Quantum Mechanical Electrical Conductivity of the One-Dimensional Landauer Model of an Impure Metal

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1. Introduction

In a paper, on localized scattering, R. Landauer called attention to the fact that "the duality between current generators and voltage generators which exists in circuit theory, also exists in transport theory". In particular, he clarified the viewpoint according to which the current entering the specimen is considered as the starting point for the calculation of the conductivity, while the field set up by the carriers through their interaction with the scattering centers is a secondary consequence of the current flow.

He used a one-dimensional model, consisting of a set of barriers to treat classically and quantum-mechanically the flow of electrons through the system. This model is excellently suited to demonstrate the usefulness of this viewpoint, and it also gives an opportunity to elucidate the origin of the irreversibility of transport phenomena.

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Extension of the model to a random collection of obstacles yields the result, that if the obstacles were classical reflectors, the conductivity is reduced by a factor equal to the number of obstacles. The same result for the quantum-mechanical obstacles, however, has not been obtained. This made the author of ref. 1 doubt the physical relevance of the one-dimensional model.

In this paper, we discuss the wave mechanical problem of transmission through a set of barriers.

The results will shed light upon two interesting questions about disordered systems.

First, it will allow us to form a clear concept as to what happens to the electronic band structure of a metal when more and more disorder is introduced in the ionic positions.

Second, it will allow us to discuss the optical problem of transmission of monochromatic (e.g. laser) light through a set of semi-transparent mirrors.

2. Transmission Through a Set of Barriers

In this section we begin the study of the transmission of a particle with sharply defined wave number k through a set of barriers. As will be explained later, the treatment presented here cannot immediately be extended to include a wave-packet, because we shall average over a quantity which is non-linear in the wave function.

When we talk about the wave number and kinetic energy of the particle we always mean the quantities in the regions between the barriers. The corresponding quantities inside the barries need not concern us.

Consider N identical barriers along the x-axis The barriers are represented by a real, symmetric potential $v(x-x_n)$ where x_n is the position of the center of the barrier. As discussed in Appendix A, the barrier located at x=0 is characterized by the transmission matrix M (A.4). The transmission matrix expresses the wave function to the right of the barrier in terms of the wave function to the left. We describe the wave function in the region $x_n < x < x_{n+1}$ by the two-component complex vector

$$\underset{\sim}{b}_n = \begin{pmatrix} b_n^1 \\ b_n^2 \end{pmatrix} , \tag{2.1}$$

whose components are the coefficients in the solution of Schrödinger's equation in the region $x_n < x < x_{n+1}$, written in the form

$$\psi_n = b_n^1 e^{ik(x-x_n)} + b_n^2 e^{-ik(x-x_n)} . \tag{2.2}$$

Consequently

$$\underset{\sim}{b}_{n+1} = M_n \underset{\sim}{b}_n , \qquad \text{for } n = 0, \ldots, N-1. \tag{2.3}$$

The matrix M_{n+1} is not of the form (A.4), because it is not symmetric with respect to x=0, but with respect to the point x_{n+1}. It is therefore convenient to introduce a new coordinate z measured from x_{n+1}:

$$x = x_{n+1} + z \,, \tag{2.4}$$

and write

$$\psi_n = a_n^1 e^{ikz} + a_n^2 e^{-ikz} \,, \qquad n = 0, \ldots, N. \tag{2.5}$$

Combining (2.2), (2.4), and (2.5), it follows

$$a_{n+1} = b_{n+1} \,,$$

and

$$\underset{\sim}{a}_n = U(x_{n+1} - x_n)\, \underset{\sim}{b}_n \,, \tag{2.6}$$

where

$$U(x) = \begin{pmatrix} e^{ikx} & 0 \\ 0 & e^{-ikx} \end{pmatrix}. \tag{2.7}$$

Clearly,

$$\underset{\sim}{a}_{n+1} = M \underset{\sim}{a}_n \,, \tag{2.8}$$

where M is now independent of the barrier position, and of the form (A.4).

Inserting (2.6) and (2.8) into (2.3), we obtain

$$\underset{\sim}{b}_{n+1} = M U(x_{n+1} - x_n)\, \underset{\sim}{b}_n \,. \tag{2.9}$$

Application of (2.9) N-times yields

$$\underset{\sim}{b}_N = \mathcal{P} \prod_{n=0}^{N-1} \left[M U(x_{n+1} - x_n) \right] \underset{\sim}{b}_0 \,. \tag{2.10}$$

Here $\mathcal{P}\Pi$ denotes the product of the matrices in the square bracket ordered with increasing n from the right to the left. We denote the total transmission matrix by $\mathcal{M}$, hence

$$\underset{\sim}{b}_N = \mathcal{M}\, \underset{\sim}{b}_0 \,. \tag{2.11}$$

We note that

$$\det \mathcal{M} = 1, \tag{2.12}$$

because det M=1 and detU(x)=1. Furthermore, induction from n to n+1 shows, that

$$\mathcal{M}_{11} = \mathcal{M}_{22}^{*} \quad \text{and} \quad \mathcal{M}_{12} = \mathcal{M}_{21}^{*} \tag{2.13}$$

which follows from the same property of $M_n = MU(x_{n+1} - x_n)$.

Therefore (A.3) applies for the total transmission and reflection coefficients t_T and r_T, and we have, resolving (A.3) into components and making use of the fact that detMU =1 we have

$$\left|\frac{r}{t}\right|^2 = |\mathcal{M}_{12}|^2. \tag{2.14}$$

3. Ensemble Averages

Equation (2.14) expresses the ratio of reflected to the transmitted current through a set of barriers located at specific positions x_n.

We are interested in this ratio for certain ensembles of randomly distributed barriers.

We shall consider two types of barrier distributions. The first type is useful in the study of a lattice, where the ion positions are slightly displaced with respect to a regular array. Since the matrix $U(x_n - x_{n-1})$ depends

on the inter-barrier distance rather then the barrier position, t is more convenient to use $x_n - x_{n-1}$ as independent random variables instead of x_n itself. Hence we set

$$x_n - x_{n-1} = \ell + \varepsilon, \tag{3.1}$$

where ℓ is the average barrier separation and assume a symmetric, but otherwise arbitrary probability distribution $f(\varepsilon)$ for the deviation of the actual inter-barrier distance from its average :

$$\left.\begin{aligned} f(\varepsilon) &= f(-\varepsilon), \\ \int_{-\infty}^{\infty} f(\varepsilon)\, d\varepsilon &= 1 \end{aligned}\right\} \tag{3.2}$$

The numerical computations will be performed using a Gaussian (normal) distribution $f(\varepsilon)$. This kind of distribution admits deviations which are larger than the average inter-barrier distance ℓ. Hence, barrier n may be located behind barrier n+1 contrary to normal ordering. However, the probability of such events is very small if the standard deviation σ (width of the distribution) is chosen sufficiently small. For instance, if $\sigma/\ell = 0.1$ the probability of such an event is less then 10^{-6}.

The second type of random distribution is representative, for instance, of the distribution of impurity ions in a

lattice. In this case there is no correlation between the position of adjacent barriers. Let the probability of having a barrier within a segment dx be $p\,dx$. If the average barrier separation is ℓ, then clearly $p=1/\ell$. Then the probability density $f_0(x)$ of a distance x between two subsequent barriers is obtained by multiplying the probability w(x) of no barrier within a distance x with the probability density $1/\ell$ of a barrier at x. To obtain w(x), divide the distance x in ν equal parts $\frac{x}{\nu}$. The probability of no barrier within $\frac{x}{\nu}$ is $1-\frac{x}{\ell\nu}$. The probability of no barrier in any of the portions is

$$w(x)=\lim_{\nu\to\infty}\left(1-\frac{x}{\ell\nu}\right)^{\nu}=e^{-\frac{x}{\ell}}.$$

Hence

$$f_0(x)=\frac{1}{\ell}e^{-\frac{x}{\ell}}\quad,\quad x\geq 0. \tag{3.3}$$

It follows from (2.14) and (2.10) that our task is the calculation of the average $\langle\cdots\rangle$ with respect to the appropriate distribution function f (ϵ) of the quantity $|r/t|^2$:

$$\left\langle\left|\frac{r}{t}\right|^2\right\rangle=\left\langle\left\{\mathcal{P}\prod_{n=0}^{N-1}MU(x_{n+1}-x_n)\right\}_{12}^{*}\left\{\mathcal{P}\prod_{m=0}^{N-1}MU(x_{m+1}-x_m)\right\}_{12}\right\rangle. \tag{3.4}$$

Since the quantities $x_{n+1}-x_n$ are considered to be independent random variables, the average of one of the curly brackets would simply be the product of the averages taken over each matrix $MU(x_{n+1}-x_n)$ separately.

However, since (3.4) represents the average of the square of a product, each variable occurs in two matrices and the averaging has to take into account the correlation of these pairs of matrices. The matrices $MU(x_{n+1}-x_n)$ do not commute for different n, therefore we rewrite (3.4) in terms of its matrix elements in order to group together those matrix elements which depend on the same random variable. We obtain

$$\left.\begin{aligned} \langle|r/t|^2\rangle &= \sum_{\beta_0\delta_0}\sum_{\beta_{N-1}\delta_{N-1}} M_{1\beta_{N-1}}M^*_{1\delta_{N-1}}\langle U_{\beta_0 2}(x_1)U^*_{\delta_0 2}(x_1)\rangle A_{\beta_{N-1}\delta_{N-1}\beta_0\delta_0}, \qquad (3.5)\\ A_{\beta_{N-1}\delta_{N-1}\beta_0\delta_0} &= \sum_{\alpha_1}^{\alpha_{N-2}}\sum_{\beta_1}^{\beta_{N-2}}\sum_{\gamma_1}^{\gamma_{N-2}}\sum_{\delta_1}^{\delta_{N-2}}\prod_{n=0}^{N-2} M_{\alpha_n\beta_n}M^*_{\gamma_n\delta_n}\langle U_{\beta_{n+1}\alpha_n}(x_{n+1}-x_n)U^*_{\delta_{n+1}\gamma_n}(x_{n+1}-x_n)\rangle. \end{aligned}\right\}$$

Note that in this expression the matrices M_{N-1} and $U(x_1)$ received special treatment, because only one of their matrix elements occurs in $\langle|r/t|^2\rangle$. All four elements of the remaining matrices occur in (3.5), and they are grouped into $A_{\beta_{N-1}\delta_{N-1}\beta_0\delta_0}$.

For the probability distributions of type (3.1) and (3.2) we obtain from (2.7).

$$Y_{\beta\alpha\delta\gamma} \equiv \langle U_{\beta\alpha}(x_n-x_{n-1})U^*_{\delta\gamma}(x_n-x_{n-1})\rangle = \int_{-\infty}^{\infty} d\varepsilon\, f(\varepsilon)\, U_{\beta\alpha}(\varepsilon)\, U^*_{\delta\gamma}(\varepsilon). \qquad (3.6)$$

From the form (2.7) of $U(\varepsilon)$ it follows that

$$\left.\begin{aligned} &Y_{1111} = Y_{2222} = 1,\\ &Y_{1122} = Y^*_{2211} = e^{2ik\ell}\tilde{\chi}(2k), \end{aligned}\right\} \qquad (3.7)$$

and all other $Y_{\alpha\beta\gamma\delta} = 0$.

Here, $\tilde{\chi}(k)$ is the characteristic function (Fourier transform) of the distribution, defined by

$$\tilde{\chi}(k)=\int_{-\infty}^{\infty} f(\varepsilon)\, e^{ik\varepsilon}\, d\varepsilon . \tag{3.8}$$

Since $\tilde{\chi}$ may be complex, we shall use the notation $\tilde{\chi}=\chi e^{-2i\nu}$ so that χ and ν are considered real.

After averaging, the factors occurring in (3.5) become independent of n, and we may set

$$M_{\alpha\rho} M_{\gamma\delta} Y_{\beta\alpha\delta_\gamma} \equiv M_{\alpha_n\beta_n} M_{\gamma_n\delta_n} Y_{\beta_{n+1}\alpha_n\delta_{n+1}\gamma_n} . \tag{3.9}$$

We can dispose of the fourth-rank tensor $Y_{\beta\alpha\delta_\gamma}$ and may rewrite (3.5) as the product of 4x4 matrices by a simple relabeling. To this end, we replace the combination of the first and third, and second and fourth Greek subscript (each ranging from 1 to 2) by a latin subscript (ranging from 1 to 4) according to the following convention:

(α,γ) or (β,δ)	(1,1)	(2,2)	(1,2)	(2,1)
k or l	1	2	3	4

(3.10)

Hence we set $Y_{kl}=Y_{\beta\alpha\delta\gamma}$ and obtain from (3.7)

$$\left.\begin{aligned} &Y_{11}=Y_{22}=1, \\ &Y_{33}=Y_{44}^{*}=c, \\ &\text{All other } Y_{kl}=0. \end{aligned}\right\} \tag{3.11}$$

As an abbreviation, we define

$$c \equiv e^{2ik(l-\nu)}\chi(2k). \tag{3.12}$$

Also we set

$$A_{kl} \equiv A_{\alpha\rho\gamma\delta}\ , \qquad M_{kl} \equiv M_{\alpha\rho} M^{*}_{\gamma\delta}\ , \tag{3.13}$$

and henceforth use boldface letters to denote the 4x4 matrices $\underset{\sim}{Y}$, $\underset{\sim}{M}$ and $\underset{\sim}{A}$.

From (A.4) and (3.10) we obtain

$$\underset{\sim}{M} = \begin{pmatrix} aa^* & bb^* & ab^* & ba^* \\ b^*b & a^*a & b^*a & a^*b \\ ab & ab & a^2 & b^2 \\ a^*b^* & a^*b^* & (b^*)^2 & (a^*)^2 \end{pmatrix}, \tag{3.14}$$

with (See Appendix A)

$$a = e^{-i\mu}\mathrm{ch}\lambda \qquad \text{and} \qquad b = -i\,\mathrm{sh}\lambda. \tag{3.15}$$

The first factor of (3.5) becomes

$$M_{1l}Y_{2k} = \sum_{\beta_0\delta_0}\sum_{\beta_{N-1}\delta_{N-1}} M_{1\beta_{N-1}} M^{*}_{1\delta_{N-1}} \langle U_{\beta_0 2}(x_1) U^{*}_{\delta_0 2}(x_1)\rangle\ ,$$

whereas the remaining factor may be writen as

$$\underset{\sim}{A} = (\underset{\sim}{M}\,\underset{\sim}{Y})^{N-2}.$$

It follows

$$\left\langle \left|\frac{r}{t}\right|^2 \right\rangle = \left[(\underset{\sim}{M}\,\underset{\sim}{Y})^{N}\right]_{12}. \tag{3.16}$$

To make further progress, we diagonalize the matrix $\underset{\sim}{\underset{\sim}{MY}}$ by means of a similarity transformation. This will enable us to write

$$\underset{\sim}{\underset{\sim}{M}}\,\underset{\sim}{\underset{\sim}{Y}} = \underset{\sim}{\underset{\sim}{S}}^{-1}\,\underset{\sim}{\underset{\sim}{D}}\,\underset{\sim}{\underset{\sim}{S}}\,, \qquad D_{kl} = E_l\,\delta_{kl} \tag{3.17}$$

and hence

$$\langle \left|\frac{r}{t}\right|^2 \rangle = (S^{-1})_{1k}\, E_k^N\, S_{k2}\,. \tag{3.18}$$

Here, E_k are the eigenvalues of $\underset{\sim}{\underset{\sim}{MY}}$ and the column vectors of $\underset{\sim}{S}$ are the eigenvectors of $\underset{\sim}{\underset{\sim}{MY}}$.

4. Eigenvalues of the Transfer Matrix

In the preceding section we reduced the calculation of the average ratio of reflected and transmitted current to the avaluation of the eigenvalues and eigenvectors of the 4x4 transfer matrix $\underset{\sim}{\underset{\sim}{MY}}$ with $\underset{\sim}{M}$ and $\underset{\sim}{Y}$ given by (3.14) and (3.11) respectively.

To facililate this task, let us pause and look at our problem from a group-theoretical point of view.

The two components (2.2) of the wave function between barriers may be regarded as vectors $\underset{\sim}{b}$ in a two-dimensional complex space L. The totality of the transformations

$$Q = MU(x_n - x_{n-1}) \tag{4.1}$$

with M and U given by (A.4) and (3.7) form a three-parameter group G acting in L. The parameters of the group are λ and μ, as well as $\varphi = x_n - x_{n-1}$. The latter generates a one-parameter

sub-group, the group of translations along x. The group G is defined by the property, that it leaves the current j invariant

$$Q \in G: \qquad j(Qb_n) = j(b_n)$$

Since the current is given as

$$j = ev\,(|b^1|^2 - |b^2|^2), \tag{4.2}$$

where e and v are the charge and the velocity of the particle, respectively, the group G is formed by all 2x2 complex matrices which leave the products

$g_{\alpha\beta} b^\alpha b^{\beta *}$ invariant, where

$$g_{\alpha\beta} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We note, that G is not the unitary group, or the group of binary transformations of spinors. Its general element is of the form (See Appendix A).

$$Q = MU = \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}; \quad a a^* - b b^* = 1. \tag{4.3}$$

Let us form the four-dimensional direct product space LxL spanned by the vectors $b^\beta b^{\delta *}$. Every group element generates a linear transformation in LxL given by $Q_{\alpha\beta} Q^*_{\gamma\delta}$ or after the relabeling (3.10), Q_{kl}. These transformations form a four-dimensional representation of G. A decomposition of LxL into sub-spaces invariant under these transformations will reduce the matrices Q_{kl} to block-diagonal form.

We introduce a basis $\underset{\sim}{e}_1, \underset{\sim}{e}_2$ in L, orthonomal with respect to the usual matric tensor $g^0_{\alpha\beta} = \delta_{\alpha\beta}$, and write

$$\underset{\sim}{b} = b^1 \underset{\sim}{e}_1 + b^2 \underset{\sim}{e}_2 . \tag{4.4}$$

According to (3.10) the matrix elements Q_{kl} refer to the basis $\underset{\sim}{g}_1=\underset{\sim}{e}_1 x \underset{\sim}{e}_1$, $\underset{\sim}{g}_2=\underset{\sim}{e}_2 x \underset{\sim}{e}_2$, $\underset{\sim}{g}_3=\underset{\sim}{e}_1 x \underset{\sim}{e}_2$, and $\underset{\sim}{g}_4=\underset{\sim}{e}_2 x \underset{\sim}{e}_1$

A one-dimensional invariant subspace of LxL is immediately found noting that the current j is itself an invariant of the group since it is conserved along the set of barriers.

According to (4.1), the current is entirely contained in the subspace L_1 of LxL , defined by

$$L_1 = \{\underset{\sim}{e}_1 x \underset{\sim}{e}_1^* - \underset{\sim}{e}_2 x \underset{\sim}{e}_2^*\} = \{\underset{\sim}{g}_1 - \underset{\sim}{g}_2\}. \tag{4.5}$$

Hence L_1 is an invariant subspace. Let us introduce the basis

$$\underset{\sim}{f}_1 = \frac{1}{\sqrt{2}}(\underset{\sim}{g}_1 - \underset{\sim}{g}_2),\ \underset{\sim}{f}_2 = \frac{1}{\sqrt{2}}(\underset{\sim}{g}_1 + \underset{\sim}{g}_2),\ \underset{\sim}{f}_3 = \underset{\sim}{g}_3 \text{ and } \underset{\sim}{f}_4 = \underset{\sim}{g}_4, \tag{4.6}$$

and express the matrix $\underset{\sim}{Q}$ in this new basis. This will reduce it to the block diagonal form $\underset{\sim}{\tilde{Q}}$ with a 1x1 and 3x3 block along the principal diagonal, because $\underset{\sim}{f}_1$ is an invariant vector. The reduction is accomplished by writing

$$\underset{\sim}{f}_l = U_{lk}\,\underset{\sim}{g}_k, \qquad \underset{\sim}{U} = (U_{lk}), \tag{4.7}$$

where the U_{1k} can be read off from (4.6). Then

$$\underset{\sim}{\tilde{Q}} = \underset{\sim}{U}\,\underset{\sim}{Q}\,\underset{\sim}{U}^{-1}. \tag{4.8}$$

Combining (3.11), (3.14), (4.1), (4.7), into (4.8), we obtain

$$\underset{\sim}{\tilde{Q}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & aa^* + bb^* & \sqrt{2}ab^*c & \sqrt{2}a^*bc^* \\ 0 & \sqrt{2}ab & a^2c & b^2c^* \\ 0 & \sqrt{2}a^*b^* & (b^*)^2c & (a^*)^2c^* \end{pmatrix} \qquad (4.9)$$

The first eigenvalue, E_o, of this matrix is unity in accordance with the fact that the current is constant along the barriers, which means that we must have $E_0^{\,n} = E_0$ for any integer n.

In general there are no other invariant sub-spaces besides L_1.

The other eigenvalues of $\underset{\sim}{Q}$ are given by the three roots of the secular equation of (4.9):

$$E^3 - E^2(a^2c + a^{*2}c^* + aa^* + bb^*) + E[(aa^* + bb^*)cc^* + a^2c + a^{*2}c^*] - cc^* = 0. \qquad (4.10)$$

At this point it is convenient to <u>specialize to δ-function type potentials</u>, which are characterized by a single parameter g (henceforth called the "stength") instead of the two parameters λ and μ.

The reader will easily verify, that for these potentials

$$g = \sinh\lambda = \tan\mu, \qquad (4.11)$$

and (3.15) may be replaced by

$$a = 1 - ig \quad \text{and} \quad b = -ig. \qquad (4.12)$$

A further quantity shall be introduced whose significance will be discussed shortly

$$\beta \equiv 4(\cos k'\ell + q \sin k'\ell)^2 - 1 \; ; \qquad k'\ell \equiv k\ell - \nu(k), \tag{4.13}$$

With (4.11), (4.12) and (4.13) the root equation (4.10) becomes

$$E^3 - E^2[\chi\beta + (1-\chi)(1+2q^2)] + E[\chi\beta - \chi(1-\chi)(1+2q^2)] - \chi^2 = 0. \tag{4.14}$$

Since its coefficients are real, the three roots of (4.14) are either all real or one is real and two are complex conjugates. The implications of this fact and the dependence of $\langle |r/t|^2 \rangle$ on the roots of this equation are discussed in the next section.

5. The Average Reflection to Transmission Ratio

Before embarking on a study of the roots of (4.14) as a function of electron wave number k, barrier strength g and the barrier distribution function f ($\mathcal{E}$), let us express the average reflection to transmission ratio in terms of the roots and eigenvectors of the transfer matrix (4.9), as indicated by (3.18).

Let us denote the principal minor of $\underset{\sim}{Q}$ (4.9) with nonzero elements by $\underset{\sim}{R}$, (R_{kl}; $k,\ell = 1,2,3$). Then combining (3.18), (4.8) and (4.9) we obtain

$$\langle \left|\frac{r}{t}\right|^2 \rangle = (Q^N)_{12} = -\frac{1}{2} + \frac{1}{2}(R^N)_{11}. \tag{5.1}$$

Finally, let us denote by $\underset{\sim}{W}$ (W_{kl}, k, l=1,2,3,) the matrix which diagonalizes $\underset{\sim}{R}$ according to

$$\underset{\sim}{\tilde{R}} = \underset{\sim}{W}^{-1}\,\underset{\sim}{R}\,\underset{\sim}{W}\,, \qquad \tilde{R}_{kl} = E_k\,\delta_{kl}\,. \tag{5.2}$$

The row vectors of $\underset{\sim}{W}$ are the eigenvectors of $\underset{\sim}{R}$ and shall be denoted by u, v, and w; they belong to the eigenvalues E_1, E_2 and E_3, respectively.

With these definitions, straightfoward algebra yields

$$\langle\left|\frac{r}{t}\right|^2\rangle = -\frac{1}{2}+\frac{1}{2}(\det W)^{-1}\left[E_1^N u_2(v_3w_1-v_1w_3)+E_2^N v_2(u_1w_3-u_3w_1)+\right. \\ \left.+E_3^N w_2(u_3v_1-u_1v_3)\right]. \tag{5.3}$$

More insight is gained with regard to the behavior of $\langle|r/t|^2\rangle$, if we recognize certain properties of the eigenvectors u, v and w. A glance at the explicit form (4.9) of the coefficient matrix of the linear equations which yield these eigenvectors shows, that

(a) for a <u>real</u> eigenvalue E, the complex conjugate equations become identical to the original equations if we make the substitutions

$$u_3 \to u_1\,, \quad u_2 = u_2 \quad \text{and} \quad u_1 \to u_3\,.$$

Hence the eigenvector for a real eigenvalue has the form

$$u = (u_1, u_2, u_1^*)\,; \quad u_2 \text{ real}\,. \tag{5.4}$$

(b) for a complex eigenvalue E with eigenvector u, and associated complex conjugate eigenvalue E* with eigenvector v a similar argument yields

$$v_1 = u_3^* \,, \quad v_2 = u_2^* \quad \text{and} \quad v_3 = u_1^* \,. \tag{5.5}$$

Using (5.4) and (5.5) we arrive at the conclusion that

(a) If all three eigenvalues E_i are real, then the determinant of W is purely imaginary, i.e., det $W = i\Delta$, with Δ = real, which reduces (5.3) to

$$\left\langle \left|\frac{r}{t}\right|^2 \right\rangle = -\frac{1}{2} + \Delta^{-1}\left[E_1^N u_2 \mathfrak{J}(v_1^* w_1) + E_2^N v_2 \mathfrak{J}(u_1 w_1^*) + E_3^N w_2 \mathfrak{J}(u_1^* v_1)\right]. \tag{5.6}$$

Here $\mathfrak{J}$ denotes the imaginary part of the bracketed quantity.

(b) If two eigenvalues are complex conjugates, and the third one, E_3 is real we set

$$\left.\begin{aligned} &E_1 = |E_1| e^{i\varphi}, \quad \det W = \Delta, \quad u_2(u_1^* w_1 - u_3^* w_1^*) \equiv u e^{i\psi}, \\ &w_2\,(|u_3|^2 - |u_1|^2) \equiv w \end{aligned}\right\} \tag{5.7}$$

with

φ, Δ, u, ψ and w all real, and (5.3) becomes

$$\left\langle \left|\frac{r}{t}\right|^2 \right\rangle = -\frac{1}{2} + \frac{1}{2}\Delta^{-1} w E_3^N + \Delta^{-1} u |E_1|^N \cos(N\varphi + \psi). \tag{5.8}$$

The dependence on the number of barriers N is completely explicit in (5.6) and (5.8): N occurs only as an exponent of a real quantity and in the argument of a cosine.

We reach the conclusion that the average reflection-to-transmission ratio can only have a dependence on the number of barriers which is exponential or oscillatory or the combination of the two.

In order to understand the dependence of $\langle |r/t|^2 \rangle$ on the parameters of the problem, let us return to the root equation (4.14).

6. The Perfect Lattice

In the perfect lattice the probability of a deviation ε from the lattice constant ℓ is given by $f(\varepsilon) = \delta(\varepsilon)$. Hence

$$\chi(2k) = 1, \qquad \text{for all } k. \tag{6.1}$$

Equation (4.14) has the root $E_1 = 1$ for any β, and the roots

$$E_{2,3} = \tfrac{1}{2}(\beta - 1) \pm \tfrac{1}{2}\sqrt{(1-\beta)^2 - 4}. \tag{6.2}$$

It is clear, that $E_{2,3}$ are complex roots of unity as long as

$$-1 < \beta < 3. \tag{6.3}$$

The condition (6.3) combined with the definition (4.13) of β becomes

$$|\cos k'\ell + q \sin k'\ell| < 1, \tag{6.4}$$

which is the well-known KRONIG-PENNEY condition for the allowed energy bands of an electron in a one-dimensional array of δ-function potentials.

Therefore, an electron with energy in the allowed band has a $\langle|r/t|^2\rangle$ -ratio, which oscillates periodically between some maximum and zero as a function of the number of barriers. The frequency of this oscillation is not, in general, an integer but is given by

$$\frac{\varphi}{2\pi} = \arctan \frac{\sqrt{4-(1-\beta)^2}}{\beta-1}, \quad \text{for } -1<\beta<3. \qquad (6.5)$$

For an electron with energy in a forbidden band the roots $E_{2,3}$ of (6.2) are real. One of the roots is always greater than one as is easily seen: Hence the electron will be exponentially attenuated because $\langle|r/t|^2\rangle$ contains a term which grows exponentially with N.

In conclusion we show that $\chi=1$ is a necessary and sufficient condition for all roots of (4.14) to be roots of unity, i.e. the perfect lattice is the only one which, for certain energies, allows a non-exponential dependence of $\langle|r/t|^2\rangle$ on N.

This immediately follows from (4.14). The constant term χ^2 is the product of the three roots. Hence if $\chi^2\neq 1$ at least one of the roots must be different from 1. We cannot, at this point, ascertain whether a term in $\langle|r/t|^2\rangle$

is exponentially decreasing or increasing with N. This question, as well as the dependence of maximum attenuation $\max \langle |r/t|^2 \rangle$ on the wave number, and other features of the finite perfect lattice will be investigated in a forthcoming paper.

7. Transmission of the Disordered Lattice

A Gaussian distribution of the departures ε from the perfect lattice position with a standard deviation σ is being extensively studied. These studies will be published separately and hence, only qualitative remarks will be made here. Comparing our results with those obtained by other authors, we find ourselves in a basic disagreement concerning allowed and forbidden energy bands.

According to these authors, there exist ranges of the real wave vector k for which the transmitted and incident wave functions differ only by a phase factor. This means, that there is no reflection, and the wave vector belongs to an allowed band.

As has been shown in section 6, no such wave vectors exist in a disorded structure ($\chi \neq 1$). For every value of k the wave amplitude decreases exponentially along the lattice: the decrease is small in the regions which form the allowed bands in the perfect crystal, and is large in the regions which form the forbidden bands in the perfect crystal.

The disagreement is attributed to the incorrect averaging [)] of the wave amplitudes (transfer matrix) instead of the wave intensities (square of the transfer matrix). Thereby important interference effects are lost.

8. Optical and Mechanical Problems - The Classical Limit

We wish to discuss the relationship between the following three related problems.

1) A mono energetic particle beam passes through a succession of randomly positioned potential barriers.

2) A monochromatic light beam traverses a sequence of randomly positioned semitransparent mirrors.

3) A monoenergetic beam of macroscopic (classical) particles dashes through an array of randomly positioned mechanical shutters. Each shutter has the same reflection to transmission ratio for the beam intensity.

The first problem is dealth with in the previous sections.

There is an immediate translation of the quantum mechanical problem into the optical one if we denote by t or r the complex transmission and reflection coefficients of the semitransparent mirrors for light of the particular wave length chosen. The properties of the transmission matrix M depend only upon the invariance of the properties of the beam interceptor with respect to space inversion and time reversal, and conservation of current density (in this case, Poynting's vector). Quantum mechanics

enters only insofar, as it determines the detailed dependence of the transmission matrix elements on the parameters which characterize the potential barrier, and on the wave number of the particle beam.

The latter relations are - in the optical case - replaced by other phenomenological relations: the general properties of the transmission matrix as stated in Appendix A remain the same.

The optical problem permits a clear visuatization of the experiment which measures the pertinent quantities calculated in the other sections.

In Fig. 1 we show the experiment performed on one member (denoted by box ℓ) of a statistical ensemble. The ensemble consists of a large number (m) of boxes, each box with an entrance and exit slit. In the box there are N semitransparent mirrors, whose spacing $(x_n - x_{n-1})$ is governed by some random distribution function f $(x_n - x_{n-1})$ described in section 3 .

If we denote the amplitude of the wave at the entrance slit A by

$$\psi_o = b_o' e^{ikx} + b_o'' e^{-ikx} \quad , \tag{8.1}$$

and at the exit B by

$$\psi_N = b_N' e^{ikx} \tag{8.2}$$

then the detector D_o measures $s_1|b_o'|^2$, D_t measures $|b_N'|^2$, and D_r measures $s_2|b_o''|^2$. The coefficients s_1 and s_2 are determined by the properties of the two deflectors S_1 and S_2. They are found by calibration: Complete removal of the box determines s_1, then replacement of the box by a perfect mirror determines s_2. The transmission coefficient $\tau_N(\ell)$ and reflection coefficient $\rho_N(\ell)$ of the ℓ-th box are defined as

$$\tau_N(\ell) = |t_N(\ell)|^2 = |b_N'(\ell)|^2 / |b_o'(\ell)|^2, \tag{8.3}$$

and

$$\rho_N(\ell) = |r_N(\ell)|^2 = |b_o''(\ell)|^2 / |b_o'(\ell)|^2. \tag{8.4}$$

We also define the reflection-to-transmission ratio σ, henceforth called <u>resistance</u>, as

$$\sigma_N(\ell) = \frac{\rho_N(\ell)}{\tau_N(\ell)}. \tag{8.5}$$

Furthermore, conservation of energy leads to

$$\rho_N(\ell) + \tau_N(\ell) = 1. \tag{8.6}$$

For each box we determine the three quantities τ_N, ρ_N and σ_N (of course, it is sufficient to measure either τ_N or ρ_N), and form the averages over the ensemble of m boxes

$$\langle \rho_N \rangle = \frac{1}{m} \sum_{l=1}^{m} \rho_N(l) \ , \quad \langle \tau_N \rangle = \frac{1}{m} \sum_{l=1}^{m} \tau_N(l) \ , \tag{8.7}$$

and

$$\langle \sigma_N \rangle = \frac{1}{m} \sum_{l=1}^{m} \frac{\rho_N(l)}{\tau_N(l)} = \left\langle \frac{\rho_N}{\tau_N} \right\rangle . \tag{8.8}$$

As has been shown in the previous sections, the quantity $\langle \sigma_N \rangle$ is either an oscillatory, or exponential or a combination-of-both type function of the number N of semitransparent mirrors. The same cannot be asserted about the ratio

$$\overline{\sigma}_N = \frac{\langle \rho_N \rangle}{\langle \tau_N \rangle} .$$

The dependence of $\overline{\sigma}_N$ on N will be given in a forthcoming paper.

These remarks lead to the question: Which of the two averages $\langle \sigma_N \rangle$ or $\overline{\sigma}_N$ should be considered as more representative of the "resistance" of the system?

For the monoenergetic quantum-mechanical particle beam and for the monochromatic light beam both quantities are equally representative, and as demonstrated in Fig. 1, both quantities can be measured. Therefore it seems a matter of taste, which one is considered to be the resistance.

For classical particles as will be shown in a later paper, the quantities $\langle\sigma\rangle$ and $\bar{\sigma}$ are the same, and therefore this question does not arise.

It is important to realize, that (2.14) does not hold for the calculation of $\langle\sigma\rangle$ for a classical particle (wave packet), and therefore all conclusions about $\langle\sigma\rangle$ pertaining to a monochromatic beam do not apply. This will be clarified in the next section.

9. The Classical Model - Wave Packets

A classical model may be thought of as follows: Consider a succession of discs with an equal number of randomly distributed holes through each disc. A classical particle of velocity v impinging upon a disc will be transmitted or reflected with the probabilities t^c and r^c, respectively. The two real quanitites are connected by the relation.

$$t^c + r^c = 1. \tag{9.1}$$

The N discs are located at random positions x_n in the box previously considered, and they rotate with angular frequencies which are incommensurable with the frequencies $\nu_n = (x_n - x_{n-1})/v$. A particle of the uniform beam of velocity v will bounce back and forth with frequency ν_n between the disc n and the disc n+1, until it goes through one of them. The rotation of the discs prevents any correlation between successive transmissions of the same particle.

Since there is no phase angle in the classical problem, the location x_n of the discs has no bearing on the results. Each box will have the same transmission and reflection probabilities, which depend only on the number N of discs, and on t^c.

It is easy to see, that

the transmission t^c_{N+1} through N+1 discs in terms of t^c_N is given by

$$t^c_{N+1} = \frac{t\,t_N}{1 - r\,r_N}\,, \tag{9.2}$$

and

$$r^c_{N+1} = \frac{r + (t-r)\,r_N}{1 - r\,r_N} = \frac{t\,r_N + r\,t_N}{1 - r\,r_N}\,. \tag{9.3}$$

Therefore

$$\frac{r^c_{N+1}}{t^c_{N+1}} = \frac{t\,r_N + r\,t_N}{t\,t_N} = \frac{r_N}{t_N} + \frac{r}{t}\,. \tag{9.4}$$

Hence the ratios r^c_N/t^c_N are additive, and it follows [1]

$$\langle \sigma_N \rangle = \bar{\sigma}_N = \sigma_N = \frac{r^c_N}{t^c_N} = N\,\frac{r}{t}\,. \tag{9.5}$$

It is certainly difficult to calculate the properties of this shutter-system quantum mechanically, since it is time-dependent. We were unable to construct a time-independent model, which would have the same properties as the mechanical model presented above.

Nevertheless, all classical models must have one property in common: The particles must be localized in space and consequently we have to deal with the transmission of wave-packets rather than a monochromatic wave. For wave packets, the quantity $\langle \sigma \rangle$ or $\bar{\sigma}$ cannot be expressed in terms of the averaged square of transfer matrix elements. Therefore the conclusions derived in section 5 about $\langle \sigma \rangle$ for a monochromatic wave do not apply.

To understand this clearly, let us represent the beam by a wave packet of the form

$$\psi(x) = \int_0^\infty [b'(k)e^{ikx} + b''(k)e^{-ikx}]\,dk . \tag{9.6}$$

For each Fourier-component of the wave the quantum-mechanical calculation applies, and a wave-number dependent transmission and reflection coefficient results.

The impinging, the transmitted and the reflected current densities shall be denoted by j_o, j_t and j_r, respectively. Then, using $j = \frac{1}{2} i(\psi \frac{d\psi^*}{dx} - \psi^* \frac{d\psi}{dx})$, it follows:

$$j_o = \int_0^\infty |b_o'(k)|^2 k\,dk , \tag{9.7}$$

$$j_t = \int_0^\infty |b_N'(k)|^2 k\,dk \tag{9.8}$$

and

$$j_r = \int_0^\infty |b_o''(k)|^2 k\,dk . \tag{9.9}$$

The transmission matrix relates $\underset{\sim}{b}_N$ and $\underset{\sim}{b}_o$ as

$$\underset{\sim}{b}_N(k) = \mathfrak{M}(k)\,\underset{\sim}{b}_o(k); \tag{9.10}$$

hence,

$$j_t = \int_0^\infty |\mathfrak{M}_{11}(k) b_o'(k) + \mathfrak{M}_{12}(k) b_o''(k)|^2 k\,dk . \tag{9.11}$$

Note, that if ensemble averages of these current densities are required, besides the transmission matrix elements the unknown b_o'' also has to be averaged over, because it represents the reflected beam. Therefore, we eliminate b_o'' by the relation

$$\underset{\sim}{b}_o(k) = \mathfrak{M}^{-1}(k)\,\underset{\sim}{b}_N(k) . \tag{9.13}$$

Making use of

$$\left.\begin{aligned} &\mathcal{M}_{11}\mathcal{M}_{22}-\mathcal{M}_{12}\mathcal{M}_{21}=1\,, \qquad \mathcal{M}_{22}=\mathcal{M}_{11}^{*}\,,\ \mathcal{M}_{21}=\mathcal{M}_{12}^{*}\,,\\ &(\mathcal{M}^{-1})_{22}^{*}=(\mathcal{M}^{-1})_{11}=\mathcal{M}_{11}^{*} \quad \text{and} \quad (\mathcal{M}^{-1})_{12}=(\mathcal{M}^{-1})_{21}^{*}=-\mathcal{M}_{12}\,, \end{aligned}\right\} \tag{9.14}$$

we obtain

$$j_t=\int_0^\infty |\mathcal{M}_{11}(k)|^{-2}\,|b_0'(k)|^2\,k\,dk\,, \tag{9.15}$$

and

$$j_r=\int_0^\infty |\mathcal{M}_{12}(k)|^{2}\,|\mathcal{M}_{11}(k)|^{-2}\,|b_0'(k)|^2\,k\,dk\,. \tag{9.16}$$

It is clear, that only for an infinitely narrow incident wave packet

$$b_0'(k)=\delta(k-k_0)$$

do we obtain

$$\frac{j_r}{j_t}=|\mathcal{M}_{12}(k_0)|^2\,.$$

Hence the quantity $\langle|r/t|^2\rangle=\langle|\mathcal{M}_{12}(k_0)|^2\rangle$ does not represent the classical limit for a localized particle whose wave packet must be extended in k space.

To obtain the reflection to transmission ratio for the classical particle, we have to calculate the quantity j_r/j_t, as given by (9.15) and (9.16), for a suitably chosen wave packet amplitude $b_0'(k)$. This quantity may then be averaged over an ensemble of barrier distributions. However this averaging is not necessary, since we expect jr/jt to be nearly the same for all members of the ensemble.

The task of calculating $\langle j_r/j_t\rangle$ is much more formidable than the calculation of $\langle|r/t|^2\rangle$, and is the subject of another paper.

In view of the result (9.5) one expects a linear dependence of j_r/j_t on N, and also from (9.5) we expect, that the more localized the particle is, the less j_r/j_t for an individual barrier arrangement deviates from $\langle j_r/j_t \rangle$.

At present, these expectations cannot be confirmed.

Appendix A. Properties of the Transmission Matrix

We wish to prove, that besides the relation

$$|r|^2 + |t|^2 = 1, \tag{A.1}$$

the following equation connects the reflection and transmission coefficients:

$$t^2 - r^2 = e^{2i\mu} \text{ , } \mu \text{ real.} \tag{A.2}$$

Furthermore, we prove that the transmission coefficient t^1 from the right to the left equals the transmission coefficient t from the left to the right. ($t^1=t$ and not $t^1=t^*$)

To this purpose we consider the waves to the left and to the right of the barrier, each as two-component wave functions with respect to the (for this problem) complete basis e^{ikx} and e^{-ikx}. Then we may express the wave to the right in terms of the wave to the left through

$$\begin{pmatrix} t \\ o \end{pmatrix} = M \begin{pmatrix} 1 \\ r \end{pmatrix}. \tag{A.3}$$

As well known[5], the conditions, (a) real and symmetric potential, (b) time-reversal invariance, (c) conservation of the probability current density, lead to the following form of the transmission matrix M:

$$M = \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}, \tag{A.4}$$

with

$$aa^* - bb^* = 1. \tag{A.5}$$

The complex quantities a, b can be expressed by two real parameters[5] λ, μ as

$$\left.\begin{aligned} a &= e^{-i\mu} ch\lambda \ , \\ b &= -ish\lambda . \end{aligned}\right\} \quad \text{and} \qquad (A.6)$$

It follows

$$\left.\begin{aligned} r &= -ith\lambda e^{-i\mu} \ , \\ t &= \frac{1}{ch\lambda} \ e^{-i\mu} . \end{aligned}\right\} \quad \text{and} \qquad (A.7)$$

Hence there is always a phase difference $\pi/2$ between r and t, and from (A.7) one immediately obtains the required relation (A.2)

When the wave is incident from the right, we have

$$\begin{pmatrix} r^1 \\ 1 \end{pmatrix} = M \begin{pmatrix} o \\ t^1 \end{pmatrix} , \qquad (A.8)$$

with M again given by (A.4), and it follows

$$\left.\begin{aligned} r &= r^1 \ , \\ t &= t^1 \end{aligned}\right\} . \quad \text{and} \qquad (A.9)$$