Self-consistent theory of localization in $2 \leq d < 4$ dimensions

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(Submitted June 29, 1982)

Fiz. Tverd. Tela (Leningrad) **24**, 3569–3574 (December 1982)

The self-consistent theory of electron localization in disordered systems proposed by Vollhardt and Wölfle [Phys. Rev. B **22**, 4666 (1980)] is generalized to $2 \leq d < 4$ dimensions. The mobility edge position is determined and the critical behavior of various physical quantities in the vicinity of the mobility edge is discussed. It is shown that the description of the vicinity of the mobility edge in a self-consistent theory is outside the range of validity of perturbation theory and, therefore, the results obtained by perturbation theory are only qualitative. The case of $d \geq 4$ is briefly discussed and the frequency dependence of the electrical conductivity for $d = 2$ is also considered.

PACS numbers: 71.55.Jv, 71.10. + x

1. It is well known that there are fundamental difficulties in the consistent description of localization of electrons in disordered systems.[1] In particular, it has not been possible to describe the localization effect itself within the standard formalism based on averaged Green functions. The only exception is the one-dimensional case. In higher dimensions, it has been necessary to resort to nonstandard methods based on the original Anderson paper.[2] However, it is practically impossible to calculate various physical quantities within the Anderson method.[1] We believe that the recent self-consistent approach to the localization theory developed in Ref. 3 represents an important step toward the solution of the localization problem. The main advantage of this method is its simplicity and standard formulation which make it possible to generalize such a theory to include new scattering mechanisms and the effects of applied fields (see, for example, Refs. 4 and 5). Reference 3 is mainly concerned with the two-dimensional case which is of particular interest in the context of the present theory.[1] The approach of Ref. 3 is particularly suitable in the two-dimensional case since it is based on the summation of a special class of diagrams[3,6,7] which dominate the perturbation series for d = 2. However, the aforementioned method can be easily generalized to dimensions d > 2. It will be shown that such a generalization yields reasonable and qualitively correct results for all the principal physical quantities of interest near the mobility edge. The position of the mobility edge is also obtained within such theory. After the completion of the present work, Ref. 8 appeared and some of our results are quoted in Ref. 8 (without derivation and discussion). Our aim is to address ourselves to a number of questions which have not been answered satisfactorily in Refs. 3–5 and 8. In particular, we shall demonstrate explicitly that the description of the mobility edge $2 < d < 4$ in dimensions, obtained in the self-consistent theory of localization, is outside the range of validity of the self-consistent theory. We shall also discuss some special features of conduction in two-dimensional systems. The behavior of the theory for $d \geq 4$ is also briefly discussed.

2. The self-consistent theory of Ref. 3 is based on the two-electron Green function averaged over the dis-

tribution of impurities and on the related quantity

$$\varphi_E^{RA}(\omega,\ \mathbf{q}) = -\frac{1}{2\pi i}\sum_{\mathbf{p},\,\mathbf{p}'}\langle G^R(\mathbf{p}_+,\ \mathbf{p}'_+;\ E+\omega)\,G^A(\mathbf{p}'_-,\ \mathbf{p}_-;\ E)\rangle, \tag{1}$$

where G_R and G_A are the one-electron Green functions before averaging; E is the electron energy (Fermi energy); ω is the frequency; $\mathbf{p}_\pm = \mathbf{p} \pm (1/2)\mathbf{q}$; and the angular brackets indicate averaging over impurities. The quantity $\varphi_E^{RA}(\omega, \mathbf{q})$ determines the density–density response function and, therefore, the conductivity of the system.

The function $\varphi_E^{RA}(\omega, \mathbf{q})$ can be obtained as the solution of an approximate "transport equation" in the following form (m is the electron mass):

$$\varphi_E^{RA}(\omega,\ \mathbf{q}) = -N(E)\frac{\omega + M_E(\mathbf{q},\ \omega)}{\omega^2 + \omega M_E(\mathbf{q},\ \omega) - \dfrac{2E}{md}q^2}, \tag{2}$$

where $M_E(\mathbf{q}, \omega)$ is the so-called "relaxation kernel."[3] In general, the relaxation kernel is determined by the sum of diagrams for the irreducible vertex part in the two-particle (R–A) channel and N(E) is the one-electron density of states.

By considering a self-consistent generalization of the summation of Langer–Neal[6,7] diagrams which yields the dominant contribution for d = 2, Vollhardt and Wölfle[3] derived the following self-consistent equation for $M_E(\mathbf{q} = 0, \omega)$:

$$M_E(0,\ \omega) = \frac{i}{\tau} - 2\rho V^2\sum_{|\mathbf{k}|<k_0}\frac{1}{\omega - \dfrac{D_0k^2}{\tau M_E(0,\ \omega)}}, \tag{3}$$

where $1/\tau = 2\pi\rho V^2N(E)$ is the Born rate of the scattering electrons from impurities which are assumed to be randomly distributed in space with a concentration ρ; V is the Fourier transform of the impurity potential which is assumed to be completely localized; and $D_0 = 2E\tau/md$ is the classical diffusion coefficient. The choice of the cutoff momentum k_0 in Eq. (3) is discussed below.

The frequency-dependent electrical conductivity of the system is given by[3]

$$\sigma_E(\omega) = \frac{ne^2}{m}\frac{i}{\omega + M_E(0,\ \omega)}. \tag{4}$$

It can be seen that $\mathrm{Re}\,M_E(0, \omega = 0) = 0$ holds in the metallic region.

In the energy range corresponding to localized states, we obtain $\sigma_E(\omega \to 0) \to 0$ and the quantity

$$A_E(\mathbf{q}) = \frac{1}{2\pi N(E)}\lim_{\delta\to 0}\sum_{\mathbf{p},\,\mathbf{p}'}\langle G^R(\mathbf{p}_+,\ \mathbf{p}'_+;\ E+i\delta)\,G^A(\mathbf{p}'_-,\ \mathbf{p}_-;\ E-i\delta)\rangle$$
$$= -\frac{1}{N(E)}\lim_{\omega\to 0}\omega\varphi_E^{RA}(\omega,\ \mathbf{q}) = \lim_{\omega\to 0}\frac{\omega M_E(\mathbf{q},\ \omega)}{\omega M_E(\mathbf{q},\ \omega) - \dfrac{2E}{md}q^2} \tag{5}$$

which determines the "localization probability" becomes nonzero.[4,9] For $\mathbf{q} \to 0$, we obtain[10]

$$A_E(\mathbf{q}) \approx 1 - q^2R_{\mathrm{loc}}^2(E), \tag{6}$$

where the localization radius $R_{\mathrm{loc}}(E)$ is given by

$$R_{\mathrm{loc}}^2(E) = \frac{2E}{md\omega_0^2(E)};\quad \omega_0^2 = -\lim_{\omega\to 0}\omega M_E(0,\ \omega) > 0. \tag{7}$$

It follows that the localization is related in the present formalism to the divergence of the relaxation kernel $M_E(0, \omega)$ for $\omega \to 0$ (see Ref. 3).

The self-consistent equation (3) was studied in Ref. 3 only for d = 2. However, it can be easily generalized to arbitrary dimensions d. It is clear that the corresponding results can describe localization only qualitatively since Eq. (3) is based completely on the summation of Langer–Neal diagrams which are important only for d = 2. Nevertheless, such calculations are interesting since they yield a simple description of localization in arbitrary dimension and, undoubtedly, describe correctly some features of the localization. The validity of such calculations will be discussed later.

3. Introducing in Eq. (3) a dimensionless integration variable, we can write this equation in the following form which is more suitable for our further calculations:

$$M_E(\omega) = \frac{i}{\tau} + d\lambda x_0^{d-2}M_E(\omega)\int_0^1 dy\,y^{d-1}\frac{1}{y^2 - \dfrac{M_E(\omega)\,\omega d}{4(x_0E)^2}}, \tag{8}$$

$$\lambda = \frac{1}{2\pi\tau E} = \left(\frac{m}{2\pi}\right)^{\frac{d}{2}}\frac{E^{\frac{d}{2}-2}}{\Gamma\left(\frac{d}{2}\right)}\rho V^2, \tag{9}$$

where λ is a dimensionless coupling constant and $x_0 = k_0/\sqrt{2mE}$. Careful examination of the equations of Ref. 3 [prior to the introduction of $M_E(\mathbf{q}, \omega)$ in Eq. (27) of Ref. 3] indicates that $k_0 \sim p_F \sim \sqrt{2mE}$ (p_F is the Fermi momentum). Such a choice of the cutoff momentum was used in Ref. 3 although the authors of Ref. 3 do not discuss in detail their choice of k_0 (see Ref. 8, where the momentum k_0 in Ref. 4 was chosen differently). We believe that the choice of the cutoff momentum $k_0 \sim p_F \sim \sqrt{2mE}$ is unique and very important for the subsequent estimates. For such a choice, it is clear that $x_0 = \mathrm{const} \sim 1$.

Setting $\omega = 0$ in Eq. (8) and considering the metallic regime $\mathrm{Re}\,M_E(0, \omega = 0) = 0$, we find that

$$\frac{i}{M_E} = \tau\left(1 - \frac{d}{d-2}\lambda x_0^{d-2}\right). \tag{10}$$

Equations (4) and (13) yield

$$\sigma_E(\omega = 0) = \frac{ne^2}{m}\tau\left\{1 - \left(\frac{E_c}{E}\right)^{\frac{4-d}{2}}\right\};\quad 2 < d < 4, \tag{11}$$

where

$$E_c = \left\{\frac{d}{d-2}\frac{x_0^{d-2}}{2\Gamma\left(\frac{d}{2}\right)}(2\pi)^{-\frac{d}{2}}\right\}^{\frac{2}{4-d}}E_{sc}, \tag{12}$$

$$E_{sc} = m^{\frac{d}{4-d}}(\rho V^2)^{\frac{2}{4-d}}. \tag{13}$$

It can be seen that E_c plays the role of a mobility edge

$$\sigma_E \approx \frac{ne^2}{m}\tau\left(\frac{4-d}{2}\right)\left(\frac{E-E_c}{E_c}\right);\quad 2 < d < 4 \tag{14}$$

for $E \gtrsim E_c$. Our result (12) is practically identical with the estimate of E_c obtained by another method in Ref. 9. For d = 3, the mobility edge E_c lies in the "strong cou-

pling" region $E_{sc} = m^3(\rho V^2)^2$ where the set of diagrams used in the calculation of this quantity is no longer dominant[1,9] and all the diagrams of perturbation theory should be included. In fact, it follows from Eq. (9) that the condition $E \gg E_{sc}$ is equivalent to the requirement $\lambda \ll 1$, i.e., it represents the simplest condition of validity of perturbation theory. For $d \to 2$, we obtain $E_c \to \infty$, which corresponds to the currently accepted view that there is complete localization in two dimensions.[1,3,9] Moreover, as shown in Ref. 9, it is more important that Eq. (12) defines essentially the dimensions of the "Ginzburg critical region"[1,9] where higher orders of perturbation theory are important since the geometric factor $(d-2)^{2/(d-4)}$ appears in the theory. It follows that, in spite of the fact that the inequality $E_c \gg E_{sc}$ ($\lambda \ll 1$) is satisfied, the mobility edge defined by Eq. (12) falls even for $d \to 2$ in an energy range where perturbation theory (and the corresponding choice of diagrams used in the present self-consistent theory) is not valid. Nevertheless, it is reasonable to assume that Eq. (12) yields a correct order-of-magnitude estimate of the mobility edge. At the same time, the result (14) implying that the conductivity tends to zero linearly in the limit $E \to E_c$ cannot be regarded as proved.

We shall now discuss the region of localized states ($E < E_c$). We shall set [see Eq. (7)] $\operatorname{Im} M_E(0, \omega) = 0$ and $\operatorname{Re} M_E(0, \omega) = -\omega_0^2/\omega_0$ and multiply Eq. (8) by ω, which yields in the limit $\omega \to 0$ the following equation for ω_0^2:

$$1 = d\lambda x_0^{d-2} \int_0^1 dy \frac{y^{d-1}}{y^2 + z}; \quad z = \frac{d\omega_0^2}{4(x_0 E)^2}. \tag{15}$$

The integral in Eq. (15) can be expressed in terms of the hypergeometric function and Eq. (15) then assumes the form

$$1 = \lambda x_0^{d-2} \frac{1}{z} {}_2F_1\left(1, \frac{d}{2}; 1 + \frac{d}{2}; -\frac{1}{z}\right). \tag{16}$$

When the mobility edge is approached from below ($E \lesssim E_c$), we can expand Eq. (16) in powers of z (small ω_0^2). Simple transformations yield

$$\omega_0^2 = \frac{4}{d}\left\{\Gamma\left(\frac{d}{2}\right)\Gamma\left(\frac{4-d}{2}\right)\right\}^{-\frac{2}{d-2}} x_0^2 E^2 \left\{1 - \left(\frac{E}{E_c}\right)^{\frac{4-d}{2}}\right\}^{\frac{2}{d-2}}; \quad 2 < d < 4. \tag{17}$$

It follows from Eq. (7) that the localization radius is given by

$$R_{loc}(E) = \frac{1}{x_0\sqrt{2mE}}\left\{\Gamma\left(\frac{d}{2}\right)\Gamma\left(\frac{4-d}{2}\right)\right\}^{\frac{1}{d-2}}\left\{1 - \left(\frac{E}{E_c}\right)^{\frac{4-d}{2}}\right\}^{-\frac{1}{d-2}} \sim \left(\frac{E_c - E}{E_c}\right)^{-\nu}, \quad E \lesssim E_c;\ 2 < d < 4, \tag{18}$$

where the critical index of the localization radius is

$$\nu = \frac{1}{d-2}. \tag{19}$$

Equations (19) and (14) indicate that Wegner's scaling relation $s = (d-2)\nu$ is satisfied for the critical conductivity index.[1] The corresponding values of the critical indices describing the behavior of physical quantities near the mobility edge agree with the results obtained in the principal approximation in the $\varepsilon = d - 2$ expansion obtained by the field-theoretic method based on nonlinear σ models (see, for example, Refs. 11-13) and also on the basis of the ε expansion in the qualitative scaling theory.[14] We believe that these results should not be taken too seriously since they were obtained by extrapolations outside the range of validity of perturbation theory and are based on an inconsistent self-consistency procedure. Nevertheless, the self-consistent theory of localization of Ref. 3 is a powerful method since it yields quite simple results that are equivalent to the results obtained by more complex methods.[11-13]

4. We shall now discuss the results of the present self-consistent theory for $d \geq 4$. It follows from Eq. (10) that

$$\sigma_E = \begin{cases} \frac{ne^2}{m}\tau\left[1 - \left(\frac{E}{E_c}\right)^{\frac{d-4}{2}}\right] \underset{E \lesssim E_c}{\approx} \frac{ne^2}{m}\tau\left(\frac{d-4}{2}\right)\left(\frac{E_c - E}{E_c}\right); & d > 4, \\ \frac{ne^2}{m}\tau\left[1 - \left(\frac{m}{2\pi}\right)^2 x_0^2 \rho V^2\right]; & d = 4. \end{cases} \tag{20}$$

The solution defined by Eq. (20) for $d > 4$ is clearly not physical since the region of localized states and the metallic region are interchanged. For $d = 4$, we obtain metallic conduction and $m^2\rho V^2$ is the dimensionless coupling constant of the four-dimensional theory of Ref. 15. Our treatment is clearly meaningful for $m^2\rho V^2 \ll 1$. [It follows from Eq. (15) that $\omega_0^2 < 0$]. This result also follows since the quantity E_{sc} defined by Eq. (13) tends to zero for $d \to 4$ (from below) for $m^2\rho V^2 \ll 1$. The interchange of the metallic region and of the region of localized states for $d > 4$ is a natural consequence of the following fact noted already in Refs. 15 and 16: the perturbation expansion in the present theory is in powers of the parameter $(E/E_{sc})^{(4-d)/2}$ and such an expansion for $d < 4$ diverges in the limit $E \to 0$; for $d > 4$, it diverges for $E \to \infty$. Nonphysical behavior of the model for $d > 4$ indicates that a model based on a point interaction (correlation of a random potential of "white noise" type) is not adequate for $d > 4$ (see Ref. 17). The situation changes completely if we assume that the cutoff parameter k_0 in Eq. (3) is determined by the range of the potential (pair correlation function of random potential) rather than by the Fermi momentum, i.e., by R_{int}, which implies $k_0 \sim R_{int}^{-1} \ll p_F$ (long-range interactions). For $d < 4$, we obtain the same results as before but the mobility edge is now given by

$$E_c = \frac{d}{d-2}\left(\frac{m}{2\pi}\right)^{d/2}\frac{E^{d/2-1}}{\Gamma\left(\frac{d}{2}\right)}\rho V^2; \quad E_0 = \frac{k_0^2}{2m}. \tag{21}$$

For $d \geq 4$, we obtain

$$\sigma \sim \frac{ne^2}{m}\tau\frac{E - E_c}{E_c}, \quad E \gtrsim E_c, \tag{22}$$

$$\omega_0^2 \sim \frac{4}{d}\frac{d-4}{d-2}\left(1 - \frac{E}{E_c}\right). \tag{23}$$

It follows that the critical index of the localization radius is $\nu = 1/2$ for $d > 4$. In this sense, we can regard $d = 4$ as the upper bound on the dimension of space in which localization effect can occur.[1] However, we would like to point out that a choice of k_0 independent of p_F does not follow from the model under study which is applicable to $d < 4$. This important factor has not been discussed in Ref. 8.

5. Finally, we shall quote (in more detail than in Ref. 3) our results on the frequency dependence of the conductivity in the self-consistent theory applying to d = 2. A somewhat lengthy but straightforwrad analysis of Eq. (3) for d = 2 indicates that there are several frequency intervals with different behavior of the conductivity. At very low frequencies $\omega \ll (1/\lambda)e^{-1/\lambda}(1/\tau)$, we obtain

$$\sigma_E(\omega) \approx \frac{ne^2}{m}\frac{1}{\tau\lambda}\frac{e^{2/\lambda}}{4(x_0E)^4}\omega^2, \tag{24}$$

i.e., we obtain insulating behavior.[3] At somewhat higher frequencies

$$\sigma_E(\omega) \approx \frac{ne^2}{m}\frac{e^{1/\lambda}}{2(x_0E)^2}\omega. \tag{25}$$

"Quasimetallic" behavior with logarithmic corrections first derived in Ref. 7 is obtained at frequencies satisfying $(1/\lambda^2)e^{-1/\lambda}(1/\tau) \ll \omega \ll (\lambda^2/\tau)$, i.e.,

$$\sigma_E(\omega) = \frac{ne^2}{m}\tau\left(1 - \lambda\ln\frac{1}{\omega\tau}\right). \tag{26}$$

Finally, for $\lambda^2/\tau \ll \omega \ll 1/\tau$, the self-consistent theory yields

$$\sigma_E(\omega) \approx \frac{ne^2}{m}\tau\left(1 - \frac{\tilde{E}_c}{E}\right), \tag{27}$$

where

$$\tilde{E}_c \approx \frac{m}{\pi}\rho V^2\ln\frac{x_0}{2}. \tag{28}$$

The last result is especially interesting since the conductivity in this frequency range is essentially constant (independent of ω) and corresponds to metallic conduction with the mobility edge $\tilde{E}_c$ defined by Eq. (28). It is possible that this result explains the well-known discrepancy between various numerical approaches to the calculation of the two-dimensional conductivity[1]: logarithmic corrections and insulating behavior manifest themselves only at extremely low frequencies and, at the same time, there is an interval of frequencies (since λ is small) in which the system is characterized by a finite mobility edge.

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Translated by D. Mathon