

## Self-Consistent Theory of Localization for the Anderson Model

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The self-consistent theory of electron localization in a random system in the form proposed by Vollhardt and Wölfle is generalized for the analysis of localization in the Anderson model. We derive the general equations appropriate for the system with rather general form of the electronic spectrum. Explicit calculations are restricted to the lattices of cubic symmetry and use the effective mass approximation to obtain the final results. Anderson's critical ratio for the localization of all the electronic states in the tight-binding band is evaluated and found to be in surprisingly good agreement with the results of numerical analysis of localization in the Anderson model.

### 1. Introduction

The phenomenon of electron localization in disordered systems, which is actively studied in recent years [1], usually is described within the framework of the well-known Anderson model [2, 3]. In most of the papers published up to now, either quite non-traditional methods, originating from the classic paper by Anderson [2], or numerical analysis were used. But the few attempts to derive localization via more or less standard formalism of the modern many-particle theory, involving the averaged Green functions, were mostly unsuccessful. Because of this situation we believe, that the development of the so-called self-consistent theory of localization, in the form proposed by Vollhardt and Wölfle [4], deserves a great attention. This approach allows to get rather reasonable description of localization of electronic states in a two-dimensional system ( $d=2$ ), and also at least qualitatively describes the Anderson transition for  $d>2$  [5, 6], in close correspondence with the scaling picture of this transition, proposed in the famous paper by Abrahams, Anderson, Licciardello and Ramakrishnan [7]. In papers [4-6] the model of electrons scattered by the randomly distributed point-like scatterers was considered. Thus, due to the existence of rather large number of

references, devoted to the study of localization in the Anderson model (cf. the reviews [1, 8]), it seems to be interesting to generalize the self-consistent theory for the description of localization in this model. The first attempt of this kind was undertaken by Prelovšek [9], in the framework of self-consistent approach proposed by Götze [10]. In this paper we shall concentrate on the study of localization in the Anderson model within the theory of Vollhardt and Wölfle [4].

### 2. General Equations

The Hamiltonian of the Anderson model in a regular lattice has the form:

$$H = \sum_j E_j a_j^+ a_j + \sum_{ij} V_{ij} a_i^+ a_j \quad (1)$$

where  $a_j$  and  $a_j^+$  are the usual destruction and creation operators of the electron at a site  $j$ . The energy levels  $E_j$  are considered to be independently distributed on different sites of the lattice. The distribution at the given site is usually defined as [2]:

$$P(E_j) = \begin{cases} \frac{1}{W}; & |E_j| < \frac{1}{2}W \\ 0; & |E_j| > \frac{1}{2}W \end{cases} \quad (2)$$

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corresponding to the homogeneous distribution of energies in the energy interval of the width  $W$ . But in the main part of this work we shall assume the Gaussian distribution

$$P(E_j) = \frac{1}{\sqrt{2\pi} \tilde{W}} \exp\left\{-\frac{E_j^2}{2\tilde{W}^2}\right\} \quad (3)$$

which considerably simplifies the corresponding diagram technique. The transfer integral  $V_{ij}$  is assumed to be different from zero and equal to a constant  $V$  only for the transitions between the sites which are nearest neighbours in the lattice.

After the Fourier transformation (1) can be written as:

$$H = \sum_{\mathbf{p}} \varepsilon(\mathbf{p}) a_{\mathbf{p}}^+ a_{\mathbf{p}} + \sum_{\mathbf{p}\mathbf{q}} U_{\mathbf{q}} a_{\mathbf{p}+\mathbf{q}}^+ a_{\mathbf{p}} \quad (4)$$

where

$$\varepsilon(\mathbf{p}) = V \sum_{\mathbf{h}} e^{i\mathbf{p}\mathbf{h}} \quad (5)$$

is the standard electronic spectrum in a tight-binding approximation [11], and the vector  $\mathbf{h}_{ij} = \mathbf{R}_i - \mathbf{R}_j$  defines the positions of the neighboring sites in the lattice (the summation in (5) is assumed over the nearest neighbours). The Gaussian random field  $U_{\mathbf{q}}$ , entering the second term in (4) ( $N$  - is the number of sites in lattice):

$$U_{\mathbf{q}} = \frac{1}{N} \sum_j E_j e^{i\mathbf{q}\mathbf{R}_j} \quad (6)$$

has in the momentum space the correlation function of the following form:

$$\langle U_{\mathbf{q}} U_{\mathbf{q}'} \rangle = \frac{\tilde{W}^2}{N} \delta_{\mathbf{q}, -\mathbf{q}'} = \tilde{W}^2 \Omega_0 \delta_{\mathbf{q}, -\mathbf{q}'} \quad (7)$$

corresponding to the assumed form of correlation of energy levels  $E_j$  in the lattice:

$$\langle E_i E_j \rangle = \tilde{W}^2 \delta_{ij}. \quad (8)$$

In (7)  $\Omega_0$  is just the volume per single site of the lattice. In the following we are considering the lattices of cubic symmetry and put the total volume of the system equal to unity, which gives  $1/N = \Omega_0$  (the volume of primitive cell of the crystal). The higher-order correlation functions in case of the Gaussian random field are factorizable in terms of the pair correlators (7), (8), so that the form of diagram technique for the calculation of the averaged Green functions, corresponding to the Hamiltonian (4), is quite obvious [12].

The derivation of the main equations of the self-consistent theory follows the main steps of [4]. The

only complication is connected with the necessity to take rather general form of the electronic spectrum (5) into account. The formalism is based upon the Bethe-Salpeter equation for the averaged two-particle Green function  $\phi_{\mathbf{p}\mathbf{p}'}^{RA}(E\omega\mathbf{q})$ , which is used to define the function

$$\begin{aligned} \phi_E(\omega\mathbf{q}) &\equiv \sum_{\mathbf{p}\mathbf{p}'} \phi_{\mathbf{p}\mathbf{p}'}^{RA}(E\omega\mathbf{q}) \\ &= -\frac{1}{2\pi i} \sum_{\mathbf{p}\mathbf{p}'} \langle G^R(\mathbf{p} + \mathbf{p}' + E + \omega) G^A(\mathbf{p}' - \mathbf{p} - E) \rangle \\ \mathbf{p}_{\pm} &= \mathbf{p} \pm \frac{1}{2}\mathbf{q}. \end{aligned} \quad (9)$$

The Bethe-Salpeter equation takes the form (for small  $q$ )

$$\begin{aligned} \{\omega - \mathbf{q} \cdot \mathbf{v}_{\mathbf{p}} - \Sigma_{\mathbf{p}_{+}}^R(E + \omega) + \Sigma_{\mathbf{p}_{-}}^A(E)\} \phi_{\mathbf{p}\mathbf{p}'}^{RA}(E\omega\mathbf{q}) \\ = \Delta G_{\mathbf{p}} \left\{ \frac{1}{2\pi i} \delta_{\mathbf{p}\mathbf{p}'} - \sum_{\mathbf{p}''} U_{\mathbf{p}\mathbf{p}''}^E(\mathbf{q}\omega) \phi_{\mathbf{p}''\mathbf{p}'}^{RA}(E\omega\mathbf{q}) \right\} \end{aligned} \quad (10)$$

where  $\mathbf{v}_{\mathbf{p}} = \partial\varepsilon(\mathbf{p})/\partial\mathbf{p}$  is the group velocity of the electron, and

$$\Delta G_{\mathbf{p}} \equiv G^R(E + \omega, \mathbf{p}_{+}) - G^A(E, \mathbf{p}_{-}) \quad (11)$$

while the averaged one-electron Green functions are taken in the standard form:

$$G^{R,A}(E\mathbf{p}) = \frac{1}{E - \varepsilon(\mathbf{p}) - \Sigma_{\mathbf{p}}^{R,A}(E)} \approx \frac{1}{E - \varepsilon(\mathbf{p}) \pm i\gamma(E)} \quad (12)$$

where the last expression in (12) is obtained through the ordinary summation of simplest diagrams [12] (without intersecting interaction lines) and

$$\gamma(E) = \pi \tilde{W}^2 \Omega_0 N(E) \quad (13)$$

is just the scattering rate of the electron on the random levels and  $N(E)$  - is the one-electron density of states. In Eq. (10)  $U_{\mathbf{p}\mathbf{p}'}^E(\mathbf{q}\omega)$  is the irreducible (in two-particle  $R-A$  channel) vertex.

Summing both sides of (10) over  $\mathbf{p}$  and  $\mathbf{p}'$  and using the Ward identity derived in [4], we get the equation for  $\phi_E(\omega\mathbf{q})$ :

$$\omega \phi_E(\omega\mathbf{q}) - q \phi_j^E(\omega\mathbf{q}) = -N(E) \quad (14)$$

where we have introduced the function:

$$\phi_j^E(\omega\mathbf{q}) = \sum_{\mathbf{p}\mathbf{p}'} (\mathbf{v}_{\mathbf{p}} \cdot \hat{\mathbf{q}}) \phi_{\mathbf{p}\mathbf{p}'}^{RA}(E\omega\mathbf{q}) \quad (15)$$

where  $\hat{\mathbf{q}}$  is the unit vector in the direction of  $\mathbf{q}$ . To obtain the equation for  $\phi_j^E(\omega\mathbf{q})$  we multiply (10) by  $\mathbf{v}_{\mathbf{p}} \cdot \hat{\mathbf{q}}$  and sum again over  $\mathbf{p}$  and  $\mathbf{p}'$ . Then to "close up" the system of equations in terms of the functions  $\phi_E(\omega\mathbf{q})$  and  $\phi_j^E(\omega\mathbf{q})$  we use the following approxi-



mate relation:\*

$$\sum_{\mathbf{p}'} \phi_{\mathbf{p}\mathbf{p}'}^{RA}(E\omega\mathbf{q}) \simeq -[2\pi iN(E)]^{-1} \Delta G_{\mathbf{p}} \cdot \sum_{\mathbf{p}'} \left\{ 1 + \frac{(\mathbf{v}_{\mathbf{p}} \cdot \hat{\mathbf{q}})(\mathbf{v}_{\mathbf{p}'} \cdot \hat{\mathbf{q}})}{v_E^2(\hat{\mathbf{q}})} \right\} \phi_{\mathbf{p}'\mathbf{p}}^{RA}(E\omega\mathbf{q}) \quad (16)$$

where

$$v_E^2(\hat{\mathbf{q}}) = -\frac{1}{2\pi iN(E)} \sum_{\mathbf{p}} (\mathbf{v}_{\mathbf{p}} \cdot \hat{\mathbf{q}})^2 \Delta G_{\mathbf{p}} \quad (17)$$

is just the "averaged in the vicinity of the isoenergetic surface  $\varepsilon(\mathbf{p})=E$ " square of the projection of the velocity  $\mathbf{v}_{\mathbf{p}}$  on the direction of  $\hat{\mathbf{q}}$ . In the lattices of cubic symmetry (which are the only lattices considered below), due to the isotropy of their physical properties we have:

$$v_E^2(\hat{\mathbf{q}}) \equiv \frac{1}{d} v_E^2 = -\frac{1}{2\pi iN(E)d} \sum_{\mathbf{p}} v_{\mathbf{p}}^2 \Delta G_{\mathbf{p}} \approx \frac{1}{N(E)d} \sum_{\mathbf{p}} v_{\mathbf{p}}^2 \delta(E - \varepsilon(\mathbf{p})) \quad (18)$$

where the last equality is approximately valid in the limit of small disorder.

Then for  $\phi_j^E(\omega\mathbf{q})$  we get the following equation:

$$\{\omega + M_E(\mathbf{q}\omega)\} \phi_j^E(\omega\mathbf{q}) - \frac{1}{d} v_E^2 q^2 \phi_E(\omega\mathbf{q}) = 0 \quad (19)$$

where the so called "relaxation kernel"  $M_E(\mathbf{q}\omega)$  takes the form:

$$M_E(\mathbf{q}\omega) = \frac{1}{2\pi iN(E)v_E^2} \sum_{\mathbf{p}} v_{\mathbf{p}}^2 \Delta G_{\mathbf{p}} \cdot [\Sigma_{\mathbf{p}_+}^R(E+\omega) - \Sigma_{\mathbf{p}_-}^A(E)] - \frac{d}{2\pi iN(E)v_E^2} \sum_{\mathbf{p}\mathbf{p}'} (\mathbf{v}_{\mathbf{p}} \cdot \hat{\mathbf{q}}) \Delta G_{\mathbf{p}} U_{\mathbf{p}\mathbf{p}'}^E(\mathbf{q}\omega) \Delta G_{\mathbf{p}'}(\mathbf{v}_{\mathbf{p}'} \cdot \hat{\mathbf{q}}) \approx 2i\gamma(E) - \frac{d}{2\pi iN(E)v_E^2} \sum_{\mathbf{p}\mathbf{p}'} (\mathbf{v}_{\mathbf{p}} \cdot \hat{\mathbf{q}}) \Delta G_{\mathbf{p}} U_{\mathbf{p}\mathbf{p}'}^E(\mathbf{q}\omega) \cdot \Delta G_{\mathbf{p}'}(\mathbf{v}_{\mathbf{p}'} \cdot \hat{\mathbf{q}}) \quad (20)$$

where the last equality is valid in the limit of small  $\mathbf{q}$  and  $\omega$ , taking (12) into account.

Solving the system of (14) and (19) we obtain:

$$\phi_E(\omega\mathbf{q}) = -N(E) \frac{\omega + M_E(\mathbf{q}\omega)}{\omega^2 + \omega M_E(\mathbf{q}\omega) - \frac{1}{d} v_E^2 q^2} \quad (21)$$

so that the corresponding density-density response function (cf. Ref. 4) is given by:

\* This relation is the natural generalization of (25) in [4] for the case of electrons with the arbitrary spectrum  $\varepsilon(\mathbf{p})$

$$\chi_E(\mathbf{q}\omega) = \omega \phi_E(\omega\mathbf{q}) + N(E) = -\frac{\frac{1}{d} N(E) v_E^2 q^2}{\omega^2 + \omega M_E(\mathbf{q}\omega) - \frac{1}{d} v_E^2 q^2}. \quad (22)$$

Neglecting the  $\omega^2$  term in the denominator of (22) we can rewrite  $\chi_E(\mathbf{q}\omega)$  in the form:

$$\chi_E(\mathbf{q}\omega) = N(E) \frac{iD_E(\mathbf{q}\omega) q^2}{\omega + iD_E(\mathbf{q}\omega) q^2} \quad (23)$$

where we have introduced the generalized diffusion coefficient:

$$D_E(\mathbf{q}\omega) = \frac{i}{d} \frac{v_E^2}{M_E(\mathbf{q}\omega)}. \quad (24)$$

The electrical conductivity is given by (cf. Ref. 4):

$$\sigma_E(\omega) = e^2 \lim_{q \rightarrow 0} \left( -\frac{i\omega}{q^2} \right) \chi_E(\mathbf{q}\omega) = \frac{e^2}{d} N(E) v_E^2 \frac{i}{\omega + M_E(0\omega)}. \quad (25)$$

The localization is signalled by the appearance (in the corresponding energy range) of the finite limit for the following expression [3, 6, 13]:

$$A_E(\mathbf{q}) = \frac{1}{2\pi N(E)} \lim_{\delta \rightarrow 0} \sum_{\mathbf{p}\mathbf{p}'} \langle G^R(\mathbf{p}_+, \mathbf{p}'_+, E + i\delta) G^A(\mathbf{p}'_-, \mathbf{p}_-, E - i\delta) \rangle = -\frac{1}{N(E)} \lim_{\omega \rightarrow 0} \omega \phi_E(\omega\mathbf{q}) = \lim_{\omega \rightarrow 0} \left\{ 1 - \frac{v_E^2 q^2}{d M_E(\mathbf{q}\omega) \omega} \right\}^{-1}. \quad (26)$$

For  $q \rightarrow 0$  we have [14]:

$$A_E(\mathbf{q}) \approx 1 - q^2 R_{\text{loc}}^2(E) \quad (27)$$

where the localization length is defined by:

$$R_{\text{loc}}^2(E) = \frac{v_E^2}{d\omega_0^2(E)}; \quad \omega_0^2(E) = -\lim_{\omega \rightarrow 0} \omega M_E(0\omega) > 0. \quad (28)$$

It can be seen, that in this formalism the localization phenomenon is connected to the divergence of the "relaxation kernel"  $M_E(0\omega)$  for  $\omega \rightarrow 0$ , which leads to the appearance of the non-zero limit for  $\omega_0^2 > 0$  in (28).

In the self-consistent theory of Vollhardt and Wölfle the irreducible kernel  $U_{\mathbf{p}\mathbf{p}'}^E(q\omega)$  is taken as a sum of the so called Langer-Neal (or maximally crossed) diagrams [15], which for the model under consid-

ration reduces to:

$$U_{\mathbf{p}\mathbf{p}'}^E(\mathbf{q}\omega) \simeq \frac{2\gamma(E)\tilde{W}^2\Omega_0}{-i\omega + D_0^E(\mathbf{p} + \mathbf{p}')^2} \quad (29)$$

where  $D_0^E = \frac{1}{d} \frac{v_E^2}{2\gamma(E)}$  is the classical diffusion coefficient, and we assume that  $|\mathbf{p} + \mathbf{p}'|$  is small with respect to the characteristic sizes of the Fermi surface. The main idea of the self-consistent approach of the Ref. 4 was the substitution of  $D_0^E$  in (29) by the "renormalized" diffusion coefficient defined according to (24). Then Eq. (20) defines the self-consistent equation for  $M_E(0\omega)$ , which after some transformations can be written as:

$$M_E(0\omega) = \frac{i}{\tau} - 2\tilde{W}^2\Omega_0\theta_E \sum_{\mathbf{k}} \frac{1}{\omega - k^2 D_0^E/M_E(0\omega)\tau} \quad (30)$$

where

$$\theta_E = \frac{2\tilde{W}^2\Omega_0}{v_E^2} \sum_{\mathbf{p}} v_{\mathbf{p}}^2 [\text{Im} G_{\mathbf{p}}(E)]^2 \quad (31)$$

and we have denoted  $2\gamma(E) = 1/\tau$ . Equation (30) generalizes (42) of [4] for the case of general electronic spectrum  $\varepsilon(\mathbf{p})$  in the lattices of cubic symmetry. It is not difficult to write the similar expressions for the lattices of some general symmetry, when the dependence on the direction of the vector  $\mathbf{q}$  appears explicitly (cf. (16), (17)).

For  $\omega = 0$  we get from (25) and (30):

$$\begin{aligned} \sigma_E(0) &= \frac{e^2}{d} N(E) v_E^2 \frac{i}{M_E(00)} \\ &= \frac{e^2}{d} N(E) v_E^2 \tau \left\{ 1 - \frac{2d\tilde{W}^2\Omega_0}{v_E^2} \theta_E \sum_{\mathbf{k}} \frac{1}{k^2} \right\} \end{aligned} \quad (32)$$

defining mobility edge by the relation  $\sigma_{E_c}(0) = 0$  we get the equation determining its position  $E_c$ :

$$1 = \frac{2d\tilde{W}^2\Omega_0}{v_{E_c}^2} \theta_{E_c} \sum_{\mathbf{k}} \frac{1}{k^2}. \quad (33)$$

In the energy range corresponding to localized states we have [4, 6]:  $\lim_{\omega \rightarrow 0} \omega \text{Im} M_E(0\omega) = 0$ ,  $\text{Re} M_E(0\omega) = -\omega_0^2(E)/\omega$ , so that from (28) and (30) we can easily find the following equation for  $\omega_0^2(E)$ :

$$1 = 2\tilde{W}^2\Omega_0\theta_E \sum_{\mathbf{k}} \frac{1}{\omega_0^2(E) + \frac{1}{d} v_E^2 k^2}. \quad (34)$$

For  $\omega_0^2(E = E_c) = 0$  it obviously reduces to (33). Remembering that the expression (29) is valid for rather small values of  $|\mathbf{p} + \mathbf{p}'|$ , we see that the sum-

mation over  $\mathbf{k}$  in (30), (32)–(34) should be restricted to the values of  $\mathbf{k}$  lying inside of some isoenergetic surface in the momentum space with the characteristic dimensions of the order of "doubled" Fermi surface. In fact it follows automatically from (20), because of two factors of  $\Delta G_{\mathbf{p}}$  and  $\Delta G_{\mathbf{p}'}$  under the sum over  $\mathbf{p}$  and  $\mathbf{p}'$  in it, because these factors are rather sharply peaked in the vicinity of the Fermi surface.

### 3. The Effective Mass Approximation

The above relations are rather general and are valid for the arbitrary electronic spectrum  $\varepsilon(\mathbf{p})$ , with the only limitation to the lattices of cubic symmetry, which allows not to deal with the anisotropy of physical properties. The actual calculations will be performed with the use of the effective mass approximation, which allows to evaluate all the integrals in momentum space by elementary means. Near the "left" band-edge we have from (5):

$$\varepsilon(\mathbf{p}) \approx -ZV + \frac{\mathbf{p}^2}{2m^*} \quad (35)$$

where  $Z$  is the number of nearest neighbours, and the effective mass can be easily evaluated from the known expressions [11] for the electronic tight-binding spectra to be  $m^* = 1/2 Va^2$  for SC, BCC and FCC lattices ( $a$  – is the lattice constant). Using (35) it is shown by direct calculation that  $\theta_E$  defined in (31) is equal to unity in this approximation. We choose the upper cut-off for the momentum space integration in (30), (32)–(34) equal to  $k_0 = x_0 p_F$ , where  $p_F = \sqrt{2m^* \varepsilon}$  ( $\varepsilon = E + ZV$  is the energy distance from the band edge) is the Fermi momentum,  $x_0 \approx 1 \div 2$  (cf. the discussion of the cut-off in Ref. 6). Then, evaluating the integral in (32) for the  $d$ -dimensional space we obtain:

$$\begin{aligned} \sigma_E(0) &= \frac{e^2}{d} N(\varepsilon) v_F^2 \tau \left\{ 1 - \frac{d}{d-2} \lambda x_0^{d-2} \right\} \\ &= \frac{e^2}{2\pi d} \frac{v_F^2}{\tilde{W}^2\Omega_0} \left\{ 1 - \frac{d}{d-2} \lambda x_0^{d-2} \right\}; \quad 2 < d < 4 \end{aligned}$$

where

$$\lambda = \frac{1}{2\pi \varepsilon \tau} = \left( \frac{m^*}{2\pi} \right)^{d/2} \frac{\tilde{W}^2\Omega_0}{\Gamma(d/2)} \varepsilon^{\frac{d-4}{2}} \quad (37)$$

is the dimensionless "coupling constant" of this theory [6],  $v_F = p_F/m^*$ .

Similarly from (33) we get:

$$\left( \frac{\tilde{W}}{V} \right)^2 = \frac{d-2}{d} \Gamma\left(\frac{d}{2}\right) \left( \frac{m^*}{2\pi} \right)^{-\frac{d}{2}} \frac{x_0^{2-d}}{V^2\Omega_0} \varepsilon^{\frac{4-d}{2}}. \quad (38)$$



For the fixed disorder  $W/V$  this equation defines  $\varepsilon = \varepsilon_c$  – the position of the mobility edge inside the band. For the fixed  $\varepsilon$  (Fermi energy!) (38) defines the critical ratio  $(W/V)_c$ , sufficient to localize all the electronic states on the Fermi surface. For the half-filled band  $\varepsilon = ZV$  (i.e.  $E=0$ , corresponding to the standard problem of the localization of the whole band in the Anderson model [2, 3]), and we get:

$$\left(\frac{\tilde{W}}{V}\right)_c^2 = \frac{d-2}{d} \Gamma\left(\frac{d}{2}\right) \left(\frac{m^*V}{2\pi}\right)^{-2} \frac{x_0^{2-d}}{\Omega_0} Z^{\frac{4-d}{2}}. \quad (39)$$

For  $\tilde{W}/V < (\tilde{W}/V)_c$  we obtain the following expression for the mobility edge

$$\varepsilon_c = \left\{ \frac{d}{d-2} \frac{x_0^{d-2}}{\Gamma(d/2)} (2\pi)^{-\frac{d}{2}} \right\}^{\frac{2}{4-d}} E_{sc} \quad (40)$$

where

$$E_{sc} = (m^*)^{\frac{d}{4-d}} (\Omega_0)^{\frac{2}{4-d}} V^{\frac{4}{4-d}} \left(\frac{\tilde{W}}{V}\right)^{\frac{4}{4-d}} \sim V \left(\frac{\tilde{W}}{V}\right)^{\frac{4}{4-d}} \quad (41)$$

is the energy defining the strong-coupling region [1, 6, 13] for the problem under consideration. When the Fermi energy lowers in the band below this energy, we get  $\lambda \sim 1$ , and the perturbation theory clearly breaks down.

While comparing our result with the literature on the Anderson model it should be taken into account, that our parameter  $\tilde{W}^2$  is just the dispersion of the Gaussian distribution (3). For the homogeneous law (2) dispersion is equal to  $W^2/12$ . Thus, for the ‘‘Anderson’s critical ratio’’ we obtain\*:  $(W/V)_c^2 = 12(\tilde{W}/V)_c^2$ . In Table I we give the numerical values of the critical disorder for the localization of the whole band calculated from (39) for the different three-dimensional cubic lattices, for two different values of the dimensionless cut-off. Despite the obvious crudeness of the theory we get the amazingly good correspondence of these values with the results of numerical calculation for the SC lattice:  $(W/V)_c \approx 15$  [16],  $(W/V)_c = 19 \pm 0.5$  [17],  $(W/V)_c = 16 \pm 0.5$  [18], for the ‘‘Anderson’s type of disorder’’, and also with the results of the most accurate analysis of localization within the Anderson approach given by Licciardello and Economou:  $(W/V)_c \approx 14.5$  [19]. Also quite reasonable is the agreement with the only known to us result of numerical analysis of

\* It is certain, that such a procedure gives only the approximate description of the Anderson’s type of disorder (2), because we actually neglect all the perturbation theory diagrams connected with the higher-order cumulants of the random field  $E_j$ , which are clearly not equal to zero for the distribution law (2)

**Table I.** Critical disorder, corresponding to the localization of the whole band for the Gaussian distribution of energy levels  $(\tilde{W}/V)_c$  and for the Anderson’s type of distribution of levels  $(W/V)_c$ , for the lattices of cubic symmetry

Lattice	$Z$	$\Omega_0$	$(\tilde{W}/V)_c$		$(W/V)_c$	
			$x_0=1$	$x_0=2$	$x_0=1$	$x_0=2$
SC	6	$a^3$	5.67	4.01	19.67	13.91
BCC	8	$a^3/2$	8.63	6.10	29.88	21.13
FCC	12	$a^3/4$	13.50	9.55	46.78	33.08

the Gaussian disorder:  $(\tilde{W}/V)_c \approx 7$  [20]. We are not aware of any numerical calculations for the BCC and FCC lattices.

In the following we quote only the results for the  $d$ -dimensional hypercubic lattices. In particular, for the static conductivity in the half-filled band case we get from (36) ( $2 < d < 4$ ):

$$\sigma = \sigma_{mm} \frac{|(\tilde{W}/V) - (\tilde{W}/V)_c|}{(\tilde{W}/V)_c}, \quad \left(\frac{\tilde{W}}{V}\right)^2 \lesssim \left(\frac{W}{V}\right)_c^2 = \frac{d-2}{d} \Gamma\left(\frac{d}{2}\right) \frac{x_0^{2-d}}{2^{\frac{d}{2}}} Z^{\frac{4-d}{2}} (8\pi)^{d/2} \quad (42)$$

where we have introduced:

$$\sigma_{mm} = \frac{4Z}{\pi d} \frac{e^2}{a^{d-2}} \left(\frac{V}{\tilde{W}}\right)_c^2 \quad (43)$$

which practically coincides with the Mott’s ‘‘minimal metallic conductivity’’ [20]. For  $d=3$  and the Anderson’s type of disorder we get:

$$\sigma_{mm} \approx 0.013 \frac{e^2}{\hbar a} \approx 10^2 \Omega^{-1} \text{ cm}^{-1} \quad \text{for } a \approx 3 A^0.$$

It is curious to note that for  $d \rightarrow 2$   $\sigma_{mm} \sim \frac{e^2}{a^{d-2}} \frac{1}{d-2} \rightarrow \infty$ , because of  $(W/V)_c \rightarrow 0$  (39), which reflects the crossover to the complete localization of the band by the infinitesimal disorder in the two-dimensional system [1, 4-7].

Similarly, for the vicinity of some mobility edge inside the band we obtain:

$$\sigma = \sigma_0 \frac{4-d}{2} \left(\frac{\varepsilon - \varepsilon_c}{\varepsilon_c}\right); \quad \varepsilon \gtrsim \varepsilon_c \quad (44)$$

where

$$\sigma_0 = \frac{e^2 v_F^2}{d} N(\varepsilon) \tau = \frac{n e^2}{m^*} \tau \quad (45)$$

is the ordinary Drude-like conductivity of a metal ( $n$  – is the total electron density). This result coincides with that obtained in Ref. 6.

Let us now consider the results, following from (34), limiting ourselves only to the case of the half-filled band and  $(\tilde{W}/V) \gtrsim (\tilde{W}/V)_c$ , which corresponds to the



localized phase\*. In dimensionless variables this equation takes the form (use also (35)):

$$1 = d\lambda x_0^{d-2} \int_0^1 dy \frac{y^{d-1}}{y^2 + Z^2}; \quad Z_E^2 = \frac{d\omega_0^2(E)}{2m^* \varepsilon v_F^2 x_0^2}. \quad (46)$$

All the calculations are similar to that done in Ref. 6, so that using  $\varepsilon = ZV$ ,  $m^* = (2Va^2)^{-1}$  and  $v_F^2 = 4ZVa^2$ , we obtain: ( $2 < d < 4$ )

$$\begin{aligned} \omega_0^2(\varepsilon = ZV) &= \frac{4}{d} \left\{ \frac{d}{d-2} \Gamma\left(\frac{d}{2}\right) \Gamma\left(2 - \frac{d}{2}\right) \right\}^{-\frac{2}{d-2}} Z^2 V^2 x_0^2 \\ &\cdot \left\{ 1 - \frac{(\tilde{W}/V)_c^2}{(\tilde{W}/V)^2} \right\}^{\frac{2}{d-2}} \\ &\approx \frac{4}{d} \left\{ \frac{d}{d-2} \Gamma\left(\frac{d}{2}\right) \Gamma\left(2 - \frac{d}{2}\right) \right\}^{-\frac{2}{d-2}} \\ &\cdot Z^2 V^2 x_0^2 \left\{ 2 \frac{(\tilde{W}/V) - (\tilde{W}/V)_c}{(\tilde{W}/V)_c} \right\}^{\frac{2}{d-2}}. \end{aligned} \quad (47)$$

From (28) and (47) we get the following expression for the localization length in the center of the band:

$$R_{\text{loc}}(\varepsilon = ZV) \approx a \left\{ 2 \frac{(\tilde{W}/V) - (\tilde{W}/V)_c}{(\tilde{W}/V)_c} \right\}^{-\frac{1}{d-2}} \quad (48)$$

so that the critical exponent for the localization length in the self-consistent theory is:

$$\nu = \frac{1}{d-2} \quad (49)$$

also for the Anderson transition in the center of the band (Cf. Refs. 5, 6). From (49) and (42) it is seen that Wegner's scaling law  $s = (d-2)\nu$  for the conductivity exponent is also satisfied.

Thus, the critical behaviour at the mobility edge in the self-consistent approach to the Anderson model is the same, as in the model of free electrons, scattered by the random impurities [6]. Also valid are all the remarks concerning the inapplicability of perturbation theory in the vicinity of the mobility edge made in Ref. 6. Thus, the results obtained may give at best only the qualitative description of the Anderson transition (this is especially so for the critical exponents).

Finally, let us briefly analyze the two-dimensional case, when there is a total localization of the band, even for small disorder [1, 4-7]. Dealing again only with the localization in the middle of the band ( $\varepsilon = ZV$ ) and solving the (46), we find:

\* For  $\varepsilon \geq \varepsilon_c$ , i.e. in the vicinity of some mobility edge inside the band (34) essentially gives the same results, as obtained in [6], because of effective mass approximation (35)

$$\omega_0^2(\varepsilon = ZV) = 2Z^2 V^2 x_0^2 \exp \left\{ -2Z \left( \frac{V}{\tilde{W}} \right)^2 \right\} \quad (50)$$

so that for the localization length in the center of the band of a square ( $Z=4$ ) lattice we get:

$$\begin{aligned} R_{\text{loc}}(\varepsilon = ZV) &= aV\sqrt{2Z} \omega_0^{-1}(\varepsilon = ZV) \\ &= \frac{a}{2x_0} \exp \left\{ 4 \left( \frac{V}{\tilde{W}} \right)^2 \right\}. \end{aligned} \quad (51)$$

De-Broglie wave length for the electron in this case is  $\sim a/2$  and from (51) it is clearly seen, that  $R_{\text{loc}}$  grows exponentially, starting with the value of  $a/2$  with  $\tilde{W}/V$  diminishing from  $(\tilde{W}/V)_c^2 = 4/\ln x_0$ , which gives  $(\tilde{W}/V)_c \simeq 2.40$  for  $x_0 = 2$ . Note, that the value of  $(\tilde{W}/V)_c$  defined in this way is rather sensitive to the change of  $x_0$  in the interval  $1 \leq x_0 \leq 2$ . It is probable, that such a behaviour "explains" the results of most numerical calculations, giving for  $d=2$  the finite value of Anderson's critical ratio  $(W/V)_c \simeq 6$  [16, 22-24] for the square Anderson lattice (Cf. the similar behaviour of the frequency dependent conductivity, discussed in [6], and giving a kind of a "quasitransition" at a finite "mobility edge").

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## Appendix

The above discussion is slightly imprecise. The reason for this is that the parameter  $E$  in the second equality in (12) is, in fact, a "renormalized" energy, which includes  $\text{Re} \Sigma^{R,A}(E)$ , defined in the simplest approximation, taking into account the diagrams with no intersecting interaction lines [12]. This leads to the shift of the band edge, due to the interaction with random field. We have:

$$\Sigma^{R,A}(E_0) = \tilde{W}^2 \Omega_0 \int \frac{d^d \mathbf{p}}{(2\pi)^d} \frac{1}{E_0 - \Sigma^{R,A}(E_0) - \varepsilon(\mathbf{p})} \quad (52)$$

where  $E_0$  denotes the "bare" energy. Defining:

$$E(E_0) = E_0 - \text{Re} \Sigma^{R,A}(E_0)$$

we can rewrite (52) in the form:

$$\begin{aligned} E_0 - E(E_0) + i \text{Im} \Sigma^{R,A}(E_0) \\ = \tilde{W}^2 \Omega_0 \int \frac{d^d \mathbf{p}}{(2\pi)^d} \frac{1}{E(E_0) - \varepsilon(\mathbf{p}) - i \text{Im} \Sigma^{R,A}(E_0)}. \end{aligned} \quad (53)$$

In terms of the "bare" energy the band edge  $E_{0c}$  is defined from the obvious condition of the vanishing density of states:

$$N(E_0) = \mp \frac{1}{\pi} \int \frac{d^d \mathbf{p}}{(2\pi)^d} \text{Im} G^{R,A}(E_0, \mathbf{p}) \xrightarrow{E_0 \rightarrow E_{0c}} 0$$



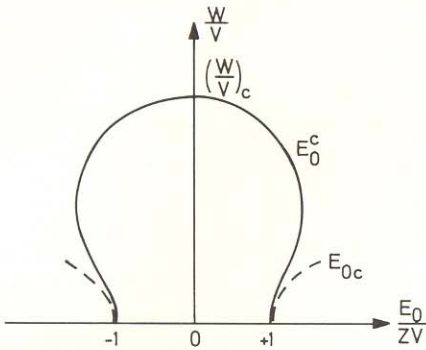


Fig. 1. "Mobility edge trajectory". Broken line shows the position of the band edge

which for our model is equivalent to the condition:

$$E(E_0) \xrightarrow{E_0 \rightarrow E_{0c}} -ZV; \quad \text{Im } \Sigma^{R,A}(E=E_{0c}) \equiv 0. \quad (54)$$

We consider here the "left" edge of the band. Then, from (53) and (54) we obtain the equation defining  $E_{0c}$ :

$$E_{0c} = -ZV - \tilde{W}^2 \Omega_0 \int \frac{d^d \mathbf{p}}{(2\pi)^d} \frac{1}{ZV + \varepsilon(\mathbf{p})}. \quad (55)$$

Analogous treatment for the free-electron case was given in [13]. In the simplest approximation (35) we get:

$$\begin{aligned} E_{0c} &= -ZV - \tilde{W}^2 \Omega_0 \int \frac{d^d \mathbf{p}}{(2\pi)^d} \frac{1}{\mathbf{p}^2/2m^*} \\ &= -ZV - \tilde{W}^2 \Omega_0 S_d \frac{2m^* p_0^{d-2}}{d-2} = -ZV - \frac{\tilde{W}^2 S_d}{V} \frac{1}{d-2} \end{aligned} \quad (56)$$

where we have introduced the upper cut-off  $p_0 = 1/a$ , and the last equality in (56) is written for hypercubic lattice, so that  $\Omega_0 = a^d$ ,  $m^* = (2Va^2)^{-1}$  and  $S_d = 2^{-(d-1)} \pi^{-d/2} / \Gamma(d/2)$ .

Remember now, that the parameter  $\varepsilon$ , entering (38) is actually the distance from the physical band edge:  $\varepsilon = E_0 - E_{0c}$ . Then, from (38) and (40) we obtain the equation, defining the mobility edge position  $E_0^c$  in terms of the "bare" energy. For hypercubic lattice we get:

$$E_0^c - E_{0c} = \left\{ \frac{d}{d-2} \frac{x_0^{d-2}}{\Gamma(d/2)} (4\pi)^{-\frac{d}{2}} \right\}^{\frac{2}{4-d}} V \left( \frac{\tilde{W}}{V} \right)^{\frac{4}{4-d}} \quad (57)$$

and for  $d=3$ , using (56) we find:

$$\frac{E_0^c}{ZV} = -1 - \frac{1}{2\pi^2 Z} \left( \frac{\tilde{W}}{V} \right)^2 + \left( \frac{3x_0^2}{4\pi^2} \right)^2 \frac{1}{Z} \left( \frac{\tilde{W}}{V} \right)^4 \quad (58)$$

defining the "mobility edge trajectory", shown in Fig. 1 (the picture is just the same near the "right" band edge), which is similar to that obtained in the Anderson's approach to localization [3, 22]. If we let  $E_0^c = 0$  in (58), we get a biquadratic equation, determining the critical ratio  $(\tilde{W}/V)_c$  for the complete localization of the band, taking the shift of the band

edge into account. The elementary solution, for  $x_0 = 2$  and  $Z=6$  (sc lattice) gives  $(\tilde{W}/V)_c \approx 4.15$ . Comparing this with the corresponding value in Table 1 shows that the influence of the shift of the band edge is rather small, which justifies the simple approach, used in the main part of this paper.

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### Note Added in Proof

We should like to add two important references which recently became known to us. The comprehensive survey of self-consistent diagrammatic theory of localization is given by Wölfle, P., Vollhardt, D.: Anderson localization. In: Springer Series in Solid State Sciences. Nagaoka, Y., Fukuyama, H. (eds.), Vol. 39, p. 26. Berlin, Heidelberg, New York: Springer-Verlag 1982. Localization in Anderson model within the self-consistent approach was also treated by Götze, W.: In: Recent developments in condensed matter. Devreese, J.T. (ed.), Vol. 1, p. 133. New York, London: Plenum Press 1981.