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## On the semiphenomenological approach in the localization theory

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**Abstract.** We propose a version of the self-consistent approach to the localization phenomena, constructed according to the following scheme. We formulate some general requirements for the second moment of the Green function. Then we find the 'simplest' expression that satisfies all these requirements. Such an expression is not unique of course, but we show that it provides quite a reasonable description of the Anderson transition.

The problems of the localization of states in disordered solids and the resulting kinetics are among the most important in solid state theory. This problem is fairly difficult, and reliable results are known only for one-dimensional systems and for large or small disorder in the multidimensional case [1–4]. As a result, in the last few years a variety of self-consistent approaches have been proposed which allow one to consider, at least qualitatively, the case of intermediate disorder and to describe in particular the metal–insulator (Anderson) transition in three-dimensional systems and the complete localization in low-dimensional ( $d = 1, 2$ ) systems (see, e.g., [5–7]). In spite of different initial prerequisites, these approaches result in essentially the same equation which provides a fairly reasonable description of the Anderson transition (the respective results are in good agreement with the exact one-dimensional calculation and with the computer simulations).

However, the procedure for the construction of self-consistent approaches in the theory of disordered systems is much less ambiguous than in the theories of critical phenomena. This is why all such approaches use hardly controllable hypotheses and approximations. It is natural therefore to make further attempts to find more convincing arguments which clarify and justify at least partially the procedure of the derivation of the self-consistent equation for the diffusion coefficient. The present paper is devoted to such an attempt. We consider the double correlator (the second moment) of the Green function and formulate some requirements which follow from the general principles and the modern state of art of the theory of disordered systems. Then we consider the 'simplest' expression for the correlator compatible with these requirements. Such an expression is not unique of course, but we show that it can be written in a form that gives in essence the same self-consistent equations that were found earlier [5–7].

As a byproduct of our scheme we can find other kinetic coefficients and obtain more detailed information on the nature of the Anderson transition. In particular we find that the short-range part of the double correlator is a singular function of frequency  $\omega$  in the

localization regime. Therefore one may expect the small-distance behaviour of the correlator to be also important to the understanding of the nature of localization.

Now we shall list and briefly discuss our requirements on the double correlator

$$K_{\omega}(r_1, r_2 | r_3, r_4) = \langle G_{E+\omega/2+i0}(r_1, r_3) G_{E-\omega/2-i0}(r_2, r_4) \rangle \quad (1)$$

where  $G_E(r, r')$  is the exact Green function of an electron in the random potential and the symbol  $\langle \dots \rangle$  denotes averaging over this potential. We shall use the Anderson model on a simple hypercubic lattice.

In what follows it is more convenient to consider the Fourier transform of (1):

$$\Phi_{\omega}(k_1, k_2 | k_3, k_4) = N^{-2} \sum_{r_1, r_2, r_3, r_4} K_{\omega}(r_1, r_2 | r_3, r_4) \exp[i(-k_1 r_1 - k_2 r_2 + k_3 r_3 + k_4 r_4)] \quad (2)$$

where  $N$  is a number of lattice sites. In view of the spatial homogeneity in the mean (see [1]) this function contains  $\Delta(k_1 + k_2 - k_3 - k_4)$  where  $\Delta(k)$  is the Kronecker symbol.

(i) *Cross symmetry.*

$$\Phi_{\omega}(k_1, k_2 | k_3, k_4) = \Phi_{\omega}(-k_3, k_2 | -k_1, k_4). \quad (3)$$

This condition is a consequence of the time-reversal symmetry of the problem resulting in the real-valuedness of the wavefunctions in the coordinate representation. Relation (3) was used earlier for the construction of self-consistent approaches (see, e.g., [6]). It can be easily proved by using the eigenfunction expansion of the Green function in the coordinate representation.

(ii) *The Hilbert identity.*

$$\delta^{-1} \text{Im} G_{E-i\delta} = G_{E+i\delta} G_{E-i\delta}. \quad (4)$$

Conditions (3) and (4) yield the following relations for the correlator (2):

$$\sum_k \Phi_{\omega}(p, k | k, p) = \sum_k \Phi_{\omega}(k, p | p, k) = \text{Im} \left( \frac{\Delta \tilde{G}(p)}{\omega} \right) \quad (5a)$$

$$\sum_k \Phi_{\omega}(p, -p | k, -k) = \sum_k \Phi_{\omega}(k, -k | -p, p) = \text{Im} \left( \frac{\Delta \tilde{G}(p)}{\omega} \right). \quad (5b)$$

Here  $\Delta \tilde{G}(p) = \langle \tilde{G}_{E-\omega/2-i0}(p) \rangle - \langle \tilde{G}_{E+\omega/2+i0}(p) \rangle$  and  $\langle \tilde{G}(p) \rangle$  is the Fourier transform of the mean Green function.

(iii) *The principle of vanishing of the correlations.* According to this principle there are no statistical correlations between infinitely distant points [1].

This principle implies that

$$K_{\omega}(r_1, r_2 + a | r_3, r_4 + a) \xrightarrow{a \rightarrow \infty} \langle G_{E+\omega/2+i0}(r_1, r_3) \rangle \langle G_{E-\omega/2-i0}(r_2, r_4) \rangle \quad (6)$$

or

$$\Phi_{\omega}(p, k | p, k) = \langle \tilde{G}_{E+\omega/2+i0}(p) \rangle \langle \tilde{G}_{E-\omega/2-i0}(k) \rangle. \quad (7)$$

Requirements (i)–(iii) are the consequences of fairly general principles. We formulate now one more requirement which has been widely used in recent years.

(iv) *The presence of the diffusion pole in correlator (2).* This requirement determines the asymptotic behaviour (the singular part) of correlator (2) for small  $\omega$  and  $q = k_1 - k_4 = k_2 - k_3$  and has the form

$$\Phi_\omega(k_1, k_2 | k_3, k_4) \underset{\omega, q \rightarrow 0}{\sim} (-i\omega + Dq^2)^{-1} \quad (8)$$

where the quantity  $D$  coincides with the full diffusion coefficient at zero temperature and depends, generally speaking, on the energy  $E$ .

Denote by  $S(q)$  the Fourier transform of the density-density correlator:

$$S(q) = \frac{1}{N} \sum_{k, k'} \Phi_\omega \left( k + \frac{q}{2}, k' - \frac{q}{2} \middle| k' + \frac{q}{2}, k - \frac{q}{2} \right).$$

Then form (8) of the singular part of  $\Phi_\omega(k_1, k_2 | k_3, k_4)$  may be considered as a natural form provided that the asymptotic expression

$$S(q) \approx 2\pi\rho(E)/(-i\omega + Dq^2)$$

which for small  $\omega$  and  $q$  follows from the fairly general phenomenological arguments (here  $\rho(E)$  is the exact density of states defined as  $\pi^{-1} \text{Im} \langle G_{E+i0}(0, 0) \rangle$ ). The asymptotic relation (8) with  $D$  replaced by the 'bare' diffusion constant  $D_0$ , given by the classical kinetic theory, follows also from the weak-disorder perturbation theory after summing of so-called 'ladder' diagrams [8, 9]. This relation is implied also by the exact Einstein relation [10]

$$D = [4\pi\rho(E)]^{-1} \lim_{\omega, q \rightarrow 0} [\omega^2 \partial^2 S(q) / \partial q^2].$$

Besides, asymptotic (8) is the simplest (but, of course, not unique) form of the correlator compatible with the exact sum rule

$$\lim_{\omega \rightarrow 0} \{\text{Re}[S(q)]\} = 2\pi^2 \rho(E) \delta(\omega) + A(\omega).$$

Here  $A(\omega) = 2(\partial/\partial E)(\text{Re} \langle G_{E+i0}(0, 0) \rangle) + O(\omega^2)$  is obviously non-singular for small  $\omega$ .

Relation (8) describes the 'diffusion' spreading of the  $\delta$ -function singularity for small  $q$  and seems very natural and useful in the delocalization region of energies.

To describe by the same formula the behaviour of correlator (2) in the localization region, we assume, based on phenomenological arguments [6], that in this region

$$D(\omega) = -i\omega\alpha \quad (9)$$

where  $\alpha$  is the polarizability that may depend on the energy.

Therefore, we suppose that the functional form (8) for small  $\omega$  and  $q$  is valid in the whole energy range, but in the localization region  $D$  has the form (9), where  $\alpha$  depends on  $E$  and tends to infinity when  $E$  approaches the mobility edge  $E_c$ .

Let us consider now to what extent requirements (i)–(iv) determine the correlator. We assume for simplicity that the random potential is the Gaussian uncorrelated random function

$$\langle U(r) \rangle = 0 \quad \langle U(r)U(r') \rangle = U_0^2 \Delta(r - r')$$

where  $\Delta(r - r')$  is the Kronecker symbol. According to the Kubo formula [11] the diffusion coefficient in this case is

$$D(\omega) = [2\pi d\rho(E)N]^{-1} \sum_{r_1, r_2, r_3, r_4} v(r_1, r_4)v(r_2, r_3)\Phi_\omega(r_1, r_2 | r_3, r_4) \quad (10)$$

where  $v(r_1, r_2) = iJ \sum_\delta \delta \Delta(r_1 - r_2 - \delta)$  is the matrix element of the velocity operator,  $J$

is the hopping amplitude of the Anderson model,  $\delta$  is the nearest-neighbour vector and  $d$  is the dimensionality of the lattice.

Our starting point will be the expression for correlator (2) given by the simplest version of the perturbation theory, the so-called 'ladder' approximation [8, 9, 12]:

$$\Phi_\omega(k_1, k_2 | k_3, k_4) = M_\omega(k_1, k_2) [\Delta(k_1 - k_3) \Delta(k_2 - k_4) + (1/N) \Delta(k_1 - k_3 + k_2 - k_4) M_\omega(k_3, k_4) P^{-1}(q)] \quad (11)$$

where

$$P(q) = U_0^2 - \frac{1}{N} \sum_p M_\omega \left( p - \frac{q}{2}, p + \frac{q}{2} \right) \quad q = k_1 - k_4$$

$$M_\omega(k_1, k_2) = \langle \tilde{G}_{E+\omega/2+i0}(k_1) \rangle \langle \tilde{G}_{E-\omega/2-i0}(k_2) \rangle \quad (12)$$

$$\langle \tilde{G}_{E \pm i0}(k) \rangle = [E - \varepsilon(k) \pm i\Gamma_0/2]^{-1}$$

$$\varepsilon(k) = J(\gamma_0 - \gamma_k) \quad \gamma_k = \sum_\delta \exp(ik\delta) \quad \Gamma_0 = 2\pi U_0^2 \rho(E) \quad (13)$$

$$\rho(E) = (2\pi N)^{-1} \Gamma_0 \sum_k |\langle \tilde{G}_E(k) \rangle|^2.$$

In particular the function  $P(k)$  in (11) for small  $k$  is

$$P(k) = 2\pi\rho(E)\Gamma_0^{-2} [-i\omega + D_0(\gamma_0 - \gamma_k)/a^2] \quad (14)$$

where  $a$  is the lattice constant and

$$D_0 = \overline{v^2}/\Gamma_0 d \quad (15)$$

is the classical diffusion coefficient in which

$$\overline{v^2} = \left( \sum_k v^2(k) M_\omega(k, k) \right) \left( \sum_k M_\omega(k, k) \right)^{-1}$$

is the mean square of the electron velocity.

In view of (8), one may try to use expressions (11)–(15) with  $D_0$  replaced by  $D$  as the simplest form of the correlator. This expression, however, does not satisfy (3) and satisfies only sum rules (5a) but not (5b). Also, by inserting (11)–(15) into (10), we can find that the diffusion pole does not give the contribution to the resulting expression for the diffusion coefficient which will coincide in this case with the classical coefficient (15). The alternative approximation, based on the summing of so-called 'fan' (maximally crossed) diagrams gives for the correlator (2) the same expressions (11)–(14) in which  $q = k_1 - k_4 = k_2 - k_3$  is replaced by  $Q = k_1 + k_2 = k_3 + k_4$ . This expression, as (11)–(14), does not satisfy (3) and satisfies only (5b) but not (5a). However, this expression, if inserted into (10), gives the well known quantum correction for the diffusion coefficient  $D(\omega)$  [3, 4].

Thus neither of these two expressions is symmetric with respect to the change  $q \leftrightarrow Q$ , i.e. neither satisfies requirement (i) following from the time reflection symmetry of the problem. To satisfy this important requirement, it is natural to replace  $P^{-1}(q)$  in (11) by the following 'interpolating' expression:

$$T_\omega(k_1, k_2 | k_3, k_4) = P^{-1}(q) + P^{-1}(Q) + g_\omega(k_1, k_2 | k_3, k_4) \quad (16)$$

where the function  $g_\omega(k_1, k_2 | k_3, k_4)$  satisfies condition (i) and has no singularities for small  $\omega$ ,  $q$  and  $Q$ .

A particle interaction, a time-dependent random potential, a magnetic field, etc, break the discussed symmetry and, as a result, (16) cannot be used in these cases. The simplest way to take into account this 'symmetry breaking' is to replace  $\omega$  by  $\omega + i\Gamma$ , where  $\Gamma > 0$ . This replacement is implied by the Kramers-Kronig relation (according to which even and odd powers of  $\omega$  should have imaginary and real coefficients, respectively) and by the causality principle (according to which  $\Gamma > 0$ ). Also, analogous replacement was found for quasi-one-dimensional electrons interacting with a random potential and three-dimensional phonons (see [13, 14]) and is exact in any dimensionality if the time-dependent part of a random potential is independent of the coordinates and is  $\delta$  correlated.

Returning to the discussion of the form of the function  $g_\omega(k_1, k_2|k_3, k_4)$  of (16) we note first that even the simplest choice  $g \equiv \text{constant}$  allows us to satisfy the relation

$$\sum_{k,p} \Phi_\omega(p, k|k, p) = \sum_{k,p} \Phi_\omega(k, -k|-p, p) = \frac{2\pi\rho(E)}{\omega} \quad (17)$$

which is the consequence of (5). Further, inserting the respective expression into (10), we find, according to [15], that the resulting self-consistent equation for the full diffusion coefficient  $D$  has no physical solutions for  $d = 1, 2$ , and for  $d = 3$  the solution exists only if  $\Gamma_0$  in (12) is small enough.

Thus we should modify our *ansatz* (16) with the constant  $g$ . We note that the first two terms in (16) are responsible for the large-distance behaviour of the correlator (1) (diffusion spreading of the wave packet according to condition (iv)), while the function  $g$  is responsible for the small-distance behaviour of (1). We correct this behaviour in the simplest way, assuming that the correction is determined by the first coordination sphere and depends only on the 'essential' variables  $q$  and  $Q$ . Then, taking into account the cubic symmetry of our problem, we obtain

$$g_\omega = C(\gamma_q + \gamma_Q) + C_1. \quad (18)$$

Since in the small-disorder limit we should have the known weak-localization formulae for the quantum corrections [3, 4] we should assume that  $C \rightarrow 0$  when  $D \rightarrow D_0$ . The simplest form of  $C$  which guarantees this property is

$$C = C_2(1 - D/D_0). \quad (19)$$

Let us find the coefficients  $C_1$  and  $C_2$ . The first equation for them follows from (17)-(19):

$$\begin{aligned} C_1 + C_2 \left(1 - \frac{D}{D_0}\right) & \left( \sum_{p,k} M_\omega(p, k) M_\omega(k, p) (\gamma_0 + \gamma_{p+k}) \right) \left( \sum_k M_\omega(k, k) \right)^{-2} \\ & = \left( \sum_{p,k} M_\omega(p, k) M_\omega(k, p) P_\omega^{-1}(p+k) \right) \left( \sum_k M_\omega(k, k) \right)^{-2}. \end{aligned} \quad (20)$$

To derive the second equation, assume that  $D$  is small (i.e. that the energy lies either in the delocalized neighbourhood of the mobility edge  $E_c$ , where  $D \rightarrow 0$  as  $E \rightarrow E_c$  or in the localized region where, according to (9),  $D \rightarrow 0$  as  $\omega \rightarrow 0$ ). Then the left-hand side

of (10) has the singularity of the form  $1/D$  due to the second term of (16). We choose the coefficient  $C_2$  so that this singularity is absent:

$$C_2 = \left( \sum_k v^2(k) M_\omega^2(k, p) \sum_Q P_\omega^{-1}(Q) \right) \left( \sum_{p,k} v(p)v(k) \gamma_{p+k} M_\omega(p, k) M_\omega(k, p) \right). \quad (21)$$

We emphasize that we impose this requirement for all energies and frequencies and not only for  $E \rightarrow E_c$  or  $\omega \rightarrow 0$ , when  $D$  is small.

Thus, we have constructed the double correlator (2). It is given by formulae (11)–(13) in which  $P_\omega^{-1}(q)$  is replaced by (16), (18)–(21).

It is worth noting that our correlator satisfies one more important and natural requirement. Namely, define the density of localized states  $\rho_l(E)$  by the relation [1]

$$\rho_l(E) = \left\langle \sum_{\text{loc. st.}} \psi_n^2(0) \right\rangle \quad (22)$$

where  $\psi_n(r)$  are the exact localized eigenfunctions of the Anderson model. According to the widely accepted point of view, we assume that

- (a) localized and delocalized states cannot coexist in the same energy region and
- (b) in the neighbourhood of the mobility edge  $E_c$  the full density of states is strictly positive and continuous (has no jumps) [16].

Then, assuming for definiteness that the localized region corresponds to  $E < E_c$ , we get

$$\begin{aligned} \rho_l(E_c - 0) &= \rho_l(E_c) > 0 & \rho_l(E_c + 0) &= 0 \\ \rho_l(E_c - 0) - \rho_l(E_c + 0) &= \rho_l(E_c) > 0. \end{aligned} \quad (23)$$

Let us show that our correlator satisfies automatically relations (23). Indeed, we can rewrite (22) in the form [1]

$$i\pi\rho_l(E) = \lim_{\omega \rightarrow 0} \left( \sum_r \omega \langle G_{E+\omega/2+i0}(0, r) G_{E-\omega/2-i0}(r, 0) \rangle \right)$$

or after the Fourier transformation

$$i\pi\rho_l(E) = \lim_{p \rightarrow 0} \left[ \lim_{\omega \rightarrow 0} \left( \frac{\omega}{N^2} \sum_{k_1, k_2, k_3} \Phi_\omega(k_1, k_2 | k_2 + p, k_3) \right) \right].$$

Now, by using (11), (14), (16), (18) and (20), setting  $p = 0$ ,  $\omega = 0$  in the non-singular terms and taking into account equation (13) for the density of states, we find that

$$\rho_l(E) = \rho(E) \lim_{p \rightarrow 0} \left\{ \lim_{\omega \rightarrow 0} [i\omega / (i\omega + Dp^2)] \right\}.$$

Since, for  $E > E_c$ ,  $D$  may depend only on  $E$  but not on  $\omega$ , the last equation implies that  $\rho_l(E) = 0$  there. On the other hand, if  $E < E_c$ ,  $D$  is given by equation (9), which implies that  $\rho_l(E) = \rho(E)$  there. Thus, the rather non-trivial looking relations (23) are provided by a fairly simple mathematical mechanism.

Now we shall derive the self-consistent equation for the diffusion coefficient and analyse its solution. We insert the constructed correlator  $\Phi_\omega$  into the Kubo formula

(10). Since this correlator contains  $D$  explicitly (see (16) and (18)–(21)), we obtain after some calculations the self-consistent equation for  $D$ :

$$\eta = 1 - \frac{\theta}{N} \sum_Q (-i\omega + J^*(\gamma_Q - \gamma_0))^{-1} \quad (24)$$

where  $\eta = D/D_0$ ,  $J^* = D_0/a^2$ ,

$$\theta = \left( U_0^2 \sum_k v^2(k) M_\omega^2(k, k) \right) \left( D_0 d \sum_k M_\omega(k, k) \right)^{-1}.$$

The form of this equation is reminiscent of the equation for the ferromagnetic order parameter in the spherical model or in the approximation of Bogolyubov and Tyablikov [17], when the density of states of the spin waves is taken in the Rayleigh–Jeans form. In our case the roles of the order parameter, the external field and the temperature are played by  $\eta$ ,  $i\omega$  and  $\theta$ , respectively; the metal–insulator transition corresponds to the phase transition from the ferromagnetic (ordered) state to the paramagnetic state. An analogous equation appears in the theory of the ideal Bose gas. There  $1 - \eta$  corresponds to the density of the condensate and  $i\omega/\eta$  corresponds to the chemical potential. Both analogies, however, are somewhat formal, because the analogues of the external field and chemical potential are imaginary. However, if we introduce damping, i.e. make the change  $\omega \rightarrow \omega + i\Gamma$ , and set  $\omega = 0$  afterwards, the analogy will become more complete.

Equations (24) for  $\omega/J^* \ll 1$  takes a simpler form:

$$\eta = \varepsilon - [b_d/\sin(\pi d/2)] R^{2-d} \quad 2 < d \leq 4 \quad (25a)$$

$$\eta = 1 - (\theta/2\pi J^*) \ln(R/a) \quad d = 2 \quad (25b)$$

$$\eta = 1 - [b_d/\sin(\pi d/2)] R^{2-d} \quad 1 \leq d < 2 \quad (25c)$$

$$\varepsilon = 1 - W\theta/zJ^* \quad R = (i\eta D_0/\omega)^{-1/2} \quad b_d = \theta\pi^{1-d/2} a^{d-2}/J^* 2^d \Gamma(d/2).$$

$W$  is the Watson integral [18] and  $z$  is the coordination number. The quantity  $\varepsilon$  in (25a) can be considered as a measure of the proximity to the mobility edge and  $R$  has the meaning of the localization radius if  $E < E_c$  and of the characteristic diffusion path length of the particle during the period of the external field if  $E > E_c$  (after the above change  $\omega \rightarrow i\Gamma$ ).

The solutions (25b) and (25c), respectively, are as follows:

$$D = \pi\rho\gamma D_0 [-i\omega \exp(1/\lambda) + \pi\rho\omega^2 \exp(2/\lambda)] \quad \lambda = a^2 U_0^2/\pi v^2 \quad d = 2$$

$$D = 4D_0 [-i\omega\tau + 8(\omega\tau)^2] \quad \tau = \Gamma^{-1} \quad d = 1.$$

These expressions coincide with the results [6], if the quadratic dispersion law is used.

Equation (25a) for  $d > 2$  is invariant with respect to the change of scales

$$\omega \rightarrow \omega L^{-d} \quad \varepsilon \rightarrow \varepsilon L^{2-d} \quad \eta \rightarrow \eta L^{2-d} \quad R \rightarrow RL. \quad (26)$$

Thus, according to (25a), the critical indices  $s$  and  $\nu$ , defined by the relations  $D \sim \varepsilon^s$ ,  $R \sim \varepsilon^{-\nu}$ , are equal (for  $2 < d \leq 4$ ) to units and  $1/(d-2)$ , respectively, and coincide with those found in [19, 20].

The quantity  $g = \eta R^{d-2}$  which is invariant with respect to the transformation (26) satisfies the equation

$$d(\ln g)/d(\ln R) = (d-2)[1 + \{b_d/[g \sin(\pi d/2)]\}].$$

A similar equation, i.e. a similar form of the Gell–Mann function, was found in [21] for



the conductance of the sample in the case of weak disorder. However, the argument of the respective equation in [21] is the sample size  $L$  and not the 'correlation' length  $R$ .

We note in conclusion that equation (25a) for  $d = 3$  can be written in the form

$$\psi^3 - \varepsilon\psi - h = 0 \quad (27)$$

where  $\psi^2 = \eta$  and  $h = (\theta/4\pi J^*)(-i\omega/J^*)^{1/2}$ . This equation is similar to that for the order parameter in the phenomenological theory of phase transitions. The quantity  $h$  is the analogue of the external field and  $\varepsilon$  is the analogue of  $T - T_c$ . Also the diffusion coefficient is related to the 'order parameter'  $\psi$  in the same way as the superfluid (or superconductor) density. The localized and delocalized phases correspond to the normal and superfluid (or superconductor) phases, respectively.

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