductance rsp. resistance. It is clear that for real conductors the selective reflection in the interval of energies close to Fermi level is sufficient to implement the resistance for *all* conductivity electrons at sufficiently low temperatures.

We'll show , that the selective reflection **is possible**, at least in principle, for small intervall of energies near k_0^2 if we form a periodic potential inlet on the infinite conductor, the amplitude of the periodic potential being defined by the interval of energies around k_0^2, where the reflection is being implemented. This selective reflection is a partial case of resonance scattering caused by the effect of interference of wave functions. In some respect it is much more delicate, than the direct tunnelling through the high barrier mentioned in the beginning of this section, but it posesses the remarkable stability under thermal fluctuations in comparing with other interferential gates (such as Aharonov - Bohm gate).

2 Spectral properties of a onedimensional conductor perturbed by a finite periodic inlet.

Let us consider the onedimensional Schrödinger operator on L_2 perturbed by inserting a sample of N periodes of the periodic potential $q(x), q(x+a) = q(x)$. We assume that the periodic potentials is real and continuous, so that the discontinuities of the resulting potential ρ_N can lie at the points of contacts $0, Na$ only.

In what follows we use the following notations.

The "standard solutions" of the Schrödinger equation

$$-\frac{d^2u}{dx^2} + q(x)u = \lambda u \equiv k^2 u$$

with the initial conditions at the origine $u_0 = 1, u_0' = 0$ or $u_0 = 0, u_0' = 1$ will be denoted by $\theta(x,\lambda)$, rsp. $\varphi(x,\lambda)$,. The corresponding Bloch solutions $\chi_\pm \in L_2(R_\pm)$ are square integrable on positive halfaxis R_+ or negative halfaxis R_- respectively for non-real λ. They are combined of θ, φ

$$\chi_+(x,\lambda) = \theta(x,\lambda) + m_+(\lambda)\varphi(x,\lambda), \chi_-(x,\lambda) = \theta(x,\lambda) + m_-(\lambda)\varphi(x,\lambda),$$

with coefficients coincining with the corresponding Weyl-Titchmarsh functions (see[2]) $m_\pm(\lambda)$. The quasymomentum p and the quasimomentum exponentials $\mu_\pm = e^{\pm iap}$ are defined by the transformation of Bloch functions under translation $\chi^q_\pm, \chi^q_\pm(x+a) = \mu^\pm \chi^q_\pm(x+a), |\mu_+(\lambda)| < 1$. They are calculated from the quadratic equation containing the Lyapunov function $l(\lambda) = \frac{\theta + \varphi'}{2}$

$$\mu + \frac{1}{\mu} = l(\lambda)$$
$$\mu_\pm = l(\lambda) \pm \sqrt{l^2 - 1}.$$

One assumes usually that $|\mu_+| < 1, |\mu_-| > 1$ on the regularity field (that is on the complement of the spectrum) of the periodic problem. The following statement is just a particular case of the general results concerning the Schrödinger equation with a decreasing potential [1]

Assertion *Consider the Schrödinger operator with the potential* ρ_N

$$-\frac{d^2u}{dx^2} + \rho_N(x)u \equiv L_{\rho_N} u \qquad (2)$$

which is defined on the Sobolev class $W_2^2(R)$ *of all* L_2*-functions with the square-integrable derivatives is a selfadjoint operator in* $L_2(R)$*. The spectrum* σ_N *of it consists of the absolutely - continuous branch, which coincides with the (absolutely - continuous) spectrum* $[0, \infty\ )$ *of the unperturbed operator* $L_0 \equiv -\frac{d^2u}{dx^2}$ *and possibly a finite set of negative eigenvalues. The scattered waves of* L_{ρ_N} *are formed of exponentials and Bloch waves. In particular for the scattered waves* $\overleftarrow{\psi}$ *iniciated by plane waves* e^{-ikx} *from the right side we have the following expression at the spectral point* $\lambda = k^2$*:*

$$\overleftarrow{\psi} = \begin{cases} Te^{-ikx}, & -\infty, x \leq 0, \\ \alpha\chi_+^q(x) + \beta\chi_-^q & ,0 < x < Na, \\ e^{-ikx} + \overrightarrow{R}\, e^{ikx}, & Na < x < \infty, \end{cases}$$

The waves $\overrightarrow{\psi}$ *iniciated from the left are constructed in a similar way.The system of all scattered waves* $\overleftarrow{\psi}$, $\overrightarrow{\psi}$ *forms a complete orthogonal base in the invariant subspace corresponding to the absolute- continuous spectrum of the operator* L_{ρ_N}*. The corresponding spectral density coincides with the spectral density of the nonperturbed operator* L_0 *for the exponential system .The corresponding expansion theorem in the space of all square integrable functions involves the scattered waves and possibly finite number of negative bound states with integrations spread over* $(0, \infty)$ *with Lebesgue measure* $dm = \frac{d\lambda}{4\pi\sqrt{\lambda}} \equiv \frac{dk}{2\pi}$

$$\delta(x-y) = \frac{1}{2\pi}\int_0^\infty \overleftarrow{\psi}\,(x)\ \bar{\overleftarrow{\psi}}(y)dk + \frac{1}{2\pi}\int_0^\infty \overrightarrow{\psi}\,(x)\bar{\overrightarrow{\psi}}(y)dk + \sum_l \psi_l(x)\bar{\psi}_l(x).$$

We calculate the transmission and reflection coefficients T, R and the scattered waves in explicite form and observe the creation of the spectral band on the absolutely-continuous spectrum.

Theorem 1. *The Weyl functions $m_\pm$ of the periodic Schrödinger Operator with the potential q on the right and left axis are equal respectively*

$$m_\pm = \frac{\mu_\pm - \theta(a)}{\varphi(a)}.$$

The reflection coefficient $\vec{R}$ is defined on the spectral bands of the periodic operator by the following formula

$$\vec{R}\,(k) = e^{-2ikaN} \frac{ik + m_+(\lambda)}{ik - m_+(\lambda)} \; \frac{\mu_+^N - \mu_-^N}{\mu_+^N - |\frac{ik+m_+(\lambda)}{ik+m_-(\lambda)}|^2 \mu_-^N}.$$

Proof of this statement can be received by the straightforward calculation. Really, from the condition of smotheness of the scattered wave we have :

$$\begin{aligned} &T = \alpha + \beta; \;\; -ikT = \alpha m_+ + \beta m_-, \\ &\alpha \mu_+^N + \beta \mu_-^N = e^{-ikNa} + \vec{R}\,(k) e^{ikNa}, \\ &\alpha m_+ \mu_+^N + \beta m_- \mu_-^N = -ike^{-ikNa} + ik\,\vec{R}\,(k) e^{ikNa}. \end{aligned}$$

We have now:

$$\frac{\beta}{\alpha} = -\frac{ik + m_+}{ik + m_-},$$

and

$$\vec{R}\,(k) = e^{-ikNa} \frac{\alpha}{2ik} (m_+ + ik)[\mu_+^N - \mu_-^N].$$

From the second pair of equations we find α

$$\alpha = \frac{2ike^{-ikNa}}{(ik - m_-)[\mu_+^N \frac{ik-m_+}{ik-m_-} - \mu_-^N \frac{ik+m_+}{ik+m_-}]}.$$

Combiming last two formulas we get the following expression for the reflection coefficient :

$$\vec{R}\,(k) = e^{-2ikNa} \frac{ik + m_+}{ik - m_+} \; \frac{\mu_+^N - \mu_-^N}{\mu_+^N - \frac{(ik+m_+)(m_- - ik)}{(ik+m_-)(m_+ - ik)} \mu_-^N}.$$

Using the the connection between the Weyl-functions $m_\pm$ on the spectral bands of the periodic operator $m_-(\lambda) = \bar{m}_+(\lambda)$ we see that the last equation coincides with the announced one .

Remark. Note that the similar expression for lattice model was suggested in [10]. The typical feature of both expressions is the presence of zeroes of the reflection coefficient on each "future" spectral band (the spectral band of the periodic Schrödinger operator on the infinite axis). It is a remerkable fact, that these zeroes divide each future spectral band into N equal intervals in quasimomentum scale. This fact was noticed first in [11]. The expression for the reflection coefficient permitts to calculate the conductivity using the Landauer formula:

$$\sigma = \frac{e^2}{\hbar}\frac{|T|^2}{1-|R|^2}.$$

Due to the unitarity of the scattering matrix the last expression is equal to

$$\sigma = \frac{e^2}{\hbar}\frac{1-|R|^2}{|R|^2}.$$

Generally the spectral problem for the Schrödinger operator with the potential vanishing on a half - axis (or the whole real axis) can be considered in terms of Resonance Scattering and Lax - Phillips theory, see for instance [12]. This gives the interpretation of the reflection and transmission coefficients as characteristic functions of some contracting semigroups or eigenvalues of the dissipative operators, which generate the reduced dynamics. In particular the zeroes of the reflection coefficient are the spectral singularities of this generator. In terms of this theory the spectral band of the Schrödinger operator with the "semi - infinite" periodic potential (where the reflection coefficient is modulo less than 1) are developed when N goes to infinity from the intervals, divided into N equal parts (in quasimomentum scale) by these spectral singularities - the zeroes of the reflection coefficient. Note that the conductivity calculated from Landauer formula is infinite at these points .

From the point of view of the theory of nonselfadjoint operators the spectral singularities are generallly very difficult to localize . But in the model we consider now they have extremely clear and important physical meaning mentioned above.

Theorem 2 *Inside the spectral band the conductivity is represented in form*

$$\sigma = \frac{e^2}{\hbar}\frac{|sin(Np+i\beta)|^2 - sin^2 Np}{sin^2(Np)},$$

where $\beta = \log |\frac{ik+m_+}{ik-m_+}|$.

On the complementary intervals of real axis - spectral lacunas - the conductivity is exponentially small for large N and is represented by formula:

$$\sigma = 4\frac{e^2}{\hbar}\mu_+^{2N}\frac{sin^2\Delta}{|1-\mu_+^{2N}|^2},$$

where $2\Delta = \arg(\mu_+ - \theta - ik\varphi) - \arg(\mu_- - \theta - ik\varphi) \equiv \psi_+ - \psi_-$ *and both* $\mu_+, \mu_- = \mu_+^{-1}$ *are positive functions on even lacunas and negative on odd ones,* $|\mu_+| < 1$.

Proof. Really, on the spectral band we have $m_- = \bar{m}_+$, hence

$$\overline{ik - m_+} = -ik - m_-, \ \overline{ik - m_-} = -ik - m_+,$$

and for some positive β

$$\frac{ik - m_+}{ik - m_-} \ \frac{ik + m_-}{ik + m_+} \equiv e^{-2\beta} < 1.$$

Then for the corresponding conductivity σ we have:

$$\sigma = \frac{e^2}{\hbar}\left(|\frac{ik - m_-}{ik + m_-}|^2\frac{|\mu_+^N e^{-2\beta} - \mu_-^N|^2}{|\mu_+^N - \mu_-^N|^2} - 1\right) =$$
$$\frac{e^2}{\hbar}\left(\frac{|\mu_+^N e^{-\beta} - \mu_-^N e^{\beta}|^2}{|\mu_+^N - \mu_-^N|^2} - 1\right) = \frac{e^2}{\hbar}\frac{|\sin(Np + i\beta)|^2 - \sin^2 Np}{\sin^2(Np)},$$

since $|e^{2ikNa}| = 1$.

Considering the lacunas, we take into account that both periodic Weyl-functions are real, $m_+ = \bar{m}_+, m_- = \bar{m}_-$, and

$$\frac{m_+ - ik}{m_+ + ik} = e^{2i\arg(\mu_+ - \theta - ik\varphi)} \equiv e^{ik\psi_+},$$
$$\frac{m_- - ik}{m_- + ik} = e^{2i\arg(\mu_- - \theta - ik\varphi)} \equiv e^{ik\psi_-},$$
$$|R|^2 = \frac{|\mu_+^N - \mu_-^N|^2}{|\mu_+^N e^{i\psi_+} - \mu_-^N e^{i\psi_-}|^2}.$$

Now we have for the conductivity inside the lacuna:

$$\sigma = \frac{e^2}{\hbar}\left(\frac{1}{|R|^2} - 1\right) = \frac{e^2}{\hbar}\left(\frac{|1 - \mu_+^{2N} e^{i(\psi_+ - \psi_-)}|^2}{|1 - \mu_+^{2N}|^2} - 1\right) =$$
$$4\mu_+^{2N}\frac{\sin^2\left(\frac{\psi_+ - \psi_-}{2}\right)}{|1 - \mu_+^{2N}|^2}.$$

3. Explicite expressions for conductivity inside the lacuna and the band in terms of the potential.

The standard perturbation technique permitts to calculate the relevant spectral quantities in terms of the potential. Actually we need the spectral data for the periodic potential $q(x)$ only. All relevant spectral data can be recovered from the behaviour of the standard solutions θ, φ, which satisfy the initial conditions $\theta(0) = 1, \theta'(0) = 0, \varphi(0) = 0, \varphi(0) = 1$. On the other hand these solutions fulfill Volterra-type integral equations which can be solved by succesive approximation method. Really, for the standard solutions θ, φ of the homogeneous equation

$$-y'' + q(x)y = \lambda y \equiv k^2 y,$$

we have, see [2]:

$$\theta(k,x) = \cos kx + \int_0^x \frac{\sin k(x-t)}{k} q(t)\theta(k,t)dt,$$
$$\varphi(k,x) = \frac{\sin kx}{k} + \int_0^x \frac{\sin k(x-t)}{k} q(t)\varphi(k,t)dt.$$

We use these integral equations to calculate the elements of the monodromy matrix

$$M(k) = \begin{pmatrix} \theta(k,a) & \varphi(k,a) \\ \theta'(k,a) & \varphi'(k,a) \end{pmatrix}.$$

The spectral bands coincide with the intervals, where $|\mathrm{Trace} M(k)| = |\theta(k,a) + \varphi'(k,a)| \leq 2$. Taking into account the terms of the first and second order of the perturbation series for the solutions of the previous integral equations in respect to the potential q we get the following "explicite" expression for the Lyapunov function $l(\lambda) = \frac{1}{2}\mathrm{Trace} M(k)$:

$$\cos ak + \frac{\sin ak}{2k}\int_o^a q(t)dt - \frac{\cos ka}{4}(\int_o^a q(t)dt)^2$$
$$\frac{\cos ka}{4}\left[(\int_0^a q(t)\cos 2kt dt)^2 - (\int_0^a q(t)\ \sin 2kt dt)^2\right] -$$
$$\frac{\sin ka}{4}\int_0^a q(t)dt \int_0^t q(s)ds\ \sin 2k(s-t).$$

The approximate positions of spectral bands and the values of quasimomentum and Weyl functions can be found from the last formula. But here we just consider two simplest examples.

Example 1 Dirac "Comb" (periodic δ - potential, see [9]) After proper change of variables we rewrite the corresponding Sturm-Liouvilles problem in the following form :

$$-\frac{d^2u}{dx^2} + Q \sum \delta(x - la)u = \lambda u.$$

Note that the half-trace of the monodromy matrix - the Lyapunov function - in this case is just

$$l(k) = \cos\, ak + \frac{\sin\, ak}{2k}\, Q \ ,$$

which coincides with the main part of our general expression when $Q = \int_0^a q(t)dt$. We calculate now the conductivity which corresponds to the finite periodic inlet on the infinite axis

$$\rho(x) = \sum_0^N \ Q\ \delta(x - al).$$

The equation for the end-points of spectral lacunae on k-axis, $k^2 = \lambda$, $(\frac{\pi l}{a}, \frac{\pi l}{a} + \delta_l)$ which correspond to "infinite" periodic potential can be reduced to the form

$$\frac{Q}{\frac{\pi l}{a} + \delta_l} = 2\ \mathrm{tg} \frac{\delta}{2}$$

Assuming that $\frac{aQ}{\pi l} << 1$ we get for the width of the l-th lacuna,$l \geq 1$, the approximate expression $\delta_l \approx \frac{aQ}{\pi l}$ Strictly inside the l-th lacuna where $|\cos\, ak + Q\frac{\sin\, ak}{2k}| > 1$ or inside the spectral band $|\cos\, k + Q\frac{\sin\, ka}{2k}| < 1$ we get respectively from the equations

$$\cos\, ak + Q\frac{\sin\, ak}{2k}\ Q\ = \cosh\, ap,$$

$$\cos\, ak + Q\frac{\sin\, ak}{2k}\ Q\ = \cos\ ap$$

the following approximate expression for the quasimomentum $p \equiv (\frac{\pi l}{a} + \delta_p)$ as a function of energy $\lambda = k^2 \equiv (\frac{\pi l}{a} + \delta_k)^2$ (for positive Q)

$$\delta_p \approx \sqrt{(\delta_k)^2 - \frac{Qa\delta_k}{\pi e}},$$

which takes imaginary values on the lakuna and real values on the band. In particular this gives due to the Theorem 2 the following expressions for the conductivity inside the lacuna :

$$\sigma(k) \approx 4\frac{e^2}{\hbar} e^{-N\sqrt{\frac{aQ\delta_k}{\pi l}}} (\sin\Delta_k)^2,$$

where

$$(\sin\Delta_k)^2 = \frac{(\delta_k)^2}{(\delta_k)^2 + \sqrt{\frac{aQ\delta_k}{\pi l}} - (\delta_k)^2}$$

Example 2 Periodic Kronig - Penny potential. Consider the Sturm - Liouvilles problem with the potential $\sum_{l=-\infty}^{l=+\infty} Q(x - la)$, where

$$Q(x) = \begin{cases} H, \text{if} & x \in (0, d), d < a, \\ 0, \text{if} & x \quad \text{elsewhere.} \end{cases}$$

Then the Lyapunov function has the form

$$\begin{aligned} l(k) \equiv \frac{\theta(2\pi, k) + \varphi'(2\pi, k)}{2} = \\ \cos k(a - d) \ \cos d\sqrt{k^2 - H} d - \\ \sin k(a - d) \ \sin\sqrt{k^2 - H} d \ \frac{H}{2k\sqrt{k^2 - H}}. \end{aligned}$$

The quasimomentum inside the spectral band is the solution of the equation $l(k) = \cos ap$ and in the spectral lacuna it fulfills the equation $l(k) = \cosh ap$. In particular the second equation can be solved approximately assuming, that $\frac{k^2}{H}$ is large enough and taking into account only linear and quadratic term in respect to $\frac{k^2}{H}$ in the following exact expression:

$$\begin{aligned} \cosh pa = \cos[ka - \frac{Hd}{k + \sqrt{k^2 - H}}] - \\ \sin d\sqrt{k^2 - H} \ \sin k(a - d) \left(1 - \frac{H}{2k\sqrt{k^2 - H}}\right) \end{aligned}$$

Basing on the quasimomentum found from the previous equation and the general formulas (see theorem 2) one can easily calculate the conductivity of the quantum wire with a finite Kronig - Penny inlet $\rho_N(x) = \sum_{l=0}^{l=N} Q(x - la)$.

Remark. When considering the conductivity of the real quantum conductor we have the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + \rho(x)u = Eu,$$

where E is the energy and m is the effective mass of the electron in the given medium. This equation can be easily reduced to the previous one by the obvious change of scale $x \to \frac{\hbar x}{\sqrt{2}m}$.

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