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LETTER TO THE EDITOR

'Unusual' metals in two dimensions: one-particle model of the metal–insulator transition at $T = 0$

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Abstract

The conductance of disordered nano-wires at $T = 0$ is calculated in the one-particle approximation by reducing the original multi-dimensional problem for an open bounded system to a set of exactly one-dimensional non-Hermitian problems for mode propagators. Regarding the two-dimensional conductor as a limiting case of a three-dimensional disordered quantum waveguide, the metallic ground state is shown to result from its multi-modeness. On thinning the waveguide (in practice, e.g., by means of the 'pressing' external electric field) the electron system undergoes a continuous phase transition from metallic to dielectric state. The results predicted conform qualitatively to the observed anomalies of the resistance of different planar electron and hole systems.

In the physics of disordered systems, there was a long-standing belief initiated by scaling theory of localization [1] that in two-dimensional electron and hole systems, just as in one-dimensional ones, there could be no metallic ground state at any strength of disorder. However, numerous studies on different materials performed in recent years (see the extensive bibliography in [2]) have challenged this point of view and showed it to be apparently incomplete and maybe, in the general case, incorrect.

The inconsistency of the experimental facts with theoretical predictions has led to a vast number of publications where the observed unusual phenomena were interpreted with the use of different physical ideas. Among these were the formation of a conducting state in electron systems of very low density [3, 4], the existence of an esoteric ideal metallic state [5], non-Fermi-liquid behaviour of the conduction electrons [6], different types of superconductivity [7, 8], the effects, which are classical in nature, of trap formation at the interface of slightly different materials [9] and the temperature-dependent screening of electron–impurity scattering [10, 11].

In this letter, we focus our attention on interpreting the observed phenomena in terms of the concept of 'quantum dephasing'. Within the framework of this approach, the 'anomalous'

conducting state of two-dimensional systems is regarded as the result of phase randomization of the originally coherent localized electrons due to their interaction with systems considered as the 'environment'. The physical nature of the dephasing environment in real systems still remains controversial [12]. As the most probable cause of dephasing, some authors suggest quasi-elastic Coulomb interaction of carriers, since the 'anomalous' behaviour of the resistance is commonly observed in two-dimensional systems with low electron density ($r_s \gtrsim 10$). Note, however, that different theories evaluate this kind of interaction quite differently, some as promoting localization [13, 14] whereas some as inhibiting its origination [3, 4, 15].

Meanwhile, it has been recently shown [16] that scattering from static inhomogeneities can lead, in much the same way as different inelastic processes do, to the dephasing of quantum states properly classified with regard for the confinement of the dynamical system being considered. The arguments were based on the use of the mode representation for one-particle propagators, which seems to be most appropriate as applied to *open systems* of waveguide type. In regard to electrons (considered as quantum waves), mode states represent the *collective* excitations which describe the electron system as strongly correlated. As a matter of fact, the correlation, even without invoking Coulomb interaction, is originally embedded in the Green function formalism which explicitly takes into account the Pauli principle [17].

As was shown in [16], owing to dephasing of the coherent mode states through impurity scattering of the electrons between the *extended* modes (for which the term 'open channels' is widely used), the formation of Anderson localized states in two-dimensional conductors that are not extremely narrow (i.e. possess more than one quantum mode) is made possible under some particular, though realizable, conditions only. Meanwhile, although from the results given in [16] it follows that the metallic-like ground state should not be considered to be anomalous for two-dimensional disordered systems, the analysis did not reveal a clear mechanism for changing such systems from the conducting to insulating state and vice versa, which is observed in numerous experiments (see the bibliography in [2]).

In this letter, the method previously developed for exactly two-dimensional open systems is extended to the case of conductors of larger dimensionality in order to fit the formal statement of the problem to real experimental conditions. The approach is inspired by the fact that in practice two-dimensional conducting systems are mostly created by forming near-surface potential finite-width wells. The wells are produced either due to application of 'pressing' external electric field or due to the contact potential. The shape of the well (in most cases it is nearly triangular [15, 18]) is of no crucial importance for its principal function, namely to restrict the electron motion in the direction normal to the heterogeneity surface. Therefore, we examine below a somewhat simplified model of the conductor, which is chosen in the form of a rectangular three-dimensional quantum waveguide with 'hard' side boundaries. The length L of the waveguide along the x-axis as well as the width W, y-axis, and the height H in the direction of the z-axis will be considered as arbitrary. We assume the chemical potential (or the Fermi energy) to be constant with change in the geometrical parameters. Such a model is justified for an *open* system, i.e. the conductor attached to identical reservoirs in the equilibrium.

According to the linear response theory [19], the conductance can be expressed in terms of the retarded one-particle Green function of the electron system. This function, within the model of an isotropic Fermi liquid and with units such that $\hbar = 2m = 1$ (m is the electron effective mass), satisfies the equation

$$[\Delta + k_F^2 + \mathrm{i}0 - V(\boldsymbol{r})]G(\boldsymbol{r}, \boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{1}$$

Here, Δ is the three-dimensional Laplacian, k_F is the electron Fermi wavenumber, $V(\boldsymbol{r})$ is the static random potential specified by zero mean value, $\langle V(\boldsymbol{r})\rangle = 0$, and the binary correlation

function

$$\langle V(\boldsymbol{r})V(\boldsymbol{r}')\rangle = \mathcal{Q}\mathcal{W}(x-x')\delta(\boldsymbol{r}_\perp - \boldsymbol{r}'_\perp), \tag{2}$$

where $\boldsymbol{r}_\perp = (y, z)$. The function $\mathcal{W}(x)$ is normalized to unity and decays at the scale of r_c, the correlation radius.

Equation (1) must be supplemented with proper boundary conditions. The side boundaries of the system, 'impenetrable' for quantum waves, can be characterized by a real impedance. In contrast, the open ends of the waveguide ($x = \pm L/2$) correspond to a complex impedance owing to which the differential operation in (1) becomes non-Hermitian.

In [16], a method was proposed for solving such a non-Hermitian problem in the case of two-dimensional conducting systems. The analogous procedure is applicable to waveguide-type systems of arbitrary dimensionality as well. The essence of the method is the transition from one transport problem posed in a dimension higher than unity to an infinite set of exactly one-dimensional problems for mode Fourier components of the propagator $G(\boldsymbol{r}, \boldsymbol{r}')$. For the waveguide-type system under study, the transition to mode representation can be carried out using the whole set of eigenfunctions $|\boldsymbol{r}_\perp; \boldsymbol{\mu}\rangle$ of the 'transverse' Laplace operator, which is made up of ordinary trigonometric functions ($\boldsymbol{\mu} = (n, m)$ is the vectorial mode index specified by integer-valued components). With such an eigenset, equation (1) is transformed into a set of equations for mode components $G_{\mu\mu'}(x, x')$ of the function $G(\boldsymbol{r}, \boldsymbol{r}')$,

$$\left[\frac{\partial^2}{\partial x^2} + \kappa_\mu^2 + \mathrm{i}0 - V_\mu(x)\right] G_{\mu\mu'}(x, x') - \sum_{\nu\neq\mu} U_{\mu\nu}(x) G_{\nu\mu'}(x, x') = \delta_{\mu\mu'}\delta(x - x'). \tag{3}$$

The parameter

$$\kappa_\mu^2 = k_F^2 - (\pi n/W)^2 - (\pi m/H)^2 \tag{4}$$

in (3) has the meaning of a *longitudinal energy* of the mode $\boldsymbol{\mu}$; the potential matrix $\|U_{\mu\mu'}\|$ is composed of the functions

$$U_{\mu\mu'}(x) = \int_S \mathrm{d}\boldsymbol{r}_\perp\, |\boldsymbol{r}_\perp; \boldsymbol{\mu}\rangle V(\boldsymbol{r}) \langle \boldsymbol{r}_\perp; \boldsymbol{\mu}'|. \tag{5}$$

The diagonal components of this matrix, $V_\mu(x) \equiv U_{\mu\mu}(x)$, are responsible for the *intra-mode* whereas off-diagonal components for the *inter-mode* scattering of quantum waves.

The initial problem reformulated in terms of the 'one-coordinate' differential equations (3) cannot actually be considered as strictly one dimensional for the entanglement of overall mode components of the Green function matrix $\|G_{\nu\mu}\|$. In [16], however, it was shown that all the off-diagonal elements of this matrix can be expressed, by means of a linear operation, in terms of the corresponding diagonal elements,

$$G_{\nu\mu}(x, x') = \int_L \mathrm{d}x_1\, \mathsf{K}_{\nu\mu}(x, x_1) G_{\mu\mu}(x_1, x') \qquad \boldsymbol{\nu} \neq \boldsymbol{\mu}. \tag{6}$$

The kernel of the operator (6) can be determined exactly given the solution $G_\mu^{(V)}(x, x')$ of the truncated equation (3),

$$\left[\frac{\partial^2}{\partial x^2} + \kappa_\mu^2 + \mathrm{i}0 - V_\mu(x)\right] G_\mu^{(V)}(x, x') = \delta(x - x'), \tag{7}$$

i.e. the equation with all inter-mode potentials $U_{\mu\nu}(x)$ omitted. For (7), the requirement of waveguide openness at the ends $x = \pm L/2$ can be formulated in terms of Sommerfeld's radiation conditions [20, 21],

$$\left(\frac{\partial}{\partial x} \mp \mathrm{i}\kappa_\mu\right) G_\mu^{(V)}(x, x')\Big|_{x=\pm L/2} = 0, \tag{8}$$

which correspond to adiabatic (not resulting in scattering) attachment of the conductor at hand to the ideally conducting leads.

The auxiliary 'trial' Green function $G_{\mu}^{(V)}(x, x')$, in view of the statistical formulation of the problem, can be thought of as known precisely if one manages to find all its statistical moments $\langle [G_{\mu}^{(V)}(x, x')]^p \rangle$, $p \in \aleph$. Using the technique described in [16], these moments can be obtained provided the scattering from the potential $V(\boldsymbol{r})$ is regarded as weak. The weakness criteria can be formulated in terms of the characteristic lengths,

$$k_F, r_c \ll \ell, \tag{9}$$

where ℓ represents the quasi-classical mean free path of conducting electrons. Its value, in the particular case of completely δ-correlated random potential ($\mathcal{W}(x) = \delta(x)$ in (2)), is equal to $4\pi/\mathcal{Q}$.

For the extended modes ($\kappa_{\mu}^2 > 0$), calculation of the required moments yields

$$\langle [G_{\mu}^{(V)}(x, x')]^p \rangle = \left(\frac{-\mathrm{i}}{2\kappa_{\mu}}\right)^p \exp\left[\mathrm{i}p\kappa_{\mu}|x - x'| - \frac{p}{2}\left(\frac{p}{L_f^{(V)}(\boldsymbol{\mu})} + \frac{1}{L_b^{(V)}(\boldsymbol{\mu})}\right)|x - x'|\right]. \tag{10}$$

Here, $L_{f,b}^{(V)}(\boldsymbol{\mu})$ are the forward (f) and the backward (b) mode scattering lengths associated solely with the *intra-mode* potential $V_{\mu}(x)$,

$$L_f^{(V)}(\boldsymbol{\mu}) = \frac{4S}{9\mathcal{Q}}(2\kappa_{\mu})^2, \qquad L_b^{(V)}(\boldsymbol{\mu}) = \frac{4S}{9\mathcal{Q}}\frac{(2\kappa_{\mu})^2}{\tilde{\mathcal{W}}(\kappa_{\mu})}, \tag{11}$$

S is the conductor cross-section area and $\tilde{\mathcal{W}}(\kappa_{\mu})$ is the Fourier transform of $\mathcal{W}(x)$. As far as the evanescent modes are concerned ($\kappa_{\mu}^2 < 0$), at weak scattering the potential $V_{\mu}(x)$ in equation (7) can be omitted, thus allowing one to take advantage of the unperturbed solution,

$$G_{\mu}^{(V)}(x, x') = -\frac{1}{2|\kappa_{\mu|}} \exp(-|\kappa_{\mu}||x - x'|). \tag{12}$$

It is worth noting that if the particular functions $G_{\mu}^{(V)}(x, x')$ are used instead of the precise mode propagators, that is if for some reason the inter-mode scattering is neglected[1], the result widely known from the theory of quasi-one-dimensional conductors would be obtained. Specifically, the conductance would *exponentially* decrease as the conductor length grew when the latter exceeded a value of the order of $N_c\ell$ (where N_c is the number of open channels). It is exactly this length scale that was associated previously with the localization length in disordered two-dimensional systems [22, 23].

However, in the general case, there are no grounds for neglecting the inter-mode potentials in equation (3). Taking them into account leads to the multi-channel Lippmann–Schwinger equation [24] for the kernel of the operator (6), which can be explicitly solved if the Green function of trial equation (7) is chosen as a starting approximation for the exact mode propagator. As a result, the closed one-dimensional equation for the diagonal component $G_{\mu\mu}$ is deduced,

$$\left[\frac{\partial^2}{\partial x^2} + \kappa_{\mu}^2 + \mathrm{i}0 - V_{\mu}(x) - \hat{\mathcal{T}}_{\mu}\right] G_{\mu\mu}(x, x') = \delta(x - x'). \tag{13}$$

Here, $\hat{\mathcal{T}}_{\mu}$ is the non-local operator potential, which, with the proviso of (9), is given by $\hat{\mathcal{T}}_{\mu} \approx \boldsymbol{P}_{\mu}\hat{\mathcal{U}}\hat{G}^{(V)}\hat{\mathcal{U}}\boldsymbol{P}_{\mu}$. The operators $\hat{\mathcal{U}}$ and $\hat{G}^{(V)}$ are defined in the mixed coordinate-mode

[1] In some particular cases, for example if the conductor inhomogeneity is in the form of random strata along the x-axis, all the intermode potentials vanish exactly.

subspace $(x, \boldsymbol{\nu})$ with the excluded mode $\boldsymbol{\mu}$ and specified by the matrix elements

$$|x, \boldsymbol{\nu}\rangle\hat{\mathcal{U}}\langle x', \boldsymbol{\nu}'| = U_{\boldsymbol{\nu}\boldsymbol{\nu}'}(x)\delta(x - x'), \tag{14}$$

$$|x, \boldsymbol{\nu}\rangle\hat{G}^{(V)}\langle x', \boldsymbol{\nu}'| = G^{(V)}_{\boldsymbol{\nu}}(x, x')\delta_{\boldsymbol{\nu}\boldsymbol{\nu}'}; \tag{15}$$

$\boldsymbol{P}_{\boldsymbol{\mu}}$ is the projection operator from the above-mentioned subspace into the mode $\boldsymbol{\mu}$. Equation (13) along with (6) enables one to obtain the function $G(\boldsymbol{r}, \boldsymbol{r}')$ with the required accuracy and in so doing to determine the system conductance.

If there is more than one open channel in the conductor (at least two), the operator potential $\hat{\mathcal{T}}_{\boldsymbol{\mu}}$ results in the imaginary term $\mathrm{i}/\tau^{(\varphi)}_{\boldsymbol{\mu}}$ appearing in the spectrum of (13),

$$\frac{1}{\tau^{(\varphi)}_{\boldsymbol{\mu}}} = \frac{\mathcal{Q}}{4S}\sum_{\boldsymbol{\nu}\neq\boldsymbol{\mu}}{}' \frac{1}{\kappa_{\boldsymbol{\nu}}}[\tilde{\mathcal{W}}(\kappa_{\boldsymbol{\mu}} - \kappa_{\boldsymbol{\nu}}) + \tilde{\mathcal{W}}(\kappa_{\boldsymbol{\mu}} + \kappa_{\boldsymbol{\nu}})] \approx \frac{k_F}{2\ell}, \tag{16}$$

which indicates that phase uncertainty has arisen owing to the scattering between extended modes other than the particular mode $\boldsymbol{\mu}$. In (16), the prime indicates the summation over *open channels* only. This means that in systems with more than one conducting channel the inter-mode scattering from quenched disorder produces the same dephasing effect on the many-particle carrier states as the real inelastic scattering processes do. Still, there is some distinction consisting in that scattering from static inhomogeneities does not affect actual one-electron energy (at $T = 0$ the latter remains the Fermi energy) but it does influence the longitudinal energy of a many-particle state, i.e. the quantum (or waveguide) mode.

As a result, on increasing the length L of the multi-channel conductor the conductance does not fall exponentially, which is characteristic of Anderson-localized states, even if $L > N_c\ell$. In particular, at $N_c \gg 1$, the dimensionless (in units of $e^2/\pi\hbar$) average conductance $\langle g(L)\rangle$ is given as

$$\langle g(L)\rangle \approx N_c, \qquad L < \ell, \tag{17a}$$

$$\langle g(L)\rangle \approx (4/3)N_c\ell/L, \qquad \ell \ll L. \tag{17b}$$

If there is only one open channel in the conductor (with, say, mode index $\boldsymbol{\mu}_1$) then there are no terms in the sum of (16) and, therefore, the electron state in this channel should be thought of as coherent. In this case, the conductance is obtained from the *one-dimensional localization* theory. It varies with L according to the law

$$\langle g(L)\rangle \approx \begin{cases} 1 - 4L/\xi_1, & L/\xi_1 \ll 1 \\ A(\xi_1/L)^{3/2}\exp(-L/\xi_1), & L/\xi_1 \gg 1, \end{cases} \tag{18}$$

where $A = \pi^{5/2}/16$ and $\xi_1 = 4L^{(V)}_b(\boldsymbol{\mu}_1)$. The result (18) clearly indicates the localized character of the electron states whose spatial extent, ξ_1, is determined by the extended mode *backscattering*.

Let us discuss the obtained results from the viewpoint of their connection to the metal–insulator transition (MIT) observed in two-dimensional systems. First of all, it is worth noting that there are no signs of MIT as long as the conductor is multi-mode. The result (17*a*) is consistent with the conception of *ballistic* electron transport in short wires. In this case, the conductance exhibits evident staircase-like dependence on the electron energy as well as on the transverse dimension of the conductor (for a massive three-dimensional wire the equality $N_c = [k_F^2 S/4\pi]$ holds, where $[\cdots]$ symbolizes the integer part of the number enclosed).

The asymptotic value (17*b*) is consistent with the model of *diffusive* classical motion of electrons and coincides exactly with the conductance well known from the kinetic theory[2].

[2] In this letter, we do not touch upon *weak-localization* effects originating from the coherent scattering due to the intra-mode potential $V_{\boldsymbol{\mu}}(x)$ in (13).

The lack of the exponential dependence on L within the length region $L \gg N_c\ell$ indicates the nonexistence of the 'localized' transport of current carriers in multi-mode conductors. Although the original disorder (potential $V(\boldsymbol{r})$) is of quenched character, the T-matrix $\hat{\mathcal{T}}_{\boldsymbol{\mu}}$ in (13) describes the recurrent scattering of the $\boldsymbol{\mu}$-mode electrons through intermediate states with mode energies different from $\kappa_{\boldsymbol{\mu}}^2$. This scattering, once proceeding through the *extended* virtual modes, dephases 'parent' mode state $\boldsymbol{\mu}$ quite similarly to the actual inelastic scattering.

Now consider again the equation (13) and the expression (4) for the mode energy. Clearly, the number of extended modes can be varied by changing the quantum waveguide thickness only, keeping its width W constant. By decreasing H, one can gradually reduce the number of open channels to unity, thus passing from 'metallic' conductance, either in its ballistic form (17*a*) or diffusive form (17*b*), to 'dielectric' result (18). In practice, for the most part, by monitoring the shape of near-surface potential wells the carrier density is normally varied [15], as a function of which the resistance of two-dimensional systems is commonly measured.

On a further increase of the 'pressing' voltage (accompanied by the corresponding decrease of two-dimensional carrier density) the quantum waveguide turns into a below-cut-off one in that only *evanescent* modes ($\kappa_{\boldsymbol{\mu}}^2 < 0$) remain. These states, as can be readily seen from (12), are exponentially localized on a scale of the mode wavelength even in the absence of any disorder. Naturally, as the electron system enters such a strongly localized phase, the resistance must show a rapid increase (MIT).

To conclude, note that in most of the experimental works the conclusions about transport properties of two-dimensional electron and hole systems were made on the basis of examining the temperature dependence of their resistance. The detailed analysis of this issue is beyond the scope of the present article. Nevertheless, taking into account the above-mentioned features of (quasi-) two-dimensional system ground states, a set of qualitative predictions regarding the temperature dependence of their resistance can also be made.

First note that the transition from the metallic-type conductance (17*a*), (17*b*) to its small value in the localized phase proceeds inevitably through the *one-mode* state of the electron system. It is evident from (17*a*) and (18) that in such a transitional regime the conductance should assume a value close to one conductance quantum, irrespective of the material of the conductor. It is exactly such a value that is observed in the vicinity of the so-called 'separatrix' in the T-dependence of two-dimensional system resistivity [2]. Also, the weak temperature dependence of the separatrix can be explained if one takes into account that mode wavelengths of marginal channels, namely those which are in the state of opening or closing, are large as compared with the thermal phonon characteristic wavelength. If this is the case, the interaction between these channels and the phonon subsystem of the conductor should be ineffective.

In the insulating phase, where all of the modes are strongly localized, it is natural to anticipate the temperature dependence predicted by the percolation theory [25]. Much more intricate is the puzzle of non-monotonic dependence on T of the resistivity in the metallic phase in proximity to the separatrix. Recall, however, that on approaching the separatrix from the metallic side the electron system is certain to run through the one-mode stage, i.e. it becomes virtually one dimensional even though the width of the quantum waveguide remains macroscopic. As for one-dimensional electron systems, non-monotonic temperature dependence of their conductivity had been predicted before, in [26] for the case $T\tau \gg 1$ and in [27] for $T\tau \ll 1$.

Hence, the result obtained in this paper with the method of [16], which was extended to analyse real two-dimensional electron systems, seems to be consistent with the 'unexpected' experimental data extracted at low but non-zero temperatures. This makes it reasonable to interpret the observed peculiarities of the planar system resistance as revealing the true *continuous phase transition* [15, 28] of such systems from conducting to insulating state.

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