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ELECTRONIC PROPERTIES OF SOLID

Conductance of Finite Systems and Scaling in Localization Theory[1]

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Abstract—The conductance of finite systems plays a central role in the scaling theory of localization (Abrahams et al., Phys. Rev. Lett. **42**, 673 (1979)). Usually it is defined by the Landauer-type formulas, which remain open the following questions: (a) exclusion of the contact resistance in the many-channel case; (b) correspondence of the Landauer conductance with internal properties of the system; (c) relation with the diffusion coefficient $D(\omega, q)$ of an infinite system. The answers to these questions are obtained below in the framework of two approaches: (1) self-consistent theory of localization by Vollhardt and Wölfle, and (2) quantum mechanical analysis based on the shell model. Both approaches lead to the same definition for the conductance of a finite system, closely related to the Thouless definition. In the framework of the self-consistent theory, the relations of finite-size scaling are derived and the Gell-Mann–Low functions $\beta(g)$ for space dimensions $d = 1$, 2, 3 are calculated. In contrast to the previous attempt by Vollhardt and Wölfle (1982), the metallic and localized phase are considered from the same standpoint, and the conductance of a finite system has no singularity at the critical point. In the 2D case, the expansion of $\beta(g)$ in $1/g$ coincides with results of the σ-model approach on the two-loop level and depends on the renormalization scheme in higher loops; the use of dimensional regularization for transition to dimension $d = 2 + \epsilon$ looks incompatible with the physical essence of the problem. The results are compared with numerical and physical experiments. A situation in higher dimensions and the conditions for observation of the localization law $\sigma(\omega) \propto -i\omega$ for conductivity are discussed.

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1. INTRODUCTION

The scaling theory of localization [1] is based on consideration of the so called "Thouless number"

$$g_L = \frac{J_L}{W_L} = \frac{G_L}{e^2/\hbar}, \tag{1}$$

equal to the conductance $G_L = \sigma_L L^{d-2}$ of the cubic block of size L (σ_L is the conductivity and d is a dimension of space) in units of $e^2/\hbar$, or to the ratio of parameters J_L and W_L of the effective Anderson model, arising in the Thouless scaling construction (Fig. 1). Equivalence of two representations in (1) follows from the estimate of overlap integrals $J_L \sim \hbar/\tau_D$ through the diffusion time $\tau_D = L^2/D_L$, estimate of W_L as the mean level spacing $\Delta_L \sim 1/\nu_F L^d$ and the use of the Einstein relation $\sigma_L = e^2\nu_F D_L$ between the conductivity Δ_L and the diffusion constant D_L (ν_F is the density of states at the Fermi level).

The behavior of g_L at large L is of the main interest: if $g_L \longrightarrow \infty$ then a system is in the metallic phase, since eigenfunctions of blocks are hybridized with practically equal weights; if $g_L \longrightarrow 0$, then a system is an Anderson dielectric (hybridization of the block eigenstates is practically absent). The block of size nL can be composed from n^d blocks of size L, so g_{nL} can be recalculated through a given g_L as $g_{nL} = F(g_L, n)$, which for $n \longrightarrow 1$ can be written in the differential form

$$\frac{d\ln g}{d\ln L} = \beta(g), \tag{2}$$

i.e. in the form of the Gell-Mann–Low equation [2]. The asymptotic behavior of $\beta(g)$

$$\beta(g) = \begin{cases} d-2, & g \gg 1, \\ \ln g, & g \ll 1, \end{cases} \tag{3}$$

follows from the evident relation $G_L = \sigma_\infty L^{d-2}$ in the metallic phase and the estimate $G_L \propto \exp\{-\text{const}\, L\}$

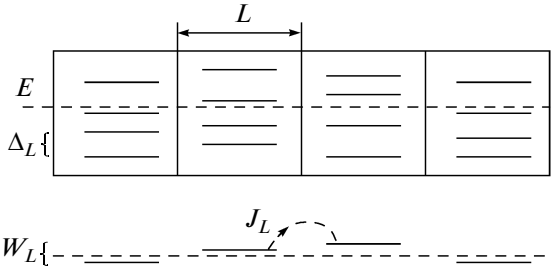

Fig. 1. The Thouless scaling construction. The infinite system is composed of finite blocks of size L; if only the level closest to the given energy E is retained in each block, the effective Anderson model arises, with the overlap integral J_L and the scattering of site energies W_L.

[1] The article was translated by the authors.

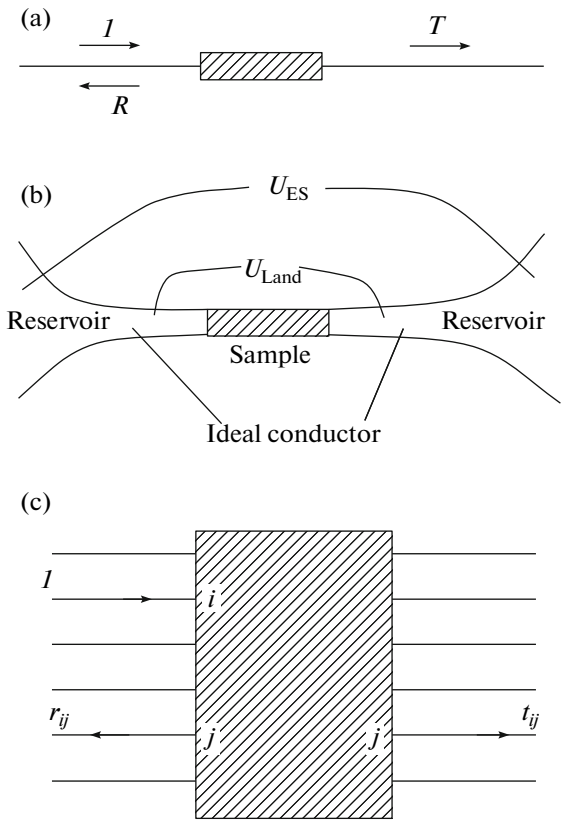

Fig. 2. (a) To derivation of the Landauer formula (4); (b) The difference between Eqs. (4) and (5) is determined by the fact, that voltage U_{ES} is measured between two reservoirs, while voltage U_{Land} between two ideal leads; (c) The many-channel scattering matrix.

for a dielectric. For $d \le 2$, the $\beta(g)$-function is always negative indicating localization of all states. For $d > 2$, it has a root g_c, corresponding to the Anderson transition point with the power law behavior $\sigma \propto \tau^s$ of the conductivity against the distance τ to the critical point.

The qualitative considerations of the paper [1] stimulated attempts to formulate them in a more quantitative form. Conductance of finite systems became a subject of a vivid discussion [3–14] (see a review article [15]) resulted in establishing of the Landauer approach [5, 12] as an adequate way of description. This approach reduces the kinetic problem of conductance to the quantum-mechanical scattering problem.

The original Landauer formula for the strictly 1D (one-channel) conductor follows from the simple considerations. If the unit flux of electrons is incident from the left to the sample under consideration (Fig. 2a), then it is transmitted with probability T and reflected with probability $R = 1 - T$ (T is a transmission coefficient). The current through the system is proportional to T, while the difference of chemical potentials is determined by the difference of electron density on the left $(1 + R)$ and on the right (T), i.e., $1 + R - T = 2(1 - T)$. Consequently the conductance is proportional to $T/(1 - T)$, and estimation of the coefficient gives [5]

$$G_{\text{Land}} = \frac{e^2}{2\pi\hbar}\frac{T}{1-T}. \tag{4}$$

A somewhat different result was obtained by Economou and Soukoulis [6] from linear response theory

$$G_{\text{ES}} = \frac{e^2}{2\pi\hbar}T. \tag{5}$$

Subsequent investigations established [12, 15], that Eq. (4) corresponds to the four-probe, while Eq. (5) to the two-probe measurement geometry (Fig. 2b): the difference between them is determined by the contact resistance $2\pi\hbar/e^2$ between the reservoir and the ideal conductor

$$\frac{1}{G_{\text{Land}}} = \frac{1}{G_{\text{ES}}} - \frac{2\pi\hbar}{e^2}. \tag{6}$$

Transition from one-dimensional to d-dimensional sample requires consideration of the many-channel scattering matrix shown at Fig. 2c: the plane wave of the unit amplitude incident to the channel i generates the transmitted and reflected waves with amplitudes t_{ij} and r_{ij} in the channel j. The multi-channel generalization of Eq. (5) has a form [3, 7, 11, 15]

$$G_{\text{ES}} = \frac{e^2}{2\pi\hbar}\sum_{ij}|t_{ij}|^2. \tag{7}$$

Subtraction of the contact resistance in analogy with (6) gives the numerical results [16] equivalent to the Thouless definition [17], relating the conductance with a reaction to boundary conditions.[2] However, multi-channel generalizations of Eq. (4) appear to be ambiguous [3, 8, 11, 13], and the problem of correct exclusion of the contact resistance remains open.

The previous discussion escapes of the fact that the conductance of a finite system is a poorly defined quantity. In a strict quantum mechanical description, a finite system has a discrete spectrum and its ground state corresponds to occupation of the lower levels (Fig. 3a).[3] If the ground state does not carry a current, then a finite conductance is related with transitions to excited states, which are separated by a finite gap Δ;

[2] The Thouless definition provides the equivalence of two representations (1). The overlap integral J_L can be estimated as the width of the band occurring from the given level in the result of the periodic repetition of the block: it is determined by the change from periodic to antiperiodic boundary conditions. The Thouless definition is physically satisfactory but requires consideration of distributions [17], being hardly formulated in terms of average quantities. By this reason it practically is not used in analytical theory.

[3] For simplicity, we have in mind non-interacting electrons in the random potential and consider one spin projection.

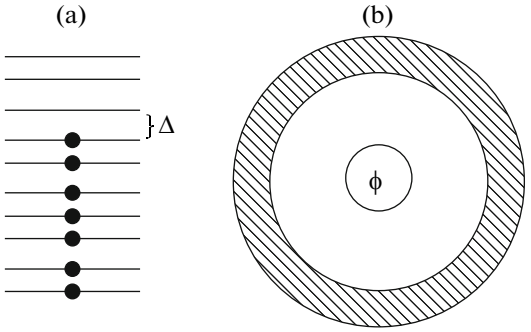

Fig. 3. In strictly quantum mechanical description, a finite system has no conductance (a) and no resistance (b).

such transitions are absent in the limit of zero frequency ω, and

$$\mathrm{Re}G_L(\omega) = 0, \quad \omega \longrightarrow 0. \tag{8}$$

It is curious, that in the Aharonov–Bohm geometry (Fig. 3b) the ground state carries a current, if the magnetic flux ϕ through the ring-shaped sample is not equal to the integer or semi-integer number of quanta $\phi_0 = \hbar c/e$ [14]; in this case, a persistent current flows through the system without external voltage and the resistance R_L is also zero,

$$\mathrm{Re}R_L(\omega) \longrightarrow 0, \quad \omega \longrightarrow 0 \tag{9}$$

(contradiction with Eq. (8) is avoided due to the presence of $\mathrm{Im}G_L(\omega)$).

In fact, this problem is well-known: the formulas of linear response theory are complemented by a prescription that the entering them δ-functions should be smeared out by the quantity γ, next the thermodynamic limit $L \longrightarrow \infty$ is taken and only then $\longrightarrow \gamma$ is set to zero. In fact, such procedure transforms the discrete spectrum into continuous density of states (Fig. 4). For a finite system such a procedure becomes impossible and attenuation γ should remain finite. The question arises on the origin of this attenuation and its dependence on parameters.

Attempts of discussing this question were made in the papers [18–21], based on the "shell model" developed in nuclear physics for description of coupling between a discrete spectrum of the "target" and a continuous spectrum of scattered particles [22]. Unfortunately, the physics of the problem remain unclear in these papers, because the σ-model formalism was introduced at the early stage of consideration. In addition, the bare diffusion coefficient was considered as a given constant, while it actually depends on the degree of the openness of a system.

In derivation of the Landauer formulas [6–8, 15] the indicated problem is avoided in a following manner. The system under consideration is connected with the ideal leads, which can be taken sufficiently massive; the spectrum becomes quasi-continuous and attenuation γ can be tended to zero. Therefore, the

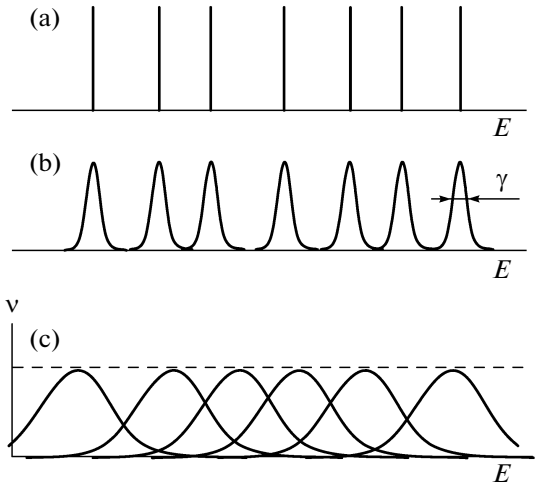

Fig. 4. The discrete levels (a) acquire width γ due to a finite lifetime (b). If the limit $L \longrightarrow \infty$ is taken before the limit $\gamma \longrightarrow 0$, the extended levels overlap strongly and form the continuous density of states (c).

Landauer conductance corresponds to the composite system "sample+external leads" and not to the system under consideration. This point is especially clear from the fact that the matrix elements entering the Kubo formula are determined by integration over the region of ideal leads.

The question arises, in what extent the formulas (4)–(7) reflect the internal properties of the system. To illustrate it more clearly, let introduce the potential barrier between the sample and ideal leads. If the height of the barrier tends to infinity, then the Landauer resistance grows unboundedly, while nothing occurs with the system itself. Contrary, if the height of the barrier tends to zero, then the boundary resistance disappears but the system is dangerously affected by its environment.

There is one more question. The infinite system is fully characterized by the diffusion coefficient $D(\omega, q)$, which generally possesses the temporal and spatial dispersion. The conductance of a finite system is evidently related to $D(\omega, q)$ but this relation is not clear in the Landauer approach.

Therefore, the following points remain unclear at the present time:

(a) exclusion of the reservoir contact resistance in the many-channel case;

(b) relation of Eqs. (4), (5), (7) with internal properties of the system;

(c) relation of the Landauer conductance with the diffusion coefficient $D(\omega, q)$ of an infinite system.

The answers to these questions are obtained below in the framework of two approaches: (1) self-consistent theory of localization by Vollhardt and Wölfle [23, 24], and (2) quantum-mechanical analysis based on the shell model [18, 22]. Both approaches lead to the same definition for the conductance of a finite system,

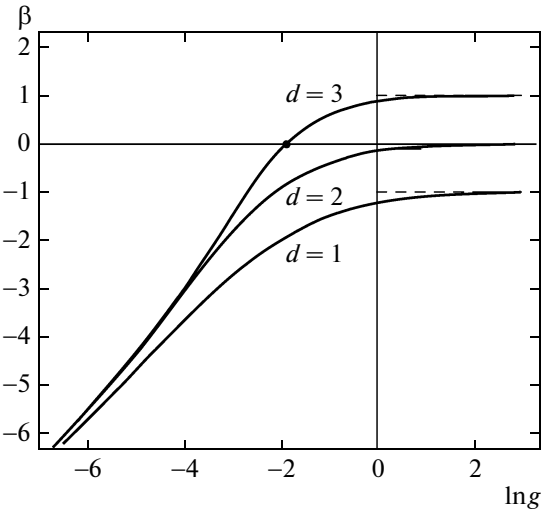

Fig. 5. Gell-Mann–Low functions $\beta(g)$ for d =1, 2, 3 obtained in the present paper.

closely related to the Thouless definition: it gives a new strong argument in favour of the self-consistent theory. Further, in the framework of this theory, we calculate the Gell-Mann–Low functions $\beta(g)$ for the space dimensions $d = 1, 2, 3$ (Fig. 5). In contrast to the analogous calculation by Vollhardt and Wölfle [24], the $\beta(g)$-function has no singularity in the fixed point g_c. The latter is related with the fact that the metallic and localized phase are considered from the same standpoint, so the conductance of a finite system has no singularity at the critical point: it is in agreement with the general principles of the modern theory of critical phenomena [25, 26].

The present theory has the following structure. A finite system is topologically quasi-zero-dimensional and its effective dimensionality is less than two. All states of this system are formally localized and one can introduce the finite correlation length ξ_{0D}; it satisfies the scaling relation

$$\frac{\xi_{0D}}{L} = F\left(\frac{L}{\xi}\right), \tag{10}$$

analogous to that for quasi-one-dimensional systems [27–30]; ξ is the correlation length of the infinite d-dimensional system. The diffusion coefficient has a behavior typical for the dielectric phase,

$$D(\omega, 0) = -i\omega\xi_{0D}^2, \tag{11}$$

and turns to zero in accordance with Eqs. (8), (9). The above statements are valid only for closed systems. In open systems the finite diffusion coefficient D_L arises, and the following result can be derived for the dimensionless conductance

$$g_L = F_1\left(\frac{\xi_{0D}}{L}\right). \tag{12}$$

Replacement of $\ln L$ by $\ln(L/\xi)$ in the Gell-Mann–Low equation (2) allows to represent g_L as a function of L/ξ. The latter can be determined from Eqs. (10), (12) and allows to reconstruct $\beta(g)$.

The paper is organized as follows. In Section 2 we discuss the early attempt of scaling by Vollhardt and Wölfle [24] and formulate the main difference between it and the present paper. In Section 3 the correlation length ξ_{0D} is discussed and the scaling relation (10) is derived for $d < 4$. In Section 4 we consider open systems and derive the result of type (12). The same result is derived in Section 5 from the shell model; its physical sense is clarified and dependence on the measurement geometry is discussed. In Section 6 the length dependence of g_L is presented in the clear form and $\beta(g)$-functions for $d = 1, 2, 3$ are calculated. Their expansion in powers of $1/g$ is compared with the results of the σ-model approach [33, 34]; the use of dimensional regularization in σ-models is found to be in conflict with the physical essence of the problem. In Section 7 the obtained results are compared with numerical [31, 32] and physical [35, 53] experiments. A situation in higher dimensions $d \geq 4$ is discussed in Section 8. In Section 9 we summarize and discuss the consequences of the present study for the conductance distribution, spatial dispersion of the diffusion coefficient and observation of the localization behavior $\sigma(\omega) \propto -i\omega$.

2. SELF-CONSISTENT THEORY AND SCALING

Self-consistent theory of localization by Vollhardt and Wölfle theory is based on existence of the diffusion pole in the irreducible four-leg vertex $U_{\mathbf{kk}'}(\mathbf{q})$, entering the Bethe–Salpeter equation and playing the role of the scattering probability $W_{\mathbf{kk}'}$ in the quantum kinetic equation. Using the estimate in the spirit of τ-approximation, $D \propto \langle U\rangle^{-1}$, where $\langle\ldots\rangle$ is averaging over momenta, one can obtain the self-consistency equation [23, 24] which can be written in the form [30][4]

$$\frac{E^2}{W^2} = \frac{D(\omega)}{D_{\min}} + \Lambda^{2-d}\int_0^{\Lambda}\frac{d^d q}{(2\pi)^d}\frac{1}{[-i\omega/D(\omega)] + q^2}, \tag{13}$$

(the limits of integration are written for the modulus of q). Here E is the energy of the bandwidth order, W is the amplitude of disorder, Λ is the ultraviolet cutoff, $D_{\min}$ is a characteristic scale of the diffusion constant corresponding to the Mott minimal conductivity.

The metallic phase is possible for $d > 2$, when a value of the basic integral

[4] Equation of type (13) can be obtained by approximate solution of the Bethe–Salpeter equation [23] or by detailed analysis of spectral properties of the quantum collision operator [37]. The possibility to neglect the spatial dispersion of the diffusion coefficient was justified in [37].

$$I(m) = \int_0^\Lambda \frac{d^d q}{(2\pi)^d} \frac{1}{m^2 + q^2} \tag{14}$$

is finite for $m = 0$. Specifying τ as a distance to a transition, one has

$$D = D_{\min}\tau, \quad \tau = \frac{E^2}{W^2} - I(0)\Lambda^{2-d}, \tag{15}$$

so the exponent of conductivity is unity. In the dielectric phase one makes substitution $D = -i\omega\xi^2$, and Eq. (13) determines the correlation length ξ; in particular, for $d > 2$

$$\xi \sim a|\tau|^{-\nu}, \quad \nu = \begin{cases} 1/(d-2), & 2 < d < 4, \\ 1/2, & d > 4. \end{cases} \tag{16}$$

The attempt of using Eq. (13) for derivation of scaling equations was made in [24] and contains two ingredients.

1. Modification of the Einstein relation. According to [24], the Einstein relation is modified in the localized phase due to non-local effects and acquires the additional exponential factor

$$\sigma_L \sim e^2 \nu_F D_L \exp(-L/\xi). \tag{17}$$

To obtain this result, one considers the change of the electron density $\rho(x)$, induced by the scalar potential $\varphi(x)$,

$$\rho(x) = \int_{-L/2}^{L/2} \alpha(x - x')\varphi(x')dx', \tag{18}$$

where $\alpha(x - x')$ is polarizability

$$\alpha(x - x') = -e^2\nu_F\left[\delta(x - x') - \frac{1}{2\xi}\exp\left(-\frac{|x - x'|}{\xi}\right)\right]. \tag{19}$$

For a closed system, the diffusion current $j_{\text{diff}}(x) = -D_L\dfrac{d\rho(x)}{dx}$ at the boundaries of the system $x = \pm L/$ is compensated by the electric current $j_e(x) = \sigma_L E$, which allows to determine σ_L. Producing such calculations for

$$\varphi(x) = \varphi_0 - Ex, \tag{20}$$

one has

$$\rho(x) = e^2\nu_F\left[E\left(\frac{L}{2} + \xi\right)\exp\left(-\frac{L}{2\xi}\right)\sinh\left(\frac{x}{\xi}\right) - \varphi_0\exp\left(-\frac{L}{2\xi}\right)\cosh\left(\frac{x}{\xi}\right)\right], \tag{21}$$

and

$$j_e\left(\pm\frac{L}{2}\right) = e^2\nu_F D_L\left[\frac{\mp\varphi_0 + E(L/2 + \xi)}{2\xi} + \frac{\pm\varphi_0 + E(L/2 + \xi)}{2\xi}\exp\left(-\frac{L}{\xi}\right)\right]. \tag{22}$$

Accepting $\varphi_0 = \pm E(L/2 + \xi)$, one obtains

$$j_e\left(\pm\frac{L}{2}\right) = e^2\nu_F D_L\left(1 + \frac{L}{2\xi}\right)\exp\left(-\frac{L}{\xi}\right)E \tag{23}$$

in accordance with (16). It is easy to see that this result is related with the unphysical response to the constant potential φ_0, which is a consequence of accepted approximations; absence of self-consistency is especially clear for $\varphi_0 \neq 0$, when estimation of σ_L using $j_e(L/2)$ and $j_e(-L/2)$ gives different results.[5]

Of course, the correct consideration recovers validity of the Einstein relation. In the framework of the self-consistent theory, $\sigma(\omega, q)$ and $D(\omega, q)$ are independent of q [37], providing the local response in the coordinate space; the relation between them has a local character and cannot be modified due to restriction of the system size. The absence of the factor $\exp(-L/\xi)$ is catastrophic for the paper [24], since it fails to obtain the result $g_L \sim \exp(-\text{const}\,L)$ in the localized phase.

2. Modification of the self-consistency equation. For a finite system, equation (13) is modified by introducing the lower cut-off,

$$\frac{E^2}{W^2} = \frac{D_L}{D_{\min}} + \Lambda^{2-d}\int_{\sim 1/L}^{\Lambda} \frac{d^d q}{(2\pi)^d}\frac{1}{m^2 + q^2}, \tag{24}$$

and rearranged by subtraction of the same equation with $L = \infty$:

$$D_L = D_\infty + D_{\min}\Lambda^{2-d}\int_0^{\sim 1/L} \frac{d^d q}{(2\pi)^d}\frac{1}{m^2 + q^2}, \quad m = \xi^{-1}. \tag{25}$$

Since $D_\infty \sim \tau$ in the metal and $D_\infty = 0$ in the dielectric phase, the diffusion coefficient D_L of a finite system acquires a singularity at the critical point. It is in conflict with general principles of the modern theory of critical phenomena [25, 26], which allow a phase transition only in the thermodynamic limit $L \longrightarrow \infty$.

The present theory is also based on Eq. (13), while indicated defects are removed in the following manner. A finite system is topologically zero-dimensional and all its states are formally localized, though the effective correlation length ξ_{0D} coincides with ξ only in the deep of the localized phase (in the metallic regime, $\xi_{0D} > L$). As a result, D_∞ turns to zero in both phases

[5] In fact, the kernel $\alpha(x, x')$ should be constructed as a binary expansion in eigenfunctions of the diffusion operator; for open systems, integration in (18) should be taken over the whole space.

and Eq. (25) becomes almost satisfactory. The correct result is obtained below,

$$D_L = D_{\min}\Lambda^{2-d}\frac{1}{L^d}\sum_q \frac{\exp(i\mathbf{q}\cdot\mathbf{x})}{m^2+q^2}\Bigg|_{|\mathbf{x}|\sim L}, \qquad (26)$$
$$m = (\xi_{0D})^{-1}$$

and differs from (25) by replacement of the integral by the discrete sum and concretization of the way of cut-off: the latter is provided by the oscillating factor $\exp(i\mathbf{q}\cdot\mathbf{x})$, which effectively restricts summation by values $|\mathbf{q}| \lesssim 1/L$. These modifications are crucial for derivation of the result $D_L \sim \exp(-L/\xi)$ in the localized phase.

The application of the quasi-zero-dimensional concept is not a pure theoretical construction, but allows to distinguish the real behavior of open and closed systems. Absence of singularities in small systems can be also verified experimentally. Therefore, the present theory differs from [24] on the level of observable consequences.

3. CORRELATION LENGTH OF QUASI-ZERO-DIMENSIONAL SYSTEM

3.1. Dimensions $2 < d < 4$

A finite system is considered as quasi-zero-dimensional and its correlation length ξ_{0D} can be studied in analogy with the quasi-one-dimensional case [30]. In a finite system, the basic integral (14) is replaced by the discrete sum

$$I(m) = \frac{1}{L^d}\sum_{|q|<\Lambda}\frac{1}{m^2+q^2}, \quad m^{-1} = \xi_{0D}, \qquad (27)$$

where allowed values of $\mathbf{q}$ has a form $2\pi\mathbf{s}/L$, and $\mathbf{s} = (s_1, s_2, ..., s_d)$ is the d-dimensional vector with integer components $s_i = 0, \pm1, \pm2, ...$ We accept the periodic boundary conditions in all directions, which correspond to the closed system (Section 4). The term with $\mathbf{q} = 0$ provides the divergency of $I(m)$ at $m \longrightarrow 0$ and the system is always in the localized regime. It is convenient to make the following decomposition

$$I(m) = \frac{1}{L^d}\frac{1}{m^2} + \frac{1}{L^d}\sum_{\substack{q\neq 0\\ |\mathbf{q}|<\Lambda}}\left(\frac{1}{m^2+q^2}-\frac{1}{q^2}\right) + \frac{1}{L^d}\sum_{\substack{q\neq 0\\ |\mathbf{q}|<L}}\frac{1}{q^2} \equiv I_1(m) + I_2(m) + I_3(0), \qquad (28)$$

where we separated the term with $\mathbf{q} = 0$, and the rest of the sum is rearranged by addition and subtraction of the analogous sum with $m = 0$. The limit $\Lambda \longrightarrow \infty$ can be taken in the second term $I_2(m)$ transforming it to the form $L^{2-d}H_0(mL)$ (neglecting contributions $\sim m^2\Lambda^{d-4}$). The third term $I_3(0)$ can be calculated at $L \longrightarrow \infty$ by the change of summation by integration, while for finite L it has a structure.[6]

$$I_3(0) = \Lambda^{d-2}\left\{b_0 + b_1\left(\frac{a}{L}\right)^{d-2} + b_2\left(\frac{a}{L}\right) + b_3\left(\frac{a}{L}\right)^2 + \ldots\right\}, \qquad (29)$$

where we accepted $a = \Lambda^{-1}$. Substitution of expressions (28), (29) into the self-consistency equation (13) gives

$$\left(\frac{L}{a}\right)^{d-2}\left[\tau + O(m^2a^2) + O\left(\frac{a}{L}\right)\right] = b_1 + H_0(mL) + \frac{1}{(mL)^2}, \qquad (30)$$

where definition $\tau = E^2/W^2 - b_0$ coincides with (15), since b_0 corresponds to the value $I(0)$, calculated in the integral approximation. According to (30), ξ_{0D} is a regular function of τ. Expressing ξ through the correlation length τ of the d-dimensional system ($\xi^{-1/\nu} \sim |\tau| = \pm\tau$) and omitting terms vanishing at $a \longrightarrow 0$, one has

$$\pm c_d\left(\frac{L}{\xi}\right)^{d-2} = H\left(\frac{L}{\xi_{0D}}\right), \qquad (31)$$

$$H(z) = b_1 + \frac{1}{4\pi^2}\sum_{\mathbf{s}\neq 0}\left(\frac{1}{|\mathbf{s}|^2 + (z/2\pi)^2} - \frac{1}{|\mathbf{s}|^2}\right) + \frac{1}{z^2}, \qquad (32)$$

which is the desired scaling relation (10), consisting of two branches (c_d are positive coefficients introduced in [30]). The asymptotical behavior of $H(z)$

$$H(z) = \begin{cases} 1/z^2, & z \ll 1,\\ -A(z-z^*), & z \quad z^*,\\ -c_d z^{d-2}, & z \gg 1, \end{cases} \qquad (33)$$

is obtained noticing that $H(z)$ at small z is determined by the last term in (32), while for large z the sum over s is approximated by the integral; the regular expansion is possible near the root z^*, corresponding to the critical point. At arbitrary z the sum over s can be calculated numerically, giving $H(z)$ for $d = 3$ shown in Fig. 6. Introducing the variables

$$y = \xi_{0D}/L, \quad x = \xi/L, \qquad (34)$$

one has for dependence $y(x)$ (Fig. 7)

$$y = \begin{cases} (c_d/x^{d-2})^{1/2}, & y \gg 1,\\ y^* \pm \text{const}/x^{d-2}, & y \longrightarrow y^*,\\ x, & y \ll 1. \end{cases} \qquad (35)$$

[6] It can be obtained using the α-representation (see Appendix) with the cut-off $|q_i| < \Lambda$.

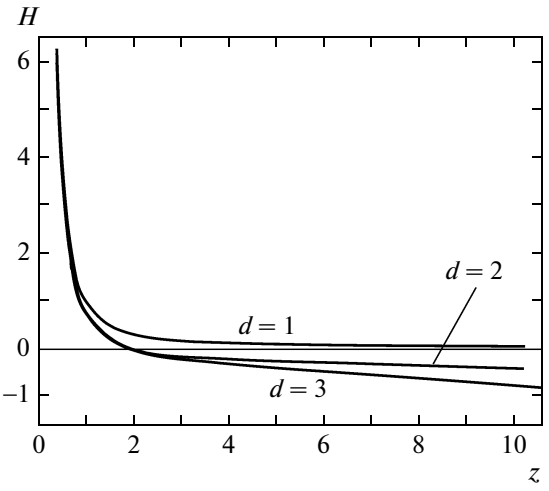

Fig. 6. Functions $H(z)$ for $d = 1, 2, 3$.

The constant b_1 in (29) is not universal and depends on the way of cut-off: a value $b_1 = -0.226$ for a spherical cut-off ($|q| < \Lambda$) is used below for $d = 3$, though in general it should be considered as an adjustable parameter.[7] Corrections to scaling can be obtained from (30) and have the same form as for quasi-one-dimensional systems: it confirms universality of their structure argued in [30].

3.2. Two-Dimensional Case

In two dimensions we have

$$I_3(0) = \frac{1}{2\pi}\ln\frac{L}{a} + b_1 + \ldots, \quad \frac{E^2}{W^2} = \frac{1}{2\pi}\ln\frac{\xi}{a}, \qquad (36)$$

and the scaling relation has the form

$$\frac{1}{2\pi}\ln\left(\frac{\xi}{L}\right) = H\left(\frac{L}{\xi_{0D}}\right) \qquad (37)$$

with the previous definition of $H(z)$ (Fig. 6). Using the asymptotic results

$$H(z) = \begin{cases} 1/z^2, & z \ll 1, \\ -(1/2\pi)\ln z, & z \gg 1, \end{cases} \qquad (38)$$

we have $y = x$ for $x \ll 1$ and $y \sim (\ln x)^{1/2}$ for $x \gg 1$ (Fig. 7). Below we use the value $b_1 = 0.1780$ obtained for the spherical cut-off.

3.3. Dimensions $d < 2$

For $d < 2$, subtraction of the term with $m = 0$ is not necessary and the limit $\Lambda \longrightarrow \infty$ can be taken immediately in (27). The scaling relation has the form

$$c_d\left(\frac{L}{\xi}\right)^{d-2} = H\left(\frac{L}{\xi_{0D}}\right),$$
$$H(z) = \frac{1}{(2\pi)^2}\sum_{\mathbf{s}}\left(\frac{1}{(z/2\pi)^2 + |\mathbf{s}|^2}\right) \qquad (39)$$

and consists of one branch, since the function $H(z)$ is positive (Fig. 6). Its asymptotic behavior

$$H(z) = \begin{cases} 1/z^2, & z \ll 1, \\ c_d/z^{2-d}, & z \gg 1 \end{cases} \qquad (40)$$

is obtained analogously and gives $y = x$ for $x \ll 1$ and $y \sim x^{(2-d)/2}$ for $x \gg 1$ (Fig. 7). In the 1D case the function $H(z)$ can be calculated exactly (see Eq. (118) below).

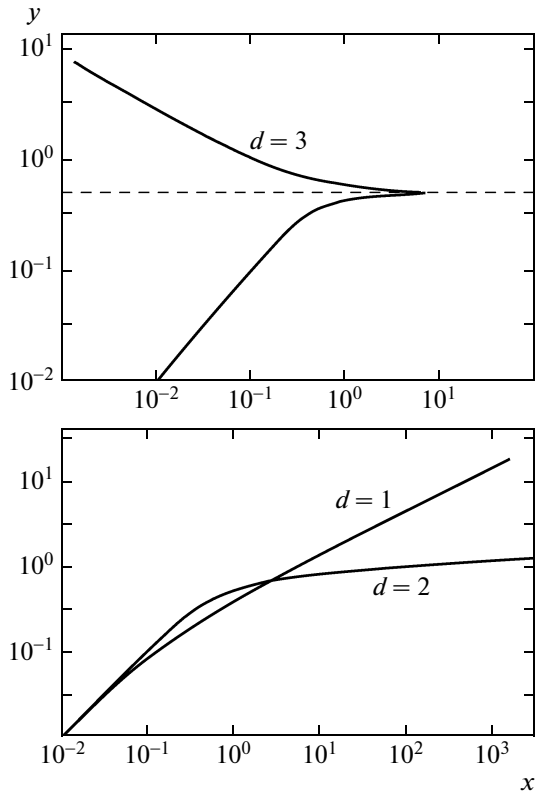

Fig. 7. Behavior of $y = \xi_{0D}/L$ versus $x = \xi/L$ for $d = 1, 2, 3$.

4. SITUATION IN OPEN SYSTEMS

4.1. Difference between Open and Closed Systems

Consider the effective diffusion equation

$$\frac{\partial f}{\partial t} - D\nabla^2 f = 0, \qquad (41)$$

describing the electron distribution $f(\mathbf{x}, t)$. In an infinite system the operator $-\nabla^2$ has eigenfunctions $e_s(\mathbf{x}) \sim \exp(i\mathbf{q}_s \cdot \mathbf{x})$ and eigenvalues $\lambda_s = q_s^2$. In a finite

[7] For the cubical cut-off ($|q_i| < \Lambda$) one has $b_1 = -0.0314$.

system $e_s(\mathbf{x})$ and λ_s become non-trivial and determine the evolution of the initial distribution $f_0(\mathbf{x})$

$$f(\mathbf{x}, t) = \sum_s A_s \exp(-D\lambda_s t) e_s(\mathbf{x}), \qquad A_s = (f_0, e_x). \tag{42}$$

The difference between open and closed systems can be formulated on a very abstract level: in the first case, the minimal eigenvalue λ_0 is zero and corresponds to the constant eigenfunction

$$\lambda_0 = 0, \quad e_0(\mathbf{x}) = \text{const}, \tag{43}$$

while in the second case

$$\lambda_0 > 0, \quad e_0(\mathbf{x}) \neq \text{const}. \tag{44}$$

In the first case one has from (42) at $t \longrightarrow \infty$

$$f(\mathbf{x}, t)|_{t\to\infty} = \text{const} = \langle f_0 \rangle, \tag{45}$$

i.e. distribution $f(\mathbf{x}, t)$ tends to the constant limit, equal to the average value of $f_0(\mathbf{x})$ in the coordinate space; consequently, environment does not affect the natural process of relaxation, and the total number of particles is conserved. In the second case

$$f(\mathbf{x}, t)|_{t\to\infty} = A_0 e_0(\mathbf{x}) \exp(-D\lambda_0 t), \tag{46}$$

i.e., distribution over $\mathbf{x}$ is stabilized, but its amplitude is decreased due to escape of the particles through boundaries of the system; by the same reason their density near boundaries is less than in the center.

Consider examples. Let the 1D system is arranged in the interval $0 \le x \le L$. For boundary conditions of the Bloch type

$$f(L) = f(0) e^{i\varphi} \tag{47}$$

the allowed values of q has a form $q_s = (2\pi s + \varphi)/L$ with integer s, so the system is closed at $\varphi = 0$, and maximally open at $\varphi = \pi$, i.e., for periodic and antiperiodic conditions correspondingly. For the more realistic boundary conditions

$$f_x'(0) = \kappa f(0), \quad f_x'(L) = -\kappa f(L) \tag{48}$$

the system is closed for $\kappa = 0$ due to the absence of flow through boundaries; the maximum openness is realized at $\kappa = \infty$, i.e. for the zero boundary conditions.

4.2. Attenuation of Electron States and Finiteness of the Diffusion Coefficient

In the open system, electrons can escape through the boundaries and their eigenstates has a finite lifetime. It can be proved quite generally, that it provides the finite diffusion constant in the static limit. Consider the density correlator

$$\mathcal{H}_\omega(\mathbf{r} - \mathbf{r}') = \langle G^R_{E+\omega}(\mathbf{r}, \mathbf{r}') G^A_E(\mathbf{r}', \mathbf{r}) \rangle, \tag{49}$$

where G^R and G^A are the retarded and advanced Green functions. Eq. 49 can be rewritten identically

$$\mathcal{H}_\omega(\mathbf{r} - \mathbf{r}') = \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\omega' \frac{1}{E + \omega - \epsilon + i0} \times \frac{1}{E - \omega' - \epsilon - i0} \rho_{\epsilon, \epsilon+\omega'}(\mathbf{r} - \mathbf{r}'), \tag{50}$$

where $\rho_{\epsilon, \epsilon+\omega}(\mathbf{r} - \mathbf{r}')$ is the Berezinsky–Gor'kov spectral density, whose Fourier transform is related with polarizability $\alpha(\omega, q)$ [37]

$$\rho_{\epsilon, \epsilon+\omega}(q) = -\frac{\mathrm{Im}\alpha_\epsilon(\omega, q)}{\pi e^2 \omega}. \tag{51}$$

Using the definitions of kinetic coefficients and analytic properties of the response functions [38], it is easy to show that [37]

$$\mathcal{H}_\omega(q) = \frac{2\pi\nu_F}{-i\omega + D(\omega, q) q^2}, \tag{52}$$

where $D(\omega, q)$ is the observable diffusion coefficient. It should be stressed, that this result has a general character and is not restricted by the metallic phase.

The finite lifetime of the electron states leads to a replacement of infinitesimal quantities $\pm i0$, entering definitions of the retarded and advanced Green functions, by $\pm i\gamma$; analogous changes occur in (50). Reproducing the indicated calculations, we come to conclusion that the replacement

$$-i\omega \longrightarrow -i\omega + 2\gamma, \tag{53}$$

should be made in (52), both in the term $-i\omega$ and in $D(\omega, q)$. In the localized phase the following combination remains invariant

$$\frac{-i\omega}{D(\omega, q)} = \frac{-i\omega}{(-i\omega)\xi^2} \longrightarrow \frac{-i\omega + 2\gamma}{(-i\omega + 2\gamma)\xi^2}, \tag{54}$$

which has a simple physical sense: attenuation of eigenstates was introduced for the permanent eigenfunctions, so the correlation length ξ characterizing the latter is also unchanged. In the static limit $D(\omega, q)$ is replaced by $D_L = 2\gamma\xi^2$, i.e., the finite diffusion constant arises.

4.3. Modification of the Self-Consistency Equation

The result $D(\omega) \longrightarrow 0$ (Section 3) is valid for closed systems, being directly related with the existence of the allowed value $\mathbf{q} = 0$; the self-consistency equation (13) has a form

$$\frac{E^2}{W^2} = \Lambda^{2-d} \frac{1}{L^d} \sum_q^{(c)} \frac{1}{m^2 + q^2}, \quad m^{-1} = \xi_{0D}. \tag{55}$$

In the open system, the diffusion constant D_L becomes finite, but the correlation length remains unchanged:

$$\frac{E^2}{W^2} = \frac{D_L}{D_{\min}} + \Lambda^{2-d}\frac{1}{L^d}\sum_q^{(o)}\frac{1}{m^2+q^2}. \quad (56)$$

The labels (c) and (o) indicate the closed and open system, which have the different sets of allowed values of $\mathbf{q}$ in the sum. Taking the difference of (55) and (56), one obtains

$$D_L = D_{\min}\Lambda^{2-d}\frac{1}{L^d}\left(\sum_q^{(c)}\frac{1}{m^2+q^2} - \sum_q^{(o)}\frac{1}{m^2+q^2}\right), \quad (57)$$

which can be considered as a definition of the diffusion coefficient for a finite system. This definition contains essential freedom, since the choice of the open and closed system is a subject of agreement. For the Bloch boundary conditions[8] (47) the natural etalon choice are the systems with $\varphi = 0$ and $\varphi = \pi$,

$$g_L = L^{d-2}\frac{1}{L^d}\left(\sum_q^{(\varphi=0)}\frac{1}{m^2+q^2} - \sum_q^{(\varphi=\pi)}\frac{1}{m^2+q^2}\right), \quad (58)$$

where we came from D_L to g_L, accepting $D_{\min}\Lambda^{2-d} = 1/\hbar\nu_F$. We shall refer Eq. (58) as the "Thouless definition", since g_L is determined by the change from periodic to antiperiodic boundary conditions.[9] We accept such a change along only one of coordinate axes, remaining periodic conditions in other directions: according to Section 5, it corresponds to the natural experimental geometry.

The definition (58) provides the exponential decrease of D_L in the localized phase (see Appendix)

$$g_L = L^{d-2}\frac{4\sqrt{\pi}}{(4\pi)^{d/2}}m^{d-2}\left(\frac{mL}{2}\right)^{(1-d)/2}e^{-mL}. \quad (59)$$

The origin of the exponential dependence can be explained in the following manner. It is well-known [39], that integration of quickly oscillating functions

$$f_\omega = \int_{-\infty}^{\infty} f(x)e^{i\omega x}dx, \quad \omega \longrightarrow \infty, \quad (60)$$

involves the analytic properties of $f(x)$. If $f(x)$ has a jump of the n-th derivative at the real axis, then $f_\omega \sim \omega^{-n-1}$; in particular, the case $n = 0$ corresponds usually to integration in finite limits. If $f(x)$ is regular at the real axis, then the integration contour is shifted to the upper half-plane and the integral is exponentially small,

$$f_\omega \sim \exp(-\text{const}\cdot\omega). \quad (61)$$

The analogous situation takes place in approximation of an integral by a discrete sum

$$\int_{-\infty}^{\infty} f(x)dx \approx h\sum_{s=-\infty}^{\infty} f(x_s)\big|_{x_s = hs}, \quad (62)$$

which becomes clear after the use of the Poisson summation formula [40]:

$$h\sum_{s=-\infty}^{\infty} f(x_s)\big|_{x_s = hs} = \sum_{k=-\infty}^{\infty}\int_{-\infty}^{\infty} f(x)\exp\left(i\frac{2\pi kx}{h}\right)dx. \quad (63)$$

The term with $k = 0$ corresponds to the integral (62), while the main correction to it has an order of $\exp(-\text{const}/h)$. Two sums over $\mathbf{q}$ in Eq. 58 are equal in the continual approximation; their difference is determined by the main effect of discreteness, which has the order of $\exp(-\text{const}\,L)$ due to $h \sim 1/L$. The definition (58) can be written in the form of the scaling relation

$$g_L = H_T\left(\frac{L}{\xi_{0D}}\right), \qquad H_T(z) = \frac{1}{(2\pi)^2}\sum_{\mathbf{t}}\frac{(-1)^{2t_1}}{|\mathbf{t}|^2 + (z/2\pi)^2}, \quad (64)$$

where we introduced a vector $\mathbf{t} = (t_1, t_2, ..., t_d)$, whose components t_i run integer values $0, \pm1, \pm2, ...$ for $i = 2, ..., d$ and semi-integer values $0, \pm1/2, \pm1, \pm3/2, ...$ for

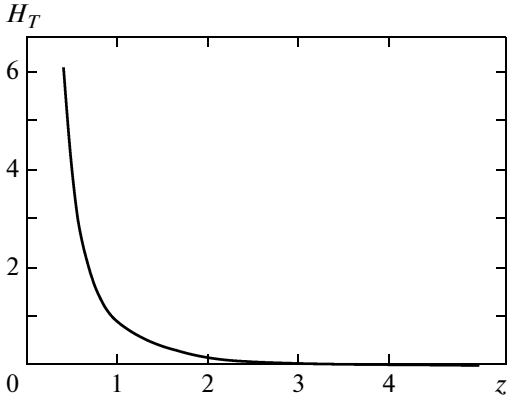

Fig. 8. Functions $H_T(z)$, corresponding to the d-dimensional "Thouless definition", for $d = 1, 2, 3$: in the scale of the figure all three curves coincide.

[8] In general, the factor L^{-d} before the sum over $\mathbf{q}$ can be replaced by the more complicated normalization factor (see Eq. (108) below), which can give the power corrections in $1/L$ (if treated inaccurately), and destroy the exponent in (59). Such problems are absent for eigenfunctions in the form of plane waves, corresponding to the Bloch conditions (47). The realistic boundary conditions (48) are considered in Section 5.7.

[9] Strictly speaking, the original Thouless definition deals with the boundary conditions for the electron wave function, and not for the effective diffusion problem. Probably, it is the most close correspondence that can be established in terms of the averaged quantities (see Footnote 4).

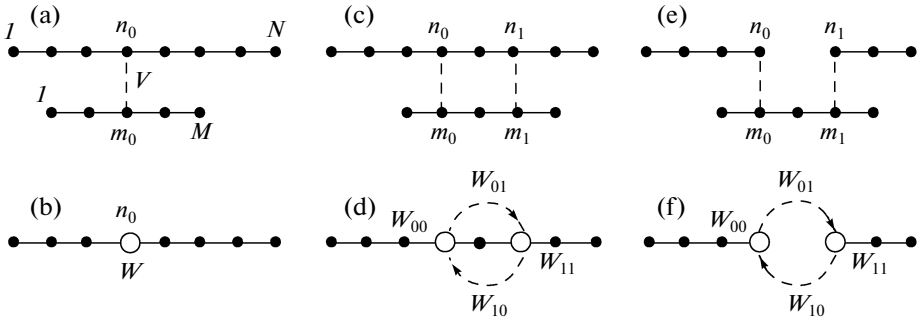

Fig. 9. (a) Weak connection V between two chains, and (b) the equivalent scheme in the subspace 1. (c) Two weak connections between chains, and (d) the corresponding equivalent scheme. (e) Broken upper chain, and (f) effective transitions between its parts.

$i = 1$. The function $H_T(z)$ is always positive (Fig. 8) and has the asymptotic behavior

$$H_T(z) = \begin{cases} 1/z^2, & z \ll 1, \\ (1/\pi)(z/2\pi)^{(d-3)/2}e^{-z}, & z \gg 1. \end{cases} \quad (65)$$

5. APPLICATION OF THE SHELL MODEL

The shell model was developed in nuclear physics for description of coupling between the discrete spectrum of the "target" with a continuous spectrum of scattered particles [22]; Iida et al. [18] suggested to use it for consideration of the combined system "sample+external leads." Below we illustrate this approach using the simple models of solid state physics and then come to consideration of the many-channel case.[10]

5.1. Connection of Infinite and Finite Chains

Consider the model consisting of two chains, upper infinite ($N \longrightarrow \infty$) and lower finite (Fig. 9a). We accept for simplicity that the chains are described by the usual Anderson model

$$J\psi_{n+1} + J\psi_{n-1} + \epsilon_n\psi_n = E\psi_n, \quad (66)$$

though it is irrelevant for the most part of discussion; the upper chain is supposed to be an ideal conductor ($\epsilon_n = 0$). As a perturbation, we include the overlap integral V between the sites n_0 and m_0 of two chains (Fig. 9a). The Hamiltonian matrix is block-diagonal in the zero approximation, while perturbation creates non-diagonal elements V in n_0-th row and m_0-th column and vice versa; so the matrix elements of the perturbation operator are

$$V_{nn'} = V(\delta_{nn_0}\delta_{n'm_0} + \delta_{nm_0}\delta_{n'n_0}). \quad (67)$$

The matrix Dyson equation $G = G_0 + G_0VG$ written in components has a form

$$G_{nn'} = G^0_{nn'} + G^0_{nn_0}VG_{m_0n'} + G^0_{nm_0}VG_{n_0n'}, \quad (68)$$

where $G_{nn'}$ is the Green function of the perturbed system and $G^0_{nn'}$ is the initial Green function corresponding to two independent chains. The index n runs values 1, 2, ..., N corresponding to the first chain, and then values $N + 1$, $N + 2$, ..., $N + M$ corresponding to the second chain; the sites of the latter will be also numerated by the index m. Equation (68) is easily solved: setting $n = n_0$ and $n = m_0$ one obtains the closed system for $G_{n_0n'}$ and $G_{m_0n'}$, and then its solution is substituted into (68). The complete expression for $G_{nn'}$ is rather lengthy, so we give only its projection on subspace 1 of the upper chain

$$G_{nn'} = G^0_{nn'} + G^0_{nn_0}\frac{V^2G^0_{m_0m_0}}{1 - V^2G^0_{m_0m_0}G^0_{n_0n_0}}G_{n_0n'} \quad (69)$$

and subspace 2 of the lower chain

$$G_{mm'} = G^0_{mm'} + G^0_{mm_0} \times \frac{V^2G^0_{n_0n_0}}{1 - V^2G^0_{m_0m_0}G^0_{n_0n_0}}G_{m_0m'}. \quad (70)$$

Investigation of relations (69), (70) reveals the following qualitative moments.

1. Effective scatterer. If we are interested only in movement along the upper chain, then perturbation (67) is equivalent to insertion of an impurity atom in the point n_0 (Fig. 9b), with the effective Hamiltonian

$$V_{nn'} = W\delta_{nn_0}\delta_{n'n_0}, \quad W = V^2G^0_{m_0m_0}. \quad (71)$$

To prove this result, it sufficient to write down the Dyson equation for the perturbation (71) and verify that its solution coincides with (69).

2. Attenuation in the finite system. The initial Green function of the lower chain has a form

$$G^0_{mm'} = \sum_s \frac{e_s(m)e^*_s(m')}{E - \epsilon_s + i0}, \quad (72)$$

[10] Section 5 contains derivation of Eq. (64) by the other method and can be omitted by the reader interesting only in results.

where ϵ_s and $e_s(m)$ are its eigenvalues and eigenvectors. In the vicinity of a level ϵ_s the sum is determined by one term; its substitution to (70) gives

$$G_{mm'} = \frac{e_s(m)e_s^*(m')}{E-\epsilon_s - V^2 G^0_{n_0n_0}\left|e_s(m_0)\right|^2}, \quad E \approx \epsilon_s. \qquad (73)$$

For the ideal chain $G^0_{nn'}$ does not depend on n, and

$$G^0_{nn} = \int \frac{dk}{2\pi}\frac{1}{E-\epsilon(k)+i0} \equiv I(E) - i\pi\nu(E), \qquad (74)$$

where $\nu(E)$ is the density of states at the energy E. Since relation (73) is valid for any level ϵ_s, and for small V we can neglect the mutual influence of different levels, then the effective Green function of the lower chain can be written as

$$\tilde{G}_{mm'} = \sum_s \frac{e_s(m)e_s^*(m')}{E-\tilde{\epsilon}_s + i\gamma_s}, \qquad (75)$$

i.e., the discrete levels acquire a finite attenuation

$$\gamma_s = \pi V^2 \nu(\epsilon_s)\left|e_s(m_0)\right|^2. \qquad (76)$$

The difference between $\tilde{\epsilon}_s$ and ϵ_s has no qualitative effect and can be neglected for small V.

3. Effective *T*-matrix. The combination entering (69),

$$T = \frac{V^2 G^0_{m_0m_0}}{1 - V^2 G^0_{m_0m_0}G^0_{n_0n_0}} \qquad (77)$$

is in fact the T-matrix of scattering [41]; by definition, its substitution into the Born expression instead of the perturbation V gives the exact scattering amplitude. Considering it in the vicinity of a level ϵ_s, one finds possibility to write it in the form

$$T \approx V^2 \tilde{G}_{m_0m_0}. \qquad (78)$$

It differs from the Born result $T = V^2 G^0_{m_0m_0}$ (following from the concept of the effective scatterer) by replacement of G^0 by $\tilde{G}$, i.e. by taking attenuation of states into account.

5.2. Several Bonds between Chains

The simplest generalization of the model contains several bonds between chains, connecting the pairs of sites n_0 and m_0, n_1 and m_1, and so on (Fig. 9c). In this case the perturbation operator is defined as

$$V_{nn'} = V\sum_i (\delta_{nn_i}\delta_{n'm_i} + \delta_{nm_i}\delta_{n'n_i}), \qquad (79)$$

and the Dyson equation reads

$$G_{nn'} = G^0_{nn'} + \sum_i (G^0_{nn_i}VG_{m_in'} + G^0_{nm_i}VG_{n_in'}). \qquad (80)$$

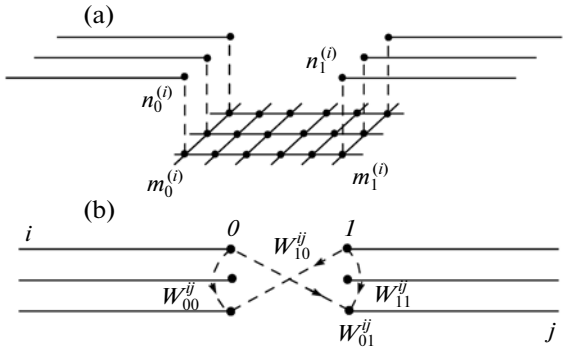

Fig. 10. (a) The modelling of the system "sample+external leads". Ideal one-dimensional chains are weakly connected with the given d-dimensional system. (b) Effective transitions between the chains corresponding to the many-channel scattering matrix (see Fig. 2c).

Let n and n' belong to the upper chain; then $G^0_{nm_i} = 0$ and (80) accepts the form

$$G_{nn'} = G^0_{nn'} + \sum_i G^0_{nn_i}VG_{m_in'}. \qquad (81)$$

On the other hand, setting $n = m_i$ in (80)

$$G_{m_in'} = \sum_j G^0_{m_im_j}VG_{n_jn'} \qquad (82)$$

and substituting in (81), we obtain

$$G_{nn'} = G^0_{nn'} + \sum_{ij} G^0_{nn_i}V^2G^0_{m_im_j}G_{n_jn'}. \qquad (83)$$

If only the upper chain is of interest, then the effective perturbation Hamiltonian

$$V_{nn'} = \sum_{ij} W_{ij}\delta_{nn_i}\delta_{n'n_j}, \quad W_{ij} = V^2G^0_{m_im_j}, \qquad (84)$$

can be used, i.e. the scatterers W_{ii} are introduced in the points n_i and the additional overlap integrals W_{ij} are included between points n_i and n_j (Fig. 9d).

5.3. Broken Upper Chain

Let us remove the portion between n_0 and n_1 in the upper chain (Fig. 9e). The above expressions formally retain, if the initial Green function $G^0_{nn'}$ is taken for the broken chain. The equivalent scheme shows (Fig. 9f), that transitions between the left and right parts of the upper chain are possible only due to overlap integrals W_{01} and W_{10}, so the transmission coefficient is proportional to $\left|W_{10}\right|^2$.

5.4. Many-Channel Case

Now introduce the model which has the immediate interest (Fig. 10a): the lower chain is replaced by a finite d-dimensional system, whose points $m_0^{(i)}$ and $m_1^{(i)}$ are related with sites $n_0^{(i)}$ and $n_1^{(i)}$ of the ideal one-dimensional chains. This model describes a situation, when the given d-dimensional system is weakly connected with the ideal leads.

Expressions (79)–(84) are formally applicable, if the index n_i runs values $n_0^{(i)}$ and $n_1^{(i)}$, while the index m_i runs values $m_0^{(i)}$ and $m_1^{(i)}$. Therefore, we can immediately introduce the equivalent scheme (Fig. 10b), according to which the i-th lead on left and the j-th lead on right are related by overlap integrals W_{00}^{ij}, W_{01}^{ij}, W_{10}^{ij}, W_{11}^{ij}. Comparing with the Landauer many-channel scattering matrix (Fig. 2c), we see that the amplitude t_{js} are determined by the quantities W_{10}^{sj},

$$t_{js} = -2i\exp(2ik_F)\sin k_F\frac{W_{10}^{sj}}{J}, \tag{85}$$

where k_F is the Fermi momentum. To derive this relation, one should write the effective Schroedinger equation

$$\begin{aligned} E\psi_n &= J\psi_{n+1} + J\psi_{n-1} + \epsilon_n\psi_n \\ &+ \sum_{sj}[W_{00}^{sj}\delta_{nn_0^{(s)}}\psi_{n_0^{(j)}} + W_{01}^{sj}\delta_{nn_0^{(s)}}\psi_{n_1^{(j)}} \\ &+ W_{10}^{sj}\delta_{nn_1^{(s)}}\psi_{n_0^{(j)}} + W_{11}^{sj}\delta_{nn_1^{(s)}}\psi_{n_1^{(j)}}] \end{aligned} \tag{86}$$

and find the solution of the scattering problem: if a wave of the unit amplitude is incident to the channel s, then the amplitude in j-th channel can be written in the form (k is a wavenumber)

$$\psi_n^{(j)} = \begin{cases} \delta_{sj}\exp[ik(n-n_0)] \\ + r_{sj}\exp[-ik(n-n_0)], & n \le n_0, \\ t_{sj}\exp[ik(n-n_1)], & n \ge n_1. \end{cases} \tag{87}$$

It leads to the system of equations

$$\begin{aligned} Je^{ik}\delta_{sj} + Je^{-ik}r_{sj} &= W_{00}^{js} + \sum_{j'}(W_{00}^{jj'}r_{sj'} + W_{01}^{jj'}t_{sj'}), \\ Je^{-ik}t_{sj} &= W_{10}^{js} + \sum_{j'}(W_{10}^{jj'}r_{sj'} + W_{11}^{jj'}t_{sj'}), \end{aligned} \tag{88}$$

whose iterations in $W_{\alpha\beta}^{js}$ give (85). Substituting (85) in the Landauer formula (7), one has

$$G_L = \frac{e^2}{2\pi\hbar}4\sin^2 k_F\frac{V^4}{J^2}\sum_{ij}\left|G^0_{m_0^{(i)}m_1^{(j)}}\right|^2. \tag{89}$$

This result corresponds to the Born approximation: to obtain the complete result, one should find the many-channel T-matrix.

5.5. T-matrix in the Many-Channel Case

If $\Phi(r) = e^{i\mathbf{k}\cdot\mathbf{r}}$ is a plane wave and $\Psi(r)$ is a solution of the scattering problem, then they are related by the Lippmann–Schwinger equation [41]

$$|\Psi\rangle = |\Phi\rangle + G_0V|\Psi\rangle, \tag{90}$$

which can be iterated as

$$\begin{aligned} |\Psi\rangle = \{1 &+ G_0V + G_0VG_0V \\ &+ G_0VG_0VG_0V + \dots\}|\Phi\rangle. \end{aligned} \tag{91}$$

Let us set $G_0 = G_1 + G_2$, where G_2 corresponds to the system under consideration, and G_1 to ideal leads; then perturbation V relates only G_1 and G_2, while combinations G_1VG_1 and G_2VG_2 turn to zero. Accepting that states $|\Psi\rangle$ and $|\Phi\rangle$ belong to subspace 1, we have

$$\begin{aligned} |\Psi\rangle = \{1 &+ G_1VG_2V \\ &+ G_1VG_2VG_1VG_2V + \dots\}|\Phi\rangle. \end{aligned} \tag{92}$$

By definition, $|\Psi\rangle$ and $|\Phi\rangle$ are related by the S-matrix, $|\Psi\rangle = S|\Phi\rangle$, and (92) gives

$$S = 1 + G_1VG_2V\frac{1}{1 - G_1VG_2V}. \tag{93}$$

The T-matrix is introduced by the relation $V|\Psi\rangle = T|\Phi\rangle$ [41], so $S = 1 + G_0T$, reducing to $S = 1 + G_1T$ in the subspace 1; so

$$\begin{aligned} T &= VG_2V\frac{1}{1 - G_1VG_2V} \\ &= V\frac{1}{E - H_2 - VG_1V}V, \end{aligned} \tag{94}$$

where the relation $G_2 = (E - H_2)^{-1}$ is used. The poles of the T-matrix are determined by eigenvalues of the operator $H_2 + VG_1V$, which can be found perturbatively

$$\lambda_s = \epsilon_s + \langle e_s|VG_1V|e_s\rangle. \tag{95}$$

Using the specific form (79) of the matrix elements of V, we have $\lambda_s = \tilde{\epsilon}_s - i\gamma_s$, where γ_s are determined by expression

$$\gamma_s = \pi V^2\nu_F\sum_i\left|e_s(m_i)\right|^2, \tag{96}$$

which is a natural generalization of (76). This result can be also obtained by induction, including connections one after another and neglecting their influence on $G^0_{nn'}$.

Below we are interested in the limit of small V. In this case we can take into account only the qualitative effect related with attenuation, neglecting influence of perturbation on eigenfunctions and eigenvalues. In the Born approximation, the T-matrix has a form VG_2V (see (94)) and has the poles at ϵ_s. Substitution of ϵ_s for $\tilde{\epsilon}_s - i\gamma_s$ corresponds to replacement of G^0 by $\tilde{G}$ in expression (89)

$$G_L = \frac{e^2}{2\pi\hbar} 4\sin^2 k_F \frac{V^4}{J^2} \sum_{r_\perp, r'_\perp} \left|\tilde{G}(\mathbf{r}, \mathbf{r}')\right|^2_{|x'-x|=L}, \qquad (97)$$

where $\tilde{G}$ is defined analogously to (75). Here we introduced the longitudinal (x) and transverse ($r_\perp$) components of vector $\mathbf{r}$, and summation occurs over the points of connection with leads. Taking the average value of the conductance, we can consider $\langle|\tilde{G}|^2\rangle$ as a zero-frequency limit of the density correlator (49) and use it in the form (52). Consequently, we have related the Landauer conductance with the diffusion coefficient $D(\omega, q)$. Since (97) corresponds to the open system, the replacement (53) is implied, leading to a finiteness of the diffusion coefficient D_L. Omitting (here and later) irrelevant constant factors we have for the dimensionless conductance

$$g_L = \frac{V^4}{J^4} \frac{J}{D_L} \sum_{r_\perp, r'_\perp} K(\mathbf{r}, \mathbf{r}')|_{|x-x'|=L},$$
$$K(\mathbf{r}, \mathbf{r}') = \frac{1}{L^d} \sum_q \frac{\exp[i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')]}{m^2+q^2}. \qquad (98)$$

5.6. Conductance of a Finite System: Definition

Let a finite system has a form of the d-dimensional cube connected to external leads, composed of N_c ideal one-dimensional chains; one should differ the "thin" and "bulk" contacts (Fig. 11). In the first case all chains are connected to the spot of a size $l \ll \sqrt{L\xi}$ (where $\sqrt{L\xi}$ is a characteristic scale where $K(r, r')$ essentially changes as a function of the transverse coordinate $r_\perp$), in the second case they are uniformly distributed along the side of the cube. For the "thin" contacts we can set $r_\perp = 0$ and write

$$g_L = \frac{V^4}{J^4} N_c^2 \frac{J}{D_L} K(x, x')|_{|x-x'|=L}. \qquad (99)$$

In the metallic state $|e_s(m)|^2 \sim L^{-d}$ and according to (96) attenuation of all states has the same order of magnitude

$$\gamma \sim V^2 \nu_F N_c L^{-d} \sim \frac{V^2}{J^2} N_c \Delta, \qquad (100)$$

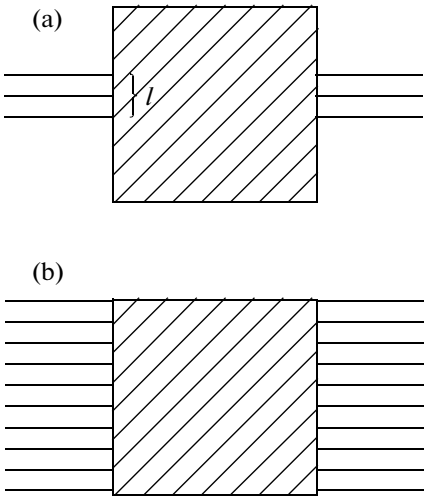

Fig. 11. The "thin" (a) and "bulk" (b) contacts attached to the system.

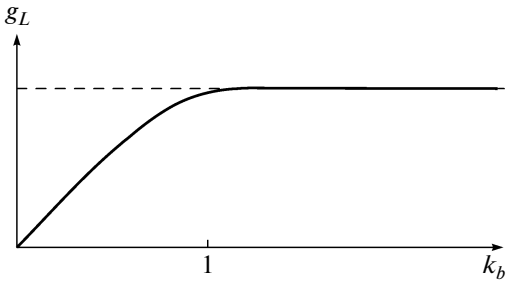

Fig. 12. Conductance g_L of a finite system versus degree of its openness.

where Δ is the level spacing. It is convenient to introduce the parameter

$$k_b = \frac{V^2}{J^2} N_c, \qquad (101)$$

having a sense of the effective transparency of an interface. According to (99), g_L contains a factor k_b^2 in the explicit form and dependence $D_L \propto \gamma \propto k_b$ in the diffusion constant, so $g_L \propto k_b$. The proportionality coefficient can be estimated from the condition that for $k_b \sim 1$ attenuation γ is of the order Δ and according to scaling theory (see Eqs. (1), (2)) the block of size L is in the critical regime, i.e. $g_L \sim 1$ and $D_L \sim JL^{2-d}$:

$$g_L = k_b L^{d-2} K(x, x')|_{|x-x'|=L}. \qquad (102)$$

This result is valid for $k_b \lesssim 1$, when perturbation theory is applicable. In the region $k_b \gtrsim 1$, one expects the absence of the k_b dependence, since $\gamma \gtrsim \Delta$ and the extended levels overlap strongly and form practically constant density of states (Fig. 4). It is easy to see (Fig. 12), that the conductance of the maximally open

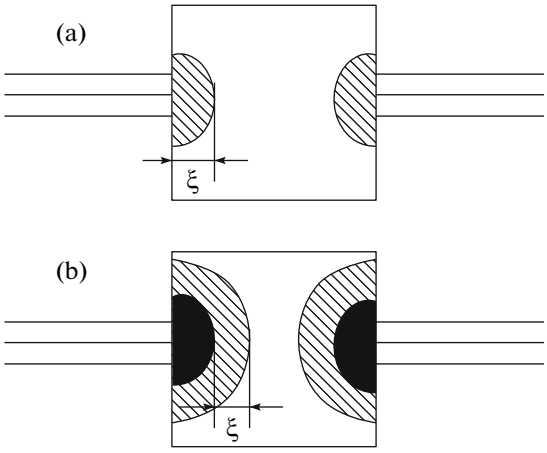

Fig. 13. A situation in the localized phase. The contacts attached to the system arouse metallization of a layer of width ~ξ around them (a). If the metallized region is replaced by the ideal conductor, then the contacts shift into the deep of the system and arouse metallization of the next layer of width $\sim g_L(L/\xi)$ (b).

system is obtained from (102) at $k_b \sim 1$.[11] However, the factor k_b can be eliminated from (102) not only setting $k_b \sim 1$, but also taking the derivative at $k_b \longrightarrow 0$:

$$g_L^{\text{open}} = \left.\frac{dg_L(k_b)}{dk_b}\right|_{k_b=0} = L^{d-2}K(x,x')\big|_{|x-x'|=L}. \tag{103}$$

We accept (103) as a definition for the conductance of a finite system: physically, it corresponds to the extremely open system, but is formulated in terms of almost closed systems. Due to the latter, such definition reflects the internal properties of the given system, not disturbed by its environment. Simultaneously, it provides the elegant solution of the contact resistance problem (Section 1): in the small k_b limit one can use the two-probe formulas (5), (7) of Economou–Soukoulis type (due to $t_{ij} \longrightarrow 0$) and there is no need in the original Landauer formula (4) or its ambiguous multichannel generalizations [3, 8, 11, 13]. The allowed values of $\mathbf{q}$ in the sum (98) for $K(\mathbf{r}, \mathbf{r}')$ correspond to the closed system and include the value $\mathbf{q} = 0$, so g_L diverges at $m \longrightarrow 0$ and the conductance of the ideal system ($\xi_{0D} = \infty$) appears to be infinite. It brightens one of the widely discussed questions [15].

In the localized phase, transition from (99) to (103) requires more complicated argumentation. The estimate (100) for γ retains for $L \lesssim \xi$; according to it, condition $k_b \sim 1$ corresponds to the critical regime for the block of size ξ. Let $k_b \gg 1$; then the block of size ξ is in the metallic state, and hence the layer of width ~ξ around contacts is metallized (Fig. 13a). Let us approximate this metallic region by the ideal conductor: then contacts shift into the deep of the system and arouse metallization of the next layer of the width ~ξ (Fig. 13b), and so on. It is easy to see that a condition $\gamma \gg \Delta$ is valid at all length scales till size L. This picture of successive metallization is valid for $k_b \gg 1$, but retains marginally at $k_b \sim 1$: in this case the blocks of size ξ are in the critical regime and the law of their composition reduces to stationarity of g_L, or $D_L \sim JL^{2-d}$, as in metallic phase. For $k_b \ll 1$ metallization does not occur and the condition $\gamma \ll \Delta$ is valid at all length scales. One can see that the estimate (102) and the k_b dependence (Fig. 12) remain the same as in the metallic phase.

5.7. Equivalence with the "Thouless Definition"

The allowed values of $\mathbf{q}$ in the sum (98) correspond to the closed system. Assuming the latter to be a system with periodical boundary conditions, it is natural to accept its size to be L in the transverse direction and $2L$ in the longitudinal direction: then for $|x-x'| = L$ the contacts are arranged at the opposite sides of the cylinder, in which the system is effectively coiled. Considering the 1D case for simplicity, we have

$$K(x,x') = \frac{1}{2L}\sum_s \left.\frac{\exp(iq_sL)}{q_s^2+m^2}\right|_{q_s=\frac{2\pi s}{2L}} \tag{104}$$

and separating odd and even s,

$$K(x,x') = \frac{1}{2L}\left(\sum_s \left.\frac{1}{q_s^2+m^2}\right|_{q_s=\frac{2\pi s}{L}} - \sum_s \left.\frac{1}{q_s^2+m^2}\right|_{q_s=\frac{2\pi s+\pi}{L}}\right). \tag{105}$$

For the Bloch boundary conditions (47), the allowed values are $q_s = (2\pi s + \varphi)/L$ and Eq. (105) contains the difference of the terms with $\varphi = 0$ and $\varphi = \pi$, being equivalent to the "Thouless definition" (58).

For the more realistic boundary conditions (48), the eigenfunctions of the operator $-\partial^2/\partial x^2$ has a form $A_s\sin(q_sx + \psi_x)$ with

$$A_s^2 = \frac{2}{L + 2\kappa/(q_s^2+\kappa^2)}, \quad \psi_s = \arctan(q_s/\kappa), \tag{106}$$

and the allowed values of q_s are determined by equation

$$q_sL + 2\arctan(q_s/\kappa) = \pi s, \quad s = 1, 2, 3, \ldots. \tag{107}$$

[11] Physically, the most adequate estimate of g_L for the extremely open system corresponds to the plateau at $k_b \gtrsim 1$ in Fig. 12; however, it is not reasonable to use very large values of k_b, since the "plateau" can in fact be a slow k_b dependence due to influence of environment on the system. Note, that numerical modelling [21] usually deals with the limit $k_b \longrightarrow \infty$.

The expression for $K(x, x')$ has a form

$$K(x, x') = \sum_{s=1}^{\infty} A_s^2 \frac{\sin(q_s x + \psi_s)\sin(q_s x' + \psi_s)}{q_s^2 + m^2}, \quad (108)$$

and for the closed system ($\kappa \longrightarrow 0$) reduces to

$$K(0, L) = \frac{1}{L}\sum_{s=-\infty}^{\infty} \frac{\cos(q_s L)}{q_s^2 + m^2}\bigg|_{q_s = \frac{\pi s}{L}}. \quad (109)$$

We have transformed the product of sines into the difference of cosines and extended the summation to negative s, using evenness in q_s. Noting that $\cos q_s L = (-1)^s$, one can separate odd and even s and obtain the result coinciding with (105) apart from the irrelevant constant factor. The accepted limitation by one dimension is not essential: the d-dimensional case differs only by summation over transverse components of $\mathbf{q}$, which is the same for two terms of the difference (105).

Below we had in mind the case of the "thin" contacts (Fig. 11a). For the "bulk" contacts (Fig. 11b) we have instead (103)

$$g_L^{\text{open}} = L^{d-2}\frac{1}{N_c^2}\sum_{r_\perp, r'_\perp} K(\mathbf{r}, \mathbf{r}')|_{|x-x'|=L}. \quad (110)$$

If the one-dimensional chains are connected to each site on the plane of the cube, then $N_c = L^{d-1}$ and summation over $r_\perp$, $r'_\perp$ removes the transverse components of the vector $\mathbf{q}$, so (110) reduces to the result for the 1D case. We see that the natural definitions for the conductance of a finite system are exhausted by d-dimensional "Thouless definitions" (see Fig. 8). The intrinsic d-dimensional case is realized for the "thin" contacts (Fig. 11a). The effective dimensionality is diminished by the unity if one-dimensional chains are connected along the line, which goes through the whole plane of the cube. For the "bulk" contacts (see Fig. 11b) the effective dimensionality is unity.

We should notice, that the physical considerations define g_L to the factor of the order of unity. Such uncertainty is natural and related with an arbitrary choice of the unit scale. Only ratios of conductances are relevant, while the choice of the absolute scale if a subject of convention.

We see that one of two scaling relations (10), (12) (written as relation (64) in Section 4) can be obtain from the pure quantum mechanical consideration without use of the self-consistent theory of localization. The second scaling relation can be also studied by other methods: in this case, the quantity ξ_{0D} should be defined by Eq. (11), where $D(\omega, 0)$ is the diffusion coefficient of the closed system.

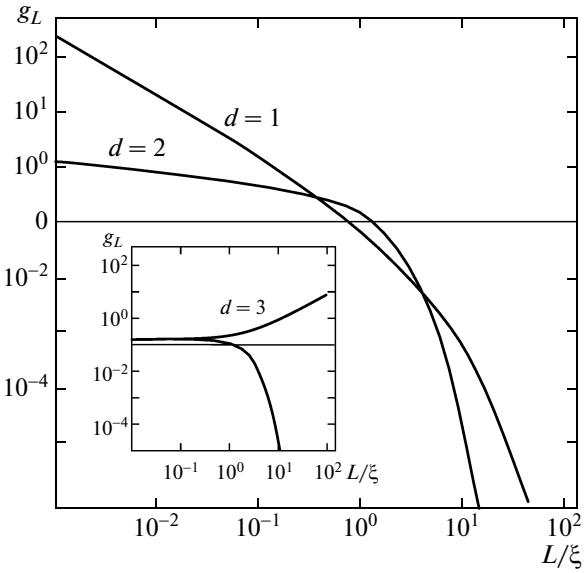

Fig. 14. Conductance g_L versus $g_L(L/\xi)$ for $d = 1, 2, 3$.

6. DISCUSSION OF SCALING EQUATIONS

According to Sections 3, 4, dependence of g_L on L/ξ is represented in the parametric form

$$\pm c_d\left(\frac{L}{\xi}\right)^{d-2} = H(z), \quad g_L = H_T(z) \quad (111)$$

for $2 < d < 4$, and

$$\frac{1}{2\pi}\ln\left(\frac{\xi}{L}\right) = H(z), \quad g_L = H_T(z) \quad (112)$$

for $d = 2$; in $d < 2$ dimensions, representation (111) holds with the upper sign and consists of one branch. Using asymptotic behavior of $H(z)$ (33), (38), (40) and $H_T(z)$ (65), one obtains for the length dependence of g_L (Fig. 14) at $d > 2$:

$$g_L = \begin{cases} c_d(L/\xi)^{d-2}, & g_L \gg 1, \\ g_c \pm B(L/\xi)^{d-2}, & g_L \longrightarrow g_c, \\ (1/\pi)(L/2\pi\xi)^{(d-3)/2}e^{-L/\xi}, & g_L \ll 1, \end{cases} \quad (113)$$

where $g_c = H_T(z^*)$, $B = c_d H'_T(z^*)/H'(z^*)$. For $d < 2$ the results for small and large g_L are formally the same, but the critical point g_c is absent. For $d = 2$, the result in the metallic phase $g_L = (1/2\pi)\ln(\xi/L)$ can be represented as a logarithmic correction to the Drude conductance g_0, $g_L = g_0 - (1/2\pi)\ln(L/a)$ [1], with the asymptotics (113) for $g_L \ll 1$.

The Gell-Mann–Low function $\beta(g)$ is determined by the derivative $d\ln g/d\ln L$ (see Eq. (2)) and can be written in the parametric form

$$g = H_T(z), \quad \beta(g) = (d-2)\frac{H(z)H'_T(z)}{H_T(z)H'(z)} \quad (114)$$

for $d \neq 2$, and

$$g = H_T(z), \quad \beta(g) = -\frac{1}{2\pi}\frac{H_T'(z)}{H'(z)H_T(z)} \tag{115}$$

for $d = 2$. Since $H_T(z)$ is positive, while $H_T'(z)$ and $H'(z)$ are negative (Figs. 6, 8), the β-function is negative for $d = 2$, and has a root for $d > 2$ due to the root of $H(z)$. The calculated β-functions for $d = 1, 2, 3$ are shown in Fig. 5.

The expansions of $H(z)$ and $H_T(z)$ in powers of z^2 has a following form for $d < 2$

$$\begin{aligned} H(z) &= 1/z^2 + a_0 - a_2 z^2 + a_4 z^4 - a_6 z^6 + \ldots, \\ H_T(z) &= 1/z^2 + \tilde{a}_0 - \tilde{a}_2 z^2 + \tilde{a}_4 z^4 - \tilde{a}_6 z^6 + \ldots, \end{aligned} \tag{116}$$

where

$$\begin{aligned} a_{2n} &= \sum_{\mathbf{s}\neq 0} \frac{1}{(2\pi|\mathbf{s}|)^{2n+2}}, \\ \tilde{a}_{2n} &= \sum_{\mathbf{t}\neq 0} \frac{(-1)^{2t_1}}{(2\pi|\mathbf{t}|)^{2n+2}}, \end{aligned} \tag{117}$$

and vectors s and t are the same as in (28) and (64). In the case $d \geq 2$, the coefficient a_0 is replaced by the parameter b_1, introduced in (29) and (36). In the case $d = 1$, the coefficients a_{2n} and $\tilde{a}_{2n}$ are expressed in terms of the Riemann ζ-function or the Bernoulli numbers [40] and can be obtained from the closed expressions

$$H(z) = \frac{1}{2z\tanh(z/2)}, \quad H_T(z) = \frac{1}{z\sinh z}, \tag{118}$$

following from (39) and (64) with the use of the Poisson summation formula.[12] Using (116), one can find the expansion of $\beta(g)$ in powers of $1/g$

$$\beta(g) = (d-2) + \frac{a_0 - \tilde{a}_0}{g} + \ldots, \quad d \neq 2, \tag{119}$$

$$\beta(g) = -\frac{1}{2\pi g} + \frac{a_2 - \tilde{a}_2}{2\pi g^3} + \ldots, \quad d = 2. \tag{120}$$

The latter result can be compared with the expansion obtained in the σ-model approach [33, 34]

$$\tilde{\beta}(t) = -2t^2 + 0\cdot t^3 + 0\cdot t^4 - 12\zeta(3)t^5 + \ldots, \tag{121}$$

which is written in terms of the variable $t \sim 1/g$. Recalculating (120) to the same form, one has

$$\tilde{\beta}(t) = -2t^2 + 0\cdot t^3 + 32\pi^4(a_2 - \tilde{a}_2)t^4 + \ldots. \tag{122}$$

The first two coefficients coincide with (121), while the third one depends on details of the g_L definition, since the parameter $\tilde{a}_2$ is different for the "thin" and "bulk" contacts (see Fig. 11). Such situation is well-known in the quantum field theory [42–44], where the structure of expansion for the β-function is the same as (121, 122): the first two coefficients are invariant, while the rest depend on the renormalization scheme. Transformation from one scheme to another corresponds to the change of variables $\tilde{t} = f(t)$, relating two different definitions of the charge; expansion of $f(t)$ in the series and the proper choice of the coefficients allows to transform (122) into (121) [43, 44]. The function $f(t)$ is well-defined in perturbation theory but can be singular at $t \sim 1$, indicating that one of two schemes is surely defective [44]. Since (122) corresponds to the physical definition of g_L, such problems can refer only to the expansion (121). In the framework of perturbation theory (121) and (122) are completely equivalent.

Such equivalence is destroyed in the space dimension $d = 2 + \epsilon$. The dimensional regularization used in the σ-models corresponds to the β-function of the form

$$\beta_{2+\epsilon}(g) = \epsilon + \beta_2(g), \tag{123}$$

i.e. the d dependence is present only in the first term of $1/g$ expansion. The exponent ν is determined by the derivative of $\beta(g)$ in the fixed point, and the corresponding result [31]

$$\nu = 1/\epsilon - (9/4)\zeta(3)\epsilon^2 + \ldots \tag{124}$$

is in conflict with (16). This fact is usually considered as a proof that the Vollhardt and Wölfle theory cannot be exact.

However, another interpretation is possible. Let us assume (in accordance with [37, 45]), that the Vollhardt and Wölfle theory is correct: then the physical reality consists in existence of the exact result $\nu = 1/\epsilon$ for $d = 2 + \epsilon$ and the non-trivial β-function for $d = 2$. The latter is related with the physical essence of the problem: the logarithmic behavior at $g \ll 1$ (see Eq. 3) makes impossible for $1/g$ expansion to be truncated at finite number of terms. Such physical reality is incompatible with the formalism of dimensional regularization: according to (123), the exact result $\nu = 1/\epsilon$ is possible only for the trivial function $\beta_2(g) = A/g$. Description of reality with such formalism should lead to unsolvable problems. Exactly such situation takes place in the modern theory: the Anderson transition problem reduces to the σ-model in a certain approximation but the corresponding renormalization group is unstable to high gradient terms [46, 47]. It is interesting to carry out renormalization of σ-models without the use of dimensional regularization: there are indications that in this case the high-gradient catastrophe is absent (see discussion of [48] in the paper [47]).

[12] These results can be used for numerical calculations in higher dimensions, in order to produce the analytic summation along one of coordinate axes.

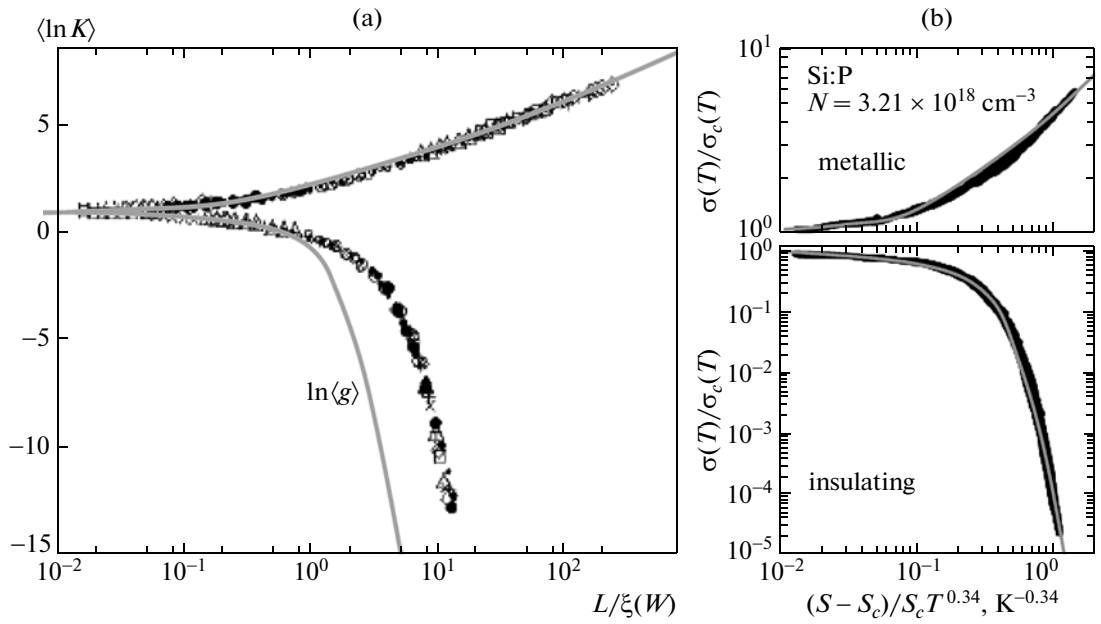

Fig. 15. (a) Comparison of the theoretical scaling curves for $d = 3$ with numerical results by Zharekeshev (symbols) [34]. The general form of the curves was determined without adjustable parameters, and only parallel shifts along two axes were made (the same for two branches), corresponding to the choice of the absolute scales for g_L and ξ. (b) Comparison of the same curves with the experimental results for Si–P [36] under assumption $L \propto T^{-\alpha}$, where α was chosen independently for two branches.

The latter asymptotics in (113) can be compared with the exact results for the 1D case [49]

$$\langle g\rangle = \frac{\pi}{2}(\alpha L/\pi)^{-3/2}e^{-\alpha L/4},$$
$$\exp\langle \ln g\rangle = 4e^{-\alpha L/4}, \qquad (125)$$
$$\langle 1/g\rangle = \frac{1}{2}e^{2\alpha L},$$

where $\alpha \propto W^2$ for weak disorder. The effective correlation length in the dependence $\exp(-L/\xi)$ is sensitive to details of the averaging procedure and determined only by the order-of-magnitude, in correspondence with its physical sense. The same uncertainty exists in the present theory, where ξ is defined by the relation $D(\omega) = (-i\omega)\xi^2$ with the ambiguous choice of the absolute scale for $D(\omega)$. Within such uncertainty, there is no sense to discuss the precise form of the pre-exponential dependence which corresponds to redefinition of ξ by the factor $1 + O(\ln L/L)$.

7. COMPARISON WITH NUMERICAL AND PHYSICAL EXPERIMENTS

Behavior of g_L versus L/ξ for $d = 3$ is compared (Fig. 15a) with numerical results by Zharekeshev [32], where g_L was estimated as "acceleration" of levels $K_s = d^2\epsilon_s/d\varphi^2$ at $\varphi = 0$ (φ is the parameter in the boundary condition (47)), which is a possible variant of the Thouless definition [17]. The agreement is satisfactory in the metallic state and the vicinity of transition, while there are expectable deviations in the localized phase: they are related with the fact that theoretical results correspond to $\ln\langle g\rangle$, while numerical to $\langle \ln g\rangle$. According to (125), the difference of two situations corresponds to redefinition of ξ by the constant factor, which reduces to the parallel shift in the logarithmic scale of Fig. 15a.

Comparison of the same dependence with the physical experiment [36] is possible under assumption that L is replaced by the length $L_{\text{in}} \propto T^{-\alpha}$, characterizing the inelastic processes. Unfortunately, there are no grounds for α to be the same in the metallic and localized phase, and it can have a slow drift as a function of disorder. In Fig. 15b it was suggested that α is the piecewise constant quantity, taking different values in the metal and insulator. Such assumption does not strongly affect the results in the critical region where the length dependence of g_L is rather slow. The latter region is poorly presented in Fig. 15b, and in fact it illustrates a situation not very close to the critical point. On the other hand, the critical behavior obtained in [36], is excellently described by the Vollhardt and Wölfle theory: the values $s = 1.0 \pm 0.1$ for the conductivity exponent and $z = 2.94 \pm 0.30$ for the dynamical exponent agree with the theoretical results $s = 1$ and $z = 3$.

The length dependence of g_L for $d = 2$ can be compared (Fig. 16a) with the numerical data by Markos [33]. There is a good agreement in the region $W > 2$, while for weak disorder numerical results display a strong violation of scaling: it can be related with the

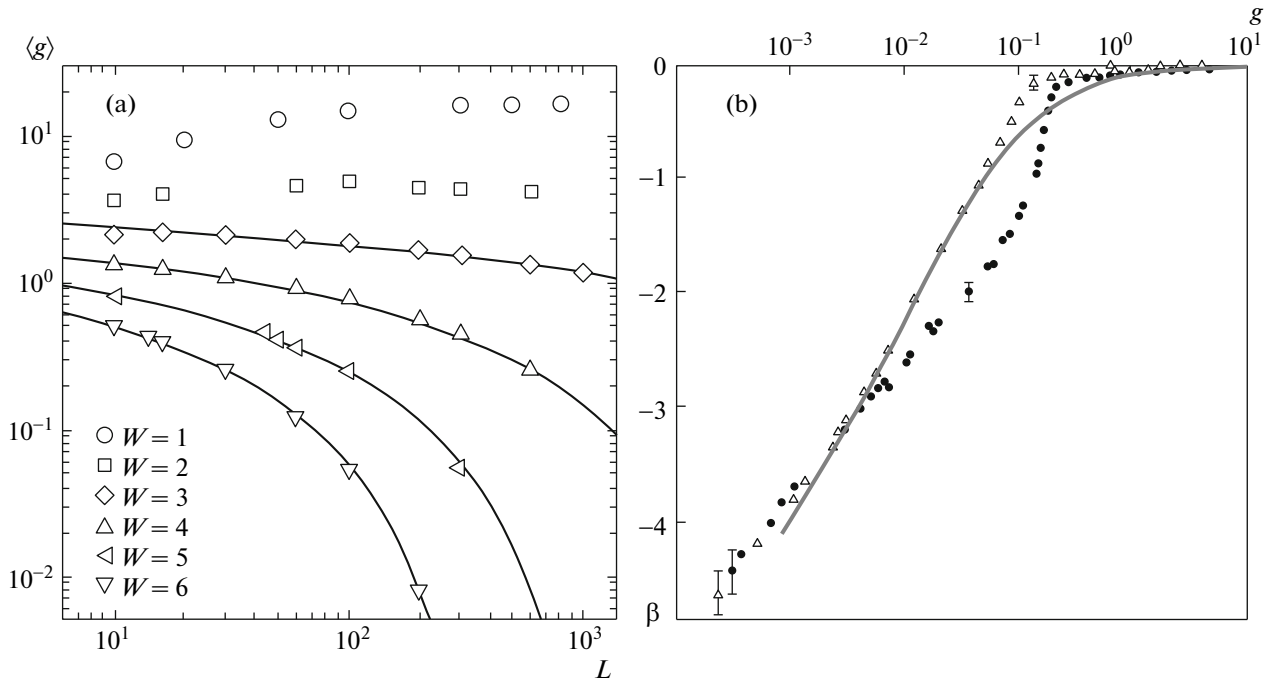

Fig. 16. (a) Comparison of the theoretical scaling curves for $d = 2$ with numerical results by Markos [33, Fig. 37]. The form of the curves was determined without adjustable parameters, only parallel shifts along two axes were made. (b) Comparison of the theoretical β-function for $d = 2$ (Fig. 5) with the empirical β-function extracted from experiment [35] under assumption $L \propto T^{-\alpha}$. The open and dark symbols corresponds to the freshly cleaved surface of Ge and to bicrystals of Ge.

protracted ballistic regime [33] or existence of the 2D metal-insulator transition. The latter, according to [29], occurs in roughly half cases and belongs to the Kosterlitz–Thouless type, compatible with scaling theory [1]. From viewpoint of the general analysis [37], a situation at $d = 2$ is special and probably reduces to the Vollhardt and Wölfle theory not in all cases.

The theoretical β-function for $d = 2$ (Fig. 5) can be compared with the empirical β-function (Fig. 16b) obtained by Zavaritskaya [35] under assumption $L \longrightarrow L_{\text{in}} \propto T^{-\alpha}$. The use of the constant α allows to describe a situation both for large and small g. Some deviations are present only in the region $g \sim 0.1$, where the experimental results are also ambiguous.

8. SITUATION IN HIGHER DIMENSIONS

8.1. Dimensions $d > 4$

For $d > 4$ we have for $I_2(m)$ in (28)

$$I_2(m) = -m^2\{c_d\Lambda^{d-4} + O(m^{d-4}, L^{4-d})\}, \qquad (126)$$

i.e., analytical calculation is possible (in the main approximation) for arbitrary values of m and L^{-1}. Indeed, for $m \gtrsim L^{-1}$ the sum can be estimated by the integral, which converges at the lower limit already for $m = 0$, so finiteness of m gives only small corrections. In the case $m \lesssim L^{-1}$, the main effect of finite L is related with absence of the term with $q = 0$, which can be estimated as restriction $|q| \gtrsim L^{-1}$ in the integral approximation.

Substitution into relation (126) reveals the possibility to neglect b_1 and leads to the scaling relation

$$\pm\frac{1}{x^2} = y^2 - \frac{1}{y^2} \qquad (127)$$

in variables

$$y = \frac{\xi_{0D}}{L}\left(\frac{a}{L}\right)^{(d-4)/4}, \quad x = \frac{\xi}{L}\left(\frac{a}{L}\right)^{(d-4)/4}, \qquad (128)$$

where we redefined the scales of ξ_{0D} and ξ, in order to obtain the unit coefficients in (127). Scaling relations (127), (128) contain the atomic scale a due to non-renormalizability of theory [30]. The critical point corresponds to $y = 1$, so that

$$\frac{\xi_{0D}}{L} \sim \left(\frac{L}{a}\right)^{(d-4)/4}, \quad \tau = 0, \qquad (129)$$

and the small z asymptotics can be used for $H_T(z)$ (see Eq. (64)). In the vicinity of transition we can replace ξ_{0D}/L by $\sqrt{g_L}$ and equations (127), (128) determine the length dependence of g_L; in particular, at the transition point

$$g_L \sim \left(\frac{L}{a}\right)^{(d-4)/2}, \quad \tau = 0. \qquad (130)$$

The physical sense of this result is clarified by the fact, that it can be obtained from the self-consistency equation for an infinite system (following from relations of Section 2)

$$D(\omega) = A\tau + B\left[\frac{-i\omega}{D(\omega)}\right]^{1/2\nu}, \quad (131)$$

if one replace $D(\omega) \longrightarrow D_L$, $-i\omega \longrightarrow \gamma$ and accept γ (for $\tau = 0$) to be of the order of level spacing $\Delta \propto L^{-d}$. For $d < 4$ it gives $g_L = \text{const}$, while for $d > 4$ it reduces to (130).

8.2. Four-Dimensional Case

For $d = 4$ we have analogously

$$I_2(m) = \begin{cases} -c_4 m^2 \ln\frac{\Lambda}{m} + O(1), & mL \gtrsim 1, \\ -c_4 m^2 \ln(\Lambda L) + O(1), & mL \lesssim 1 \end{cases} \quad (132)$$

and two results differ by $\ln(mL)$, which in the actual region reduces to the double logarithmic quantity. Neglecting such quantities, we can obtain the scaling relation (127) in variables

$$y = \frac{\xi_{0D}}{L}[\ln(L/a)]^{-1/4}, \quad x = \frac{\xi}{L}\frac{[\ln(L/a)]^{1/4}}{[\ln(\xi/a)]^{1/2}}. \quad (133)$$

In the vicinity of transition we can replace ξ_{0D}/L by $\sqrt{g_L}$ and obtain

$$g_L \sim [\ln(L/a)]^{(d-4)/2}, \quad \tau = 0. \quad (134)$$

As was explained in [30], Eqs. (127), (133) allow to produce the usual constructions of scaling curves, if the quantity y is considered as a function of the "modified length" $\mu(L) = L[\ln(L/a)]^{-1/4}$; then a change of the scale for $\mu(L)$ allows to reduce all dependences for $\tau > 0$ and $\tau < 0$ to two universal curves. It should be emphasized, that the critical point cannot be determined for $d \geq 4$ by the condition $g_L = \text{const}$.

9. CONCLUSION

The present paper continues the line initiated by the previous publication [30]: since there are serious indications [37, 45] that the Vollhardt and Wölfle theory predicts the correct critical behavior, it is desirable to derive its consequences (as many as possible) and compare them with the numerical and physical experiments on the level of raw data. Such approach already proved its value [30]: the results $\nu = 1.3$–1.6, obtained usually for $d = 3$ in numerical papers, can be explained by the fact that dependence $L + L_0$ with $L_0 > 0$ is interpreted as $L^{1/\nu}$ with $\nu > 1$, while the raw data are excellently compatible with the self-consistent theory. The finite-size scaling relations for the conductance and Gell-Mann–Low functions $\beta(g)$ obtained in the present paper are also in a good agreement with numerical and physical experiments.

In the present paper, we have elaborated a new definition for the conductance of finite systems, brightening the questions formulated in Section 1. It appears, that both self-consistent theory of localization and the quantum-mechanical analysis based on the shell model lead to the same definition, closely related with definition by Thouless. It gives one more serious argument in favour of the Vollhardt and Wölfle theory. Expansion of the β-function in $1/g$ shows that there are no contradictions on the perturbative level with the results of the σ-model approach in two dimensions. Further, in the case of validity of self-consistent theory, the formalism of dimensional regularization is incompatible with the physical essence of the problem. Probably, it is the reason both for the high-gradient catastrophe, and contradiction with the Vollhardt and Wölfle theory in the space dimension $d = 2 + \epsilon$.

The new definition will probably resolve the problem of pathological singularities in the conductance distribution [33], which cannot exist in finite systems. Their observation in numerical studies [33] is probably explained by the fact the considered system was not sufficiently isolated from environment and the thermodynamic limit $L \longrightarrow \infty$ was effectively taken along one of the coordinate axes.

The above approach suggests the simple argumentation on the spatial dispersion of the diffusion coefficient. It is easily proved for the localized phase [37], that $D(\omega, q)$ has a regular expansion in q^2. However, it does not exclude the appearance of non-integer powers of q at the critical point [50] due to possibility of constructions

$$D(\omega, q) \sim (1 + \xi^2 q^2)^{\eta}, \quad (135)$$

becoming singular in the $\xi \longrightarrow \infty$ limit. In a finite system the role of ξ is played by ξ_{0D}, which is regular at the transition point; with such replacement, Eq. (135) is valid in the metallic phase. However, the absence of such dispersion in the metallic regime is easily established from the kinetic equation. According to [37], the following result is valid instead (135)

$$D(\omega, q) = (-i\omega)\xi^2(1 + d_1 q^2 + d_2 q^4 + \ldots) \quad (136)$$

(with d_i independent of ξ), which reveals no pathologies for replacement of ξ by ξ_{0D}. It should be noted that Wegner's exact result $D(\omega, 0) \sim \omega^{(d-2)/d}$ for the critical point [51], following from (131) for $\tau = 0$, cannot be obtained in the case of essential spatial dispersion of $D(\omega, q)$. It is interesting, that the recent experiments on the spreading of wave packet [52] are in agreement with the self-consistent theory and give no evidence of the anomalous spatial dispersion.

The localization law for conductivity $\sigma(\omega) \propto -i\omega$ was predicted almost 40 years ago [53] but has never been observed experimentally. The above analysis clarifies that its observation is possible in the closed sys-

tems under approximately the same conditions as for existence of the persistent current in the Aharonov–Bohm geometry (Fig. 3) [54–56].

APPENDIX

Asymptotics of g_L for $mL \longrightarrow \infty$

Consider the sum (27) for the Bloch boundary conditions in all directions

$$I(m) = \frac{1}{L^d}\sum_{s_1,\ldots,s_d}\frac{1}{m^2+q_1^2+\ldots+q_d^2}\Big|_{q_i=\frac{2\pi s_i+\varphi_i}{L}} \tag{A.1}$$

and introduce the so called α-representation

$$\frac{1}{m^2+q^2} = \int_0^\infty d\alpha \exp[-\alpha(q^2+m^2)]. \tag{A.2}$$

Then

$$I(m) = \int_0^\infty d\alpha \exp(-\alpha m^2)\prod_{j=1}^d S_j(\alpha),$$
$$S_j(\alpha) = L^{-1}\sum_{s=-\infty}^\infty \exp(-\alpha q_s^2)\Big|_{q_s=\frac{2\pi s+\varphi_j}{L}} \tag{A.3}$$

and the use of the Poisson summation formula [40] transforms $S_j(\alpha)$ to

$$S_j(\alpha) = \frac{1}{\sqrt{4\pi\alpha}}\sum_{k_j=-\infty}^\infty \exp\left(ik_j\varphi_j - \frac{k_j^2L^2}{4\alpha}\right). \tag{A.4}$$

Then (A.3) takes a form

$$I(m) = \int_0^\infty \frac{d\alpha}{(4\pi\alpha)^{d/2}}\exp(-\alpha m^2)$$
$$\times\sum_{\mathbf{k}}\exp\left(i\mathbf{k}\cdot\boldsymbol{\varphi} - \frac{|\mathbf{k}|^2L^2}{4\alpha}\right), \tag{A.5}$$

where a vector $\mathbf{k} = (k_1, \ldots, k_d)$ is introduced and $\mathbf{k}\cdot\boldsymbol{\varphi} = \sum_j k_j\varphi_j$. The term with $\mathbf{k} = 0$ is calculated exactly and corresponds to the continual approximation. The main effect of discreteness is determined by the terms with $|\mathbf{k}| = 1$, which can be calculated for $mL \gg 1$ in the saddle-point approximation. Remaining only these terms, one has

$$I(m) = \frac{m^{d-2}}{(4\pi)^{d/2}}\left[\Gamma\left(1-\frac{d}{2}\right)\right.$$
$$\left. + \sqrt{\pi}\left(\frac{mL}{2}\right)^{(1-d)/2}e^{-mL}\sum_{j=1}^d 2\cos\varphi_j\right]. \tag{A.6}$$

Taking the difference of two such expressions with $\varphi_1 = 0$ and $\varphi_1 = \pi$,

$$I(m)\big|_{\varphi_1=0} - I(m)\big|_{\varphi_1=\pi}$$
$$= \frac{4\sqrt{\pi}}{(4\pi)^{d/2}}m^{d-2}\left(\frac{mL}{2}\right)^{(1-d)/2}e^{-mL}, \tag{A.7}$$

we come to Eq. (59).

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