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P. Wölfle, Dieter Vollhardt

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Self-Consistent Diagrammatic Theory of Anderson Localization

P. Wölfle[1,2] and D. Vollhardt[2]

[1]Physik-Department der Technischen Universität München
D-8046 Garching, Fed. Rep. of Germany and

[2]Max-Planck-Institut für Physik und Astrophysik
Werner-Heisenberg-Institut für Physik
D-8000 München, Fed. Rep. of Germany

Abstract

The model of independent electrons interacting with static, randomly distributed, pointlike scatterers is treated in the extended state perturbation theory at zero temperature. We discuss several types of infrared divergent contributions indicating the onset of Anderson localization. Beyond perturbation theory, using a novel classification scheme of diagrams for the total vertex function, a self-consistent equation for the frequency dependent diffusion coefficient is derived. Solving these equations, one finds that for $d \leqslant 2$ states are always localized, while for $d > 2$ particles are delocalized for sufficiently weak disorder. We calculate properties in the critical region, e.g. critical exponents and scaling behavior. Defining a frequency dependent conductance we derive a scaling equation and explicitly calculate the corresponding β-function. By a plausible extension we also investigate the length-dependent conductance and its β-function. Where comparison is possible the results agree with those of renormalization group calculations.

1. Introduction

Over the past three years considerable progress has been made in understanding the problem of localization of a quantum mechanical particle subject to a random potental. In his first formulation of this problem ANDERSON [1] showed the existence of a sharp transition from localized to delocalized behavior, or equivalently, from an insulating to a metallic state, as a function of disorder. Subsequently MOTT [2] introduced the concept of a mobility edge, defined as the critical energy at which the mobility as a function of the Fermi energy was assumed to drop to zero discontinuously.

Recent work has been done along two main lines. First, the analogy to phase transitions has led to the application of modern concepts of the theory of critical phenomena. In particular, the scaling theory by ABRAHAMS et al. [3], based on ideas developed earlier by THOULESS [4], treats the dimensionless conductance g as a function of sample length L as the only relevant scaling parameter. The corresponding β-function is determined for strong disorder by assuming exponential localization and for weak disorder by applying extended state perturbation theory as developed by EDWARDS [5]. By smoothly interpolating between the two limits one finds [3] a continuous conductivity near the transition and, in dimension $d = 2$, weak localization even for arbitrarily small disorder, both being in contradiction to MOTT [2]. Some of these results had been derived earlier by WEGNER [6] applying the real space renormalization group (RG) approach. The assumptions of the scaling theory are justified to some extent by mapping the original Hamiltonian onto field theoretical models like the n-orbitals per site model [7, 8] and the non-

linear σ-models of interacting matrices discussed by WEGNER [9], HIKAMI[10], EFETOV et al.[11] and others.

The second line of approach aims at an approximate description of the full range of physical properties (i.e. not only the critical region), similar in spirit to the van der Waals theory of fluids. Such a theory has first been proposed by GÖTZE [12] in the form of a self-consistent equation for the dynamic density response function. The derivation is based on a mode-coupling formalism previously applied in the theory of liquids by the same author. The theory describes a continuous Anderson transition, with the correct limiting behavior for weak and strong disorder [12] and has been applied to explain the temperature dependence [13,14] and frequency dependence [15] of the conductivity. In the theory [12], however, the conductance does not obey scaling in the sense of ABRAHAMS et al. [3], as is apparent from perturbation theory. Also the critical properties are different from the field theoretical results [9,10]. Given the promising features of this first self-consistent theory of the Anderson transition it seemed worthwhile to try (i) to understand its relation to the field-theoretical approach and (ii) on that basis, to derive a new self-consistent equation which would hopefully describe the critical behavior correctly. By carrying out a systematic analysis of the density response function in terms of diagrams of standard extended state perturbation theory for a model of point scattering centers, we have derived a self-consistent equation for the frequency dependent conductivity [16]. This equation indeed obeys scaling and yields a conductance in detailed agreement with field theoretical results [17]. The same self-consistent equation has subsequently been derived by KAWABATA [18] in a similar way. Modifying the relaxation kernel in the mode-coupling theory [12], PRELOVSEK [19] arrived at the same equation, too. The combined effect of the classical [12] localizaton mechanism and the quantum interference effect [3] has been considered by BELITZ et al. [20].

It is the purpose of this article to review the diagrammatic self-consistent theory [16,17]. In the next section the diagrammatic representation of the density response function will be introduced. The frequency dependent diffusion coefficient $D(\omega)$ is expressed in terms of the irreducible vertex function U. Infrared contributions to U are investigated in some detail in section 3. The most important of these can be expressed in terms of a momentum integral over the density propagator, supplementing the initial derivation of the self-consistent equation on a diagrammatic level. This self-consistent equation for the frequency dependent conductivity and for the length dependent conductance is solved in sections 4 and 5. A brief discussion of the effect of symmetry breaking fields is given in section 6.

2. Density Response Theory

We consider the model of independent electrons interacting with randomly distributed static impurity scattering centers (density n_i), as described by the Hamiltonian

$$H = \sum_{\vec{p},\sigma} \frac{p^2}{2m} a^+_{\vec{p}\sigma} a_{\vec{p}\sigma} + \sum_{\vec{q}} \sum_{\vec{r}_i} V(\vec{q}) e^{i\vec{q}\cdot\vec{r}_i} \rho(\vec{q}). \qquad (1)$$

Here $V(\vec{q})$ is the interaction potential and $\vec{r}_i$ is the position of a single impurity. We are using the second quantized formulation for convenience with field operators $a^+_{\vec{p}\sigma}$, $(a_{\vec{p}\sigma})$ creating (annihilating) electrons in plane wave states of momentum $\vec{p}$ and spin σ in spite of the fact that we are dealing

with a single particle problem. In (1) the electron density operator $\rho(\vec{q}) = \sum_{\vec{p},\sigma} a^{+}_{\vec{p}+\vec{q}/2,\sigma} a_{\vec{p}-\vec{q}/2,\sigma}$ has been introduced. The quantity of main interest here is the density response function $\chi(\vec{q},\omega)$ in the thermodynamic limit, averaged over the statistical impurity positions. The limit of zero temperature is considered. The neglect of mutual interactions in our model implies that $\chi(\vec{q},\omega)$ is given by the impurity average of a product of two single particle Green's functions [21,22]

$$\chi(\vec{q},\omega) = \sum_{\vec{p},\vec{p}'} \{ \int_{E_F-\omega}^{E_F} dE \phi^{RA}_{\vec{p}\vec{p}'}(E,\omega;\vec{q}) + \int_{0}^{E_F} dE [\phi^{RR}_{\vec{p}\vec{p}'}(E,\omega;\vec{q}) - \phi^{AA}_{\vec{p}\vec{p}'}(E-\omega,\omega;\vec{q})] \} \quad (2a)$$

where

$$\phi^{RA}_{\vec{p}\vec{p}'}(E,\omega;\vec{q}) = -\frac{1}{2\pi i} < G^{R}(\vec{p}_{+},\vec{p}_{+}';\, E+\omega)\, G^{A}(\vec{p}_{-}',\, \vec{p}_{-};E) > , \quad (2b)$$

and $\vec{p}_{\pm} = \vec{p} \pm \vec{q}/2$, etc; E_F is the Fermi energy. We will be interested mainly in the macroscopic properties which allow us to restrict our considerations to the regime of small $\omega,\vec{q}$. Then (2) reduces to

$$\chi(\vec{q},\omega) = \omega\phi(\vec{q},\omega) + N_F + O(\omega \frac{\partial N}{\partial E_F}, q^2) \quad (3)$$

where

$$\phi(\vec{q},\omega) = \sum_{\vec{p},\vec{p}'} \phi^{RA}_{\vec{p}\vec{p}'}(E_F,\omega;\vec{q}) \quad (4)$$

and N_F is the density of states at the Fermi level for both spin components (the density of states for a single spin component will be denoted by $N(E_F)$). In the context of (3) $\phi(\vec{q},\omega)$ may be interpreted as the Kubo density relaxaton function.

The perturbation theory for $\phi^{RA}_{\vec{p}\vec{p}'}(\vec{q}\omega)$ (in the following we shall drop the superscript RA) may be formulated in terms of exact averaged single particle Green's functions [21] $G^{R}_{\vec{p}}(E) = (G^{A}_{\vec{p}}(E))^{*}$,

$$G^{R}_{\vec{p}}(E) = [E - p^2/2m - \Sigma^{R}_{\vec{p}}(E)]^{-1} \quad (5)$$

where $\Sigma^{R}_{\vec{p}}(E)$ is the self-energy part. In the absence of mutual interactions the self-energy may be shown to be a bounded, nonsingular quantity, in particular varying smoothly as a function of energy near the mobility edge. For the purpose of calculating the leading singular contributions to the density response function it is therefore sufficient to approximate Σ by the lowest order (Born approximation) expression

$$\Sigma^{R}_{\vec{p}}(E_F) \cong -i\gamma , \quad (6)$$

where $\gamma = \pi N(E_F) \int \frac{d\Omega_{p'}}{4\pi} U_0(\vec{p}_F - \vec{p}_F')$ in $d = 3$.

Here $U_0(\vec{p}-\vec{p}') = n_i \mid V(\vec{p}-\vec{p}') \mid^2$ is the bare vertex function. In the following only short-ranged potentials will be considered, where $U_0(\vec{p}-\vec{p}') \cong U_0 = \text{const.}$

The perturbation series for $\phi_{\vec{p}\vec{p}'}$ consists of all skeleton diagrams with a parallel particle and hole line (particle-hole propagator), joined by impurity interaction lines in all possible ways. Each particle (hole) propagator represents a Green's function $G^R_{\vec{p}}(E_F+\omega)(G^A_{\vec{p}}(E_F))$, each interaction line a factor U_0. The external momenta are $\vec{p}_+$ and $\vec{p}'_+$ for the particle propagator and $\vec{p}_-$, $\vec{p}'_-$ for the hole propagator, whereas the internal momenta are given by momentum conservation at the vertices.

The following kinetic equation is obeyed [16] by the distribution function

$$\phi_{\vec{p}}(\vec{q},\omega) = \sum_{\vec{p}'} \phi_{\vec{p}\vec{p}'}(\vec{q},\omega)$$

$$\begin{aligned} &[\ \omega - \vec{p}\cdot\vec{q}/m - \Sigma^R_{\vec{p}_+}(E_F+\omega) - \Sigma^A_{\vec{p}_-}(E_F)\ ]\,\phi_{\vec{p}}(\vec{q},\omega) = \\ &= [G^R_{\vec{p}_+}(E_F+\omega) - G^A_{\vec{p}_-}(E_F)]\ [\ \frac{1}{2\pi i} - \sum_{\vec{p}'} U_{\vec{p}\vec{p}'}(\vec{q},\omega)\ \phi_{\vec{p}'}(\vec{q},\omega)]\ . \end{aligned} \tag{7}$$

The quantity of prime importance in this equation is the irreducible vertex part $U_{\vec{p}\vec{p}'}(\vec{q},\omega)$, defined as the sum of all particle-hole irreducible diagrams. It has been shown that $U_{\vec{p}\vec{p}'}$ obeys the Ward identity [16]

$$\Sigma^R_{\vec{p}_+}(E_F+\omega) - \Sigma^A_{\vec{p}_-}(E_F) = \sum_{\vec{p}'} U_{\vec{p}\vec{p}'}(\vec{q},\omega)\ [G^R_{\vec{p}'_+}(E_F+\omega) - G^A_{\vec{p}'_-}(E_F)\ ] \tag{8}$$

which is a consequence of particle number conservation. Summing (7) on $\vec{p}$ taking the identity (8) into account, one finds the continuity equation,

$$\omega\phi(\vec{q},\omega) + q\phi_j(\vec{q},\omega) = -N_F + 0\left(\omega \frac{\partial N(E_F)}{\partial E_F}, q^2\right) . \tag{9}$$

The current relaxation function

$$\phi_j(\vec{q},\omega) = \sum_{\vec{p}} (\vec{p}\cdot\vec{q}/m)\ \phi_{\vec{p}}(\vec{q},\omega) \tag{10}$$

obeys, for small $\omega,\vec{q}$, the equation [16]

$$[\ \omega + \frac{i}{\tau} K(\vec{q},\omega)]\ \phi_j(\vec{q},\omega) = q\ \frac{v_F^2}{d}\ \phi(\vec{q},\omega) . \tag{11}$$

The dimensionless current relaxation kernel $K(\vec{q},\omega)$ is defined in terms of the irreducible vertex by

$$K(\vec{q},\omega) = 1 + \frac{\tau}{\pi m n} \sum_{\vec{p},\vec{p}'} (\vec{p}\cdot\vec{q})\ \Delta G_{\vec{p}}\ [U_{\vec{p}\vec{p}'}(\vec{q},\omega) - U^0_{\vec{p}\vec{p}'}]\ \Delta G_{\vec{p}'}(\vec{p}'\cdot\vec{q}) \tag{12}$$

where $\Delta G_{\vec{p}} = G^{R}_{\vec{p}_+}(E_F+\omega) - G^{A}_{\vec{p}_-}(E_F)$.

Here n is the particle density and τ is the weak coupling transport relaxation time, given by

$$\frac{1}{\tau} = 2\gamma + \frac{d}{\pi N_F p_F^2} \sum_{\vec{p},\vec{p}'} (\vec{p}\cdot\vec{q})\Delta G_{\vec{p}} U^{\circ}(\vec{p}-\vec{p}') \Delta G_{\vec{p}'}(\vec{p}'\cdot\vec{q})$$

$$= 2\pi n_i \sum_{\vec{p}'} \delta(E_F - \frac{p'^2}{2m}) |V(\vec{p}-\vec{p}')|^2 (1-\hat{p}\cdot\hat{p}') \quad . \tag{13}$$

From (9) and (11) one obtains for small q,

$$\phi(\vec{q},\omega) = \frac{-N_F}{\omega+iD(\vec{q},\omega)q^2} \tag{14}$$

where the $\vec{q},\omega$ dependent diffusion coefficient is given by

$$D(\vec{q},\omega) = \frac{D_o}{K(\vec{q},\omega)} \quad , \tag{15}$$

and $D_o = (v_F^2/d)\tau$ is the bare diffusion constant ($v_F = p_F/m$).

The dynamical conductivity $\sigma(\omega)$ and the polarizability $\alpha(\omega)$ are obtained from the q = 0 limit of the diffusion coefficient $D(0,\omega) \equiv D(\omega)$ as

$$\sigma(\omega) = i\omega\alpha(\omega) = e^2 (nd/2E_F) D(\omega). \tag{16}$$

In the conducting regime we expect $\sigma(0) > 0$ and hence $\alpha(\omega) \propto (i\omega)^{-1}$, whereas in the insulating regime $\alpha(0) > 0$ and $\sigma(\omega) \propto i\omega$, for small ω, and hence $K(0,\omega) \propto \omega^{-1}$. Within our formalism localization is characterized by the very appearance of a $1/\omega$ -singularity in $K(0,\omega)$.

3. Infrared divergencies of the relaxation kernel $K(q,\omega)$

Infrared divergent terms are quite naturally introduced into the perturbation series of $K(\vec{q},\omega)$ by terms containing singular propagators in the limit $\vec{q},\omega \to 0$. In the model considered the only conserved quantity is the particle number, giving rise to a diffusion pole structure of the density relaxation function at small $\vec{q},\omega$ as exhibited by (14). The integral over the momentum $\vec{q}$ of $\phi(\vec{q},\omega)$ diverges for dimensions $d \leq 2$, even if $D(\omega) > 0$, for $\omega \to 0$, as is the case in the conducting regime:

$$\int dq \frac{q^{d-1}}{\omega+iD(0)q^2} \propto \begin{cases} (D(0)/\omega)^{1/2} & , \quad d=1 \\ \ell n(D(0)/\omega) & , \quad d=2 \quad . \end{cases} \tag{17}$$

Note that a factor of q^2 in the integrand removes this singularity. In the insulating regime, where $D(\omega) \propto -i\omega$, we have a $1/\omega$ singularity from the same integral

$$\int dq \; \frac{q^{d-1}}{\omega + iD(\omega)q^2} \propto \frac{1}{\omega} \int dq \; \frac{q^{d-1}}{1+\alpha(0)(d/2e^2 E_F n)\, q^2} \; . \tag{18}$$

Additional factors of q^2 in the integrand do not remove the singularity in the latter case. Obviously contributions of the form (18) may generate a $1/\omega$ singularity in the current relaxation kernel $K(\vec{q},\omega)$.

In lowest order a diffusion pole is generated by summing the particle-hole ladder diagrams shown in Fig.1, yielding

$$\Gamma^0_{\vec{p}\vec{p}'}(\vec{q},\omega) = \frac{2U_0 \gamma}{-i\omega + D_0 q^2} \; . \tag{19}$$

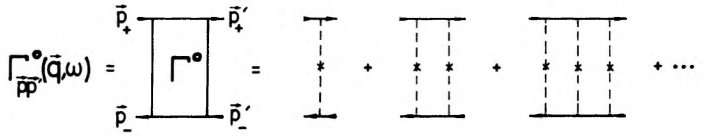

Fig. 1 Particle-hole diffusion propagator $\Gamma^0_{\vec{p}\vec{p}'}(\vec{q},\omega)$

The simplest irreducible diagrams containing Γ^0 are constructed by putting an interaction line across Γ^0 in the four possible ways, as shown in Fig. 2. Substituting $U^D_{\vec{p}\vec{p}'}$, the sum of these four irreducible diagrams, for $U_{\vec{p}\vec{p}'}(\vec{q},\omega)$ into (12) one finds the following contribution to K

$$K^D(\vec{q},\omega) = (\pi nm)^{-1} \sum_{\vec{k}} \frac{q^2 + (\vec{k}\cdot\vec{q})^2}{-i\omega + D_0 k^2} \; . \tag{20}$$

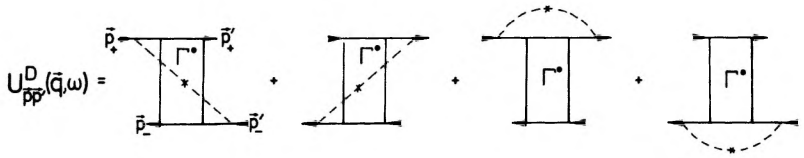

Fig. 2 Simplest irreducible diagrams containing a particle-hole diffusion propagator Γ^0

Whenever K^D is not small compared to unity the diffusion coefficient is changed from its bare value D_0. Accordingly D_0 should be replaced by $D(\vec{q},\omega)$ in the diffusion pole in (20). The resulting self-consistent equation for $D(\vec{q},\omega)$ is essentially identical with the small $\omega,\vec{q}$ limit of the self-consistent equation for $\phi(\vec{q},\omega)$ proposed by GÖTZE [12]. The solution of this equation has been discussed in detail [12-15,23]. Equation (20) has a

peculiar q-dependence: in the limit q = 0 the factor k^2 in the integrand removes the explicit infrared divergence for $d \leq 2$, but for $q \neq 0$ the divergence is present. This behavior may give rise to the expectation that the singular behavior at $q \neq 0$ is transferred to q = 0 in diagrams containing one diffusion propagator and several or many interaction lines crossing the diffusion propagator. We have shown [16], however, that the infrared divergent contributions are cancelled, i.e. a factor k^2 multiplies the diffusion propagator, within a class of diagrams that is essentially generated by cyclic permutation of the end points of interaction lines on one side of the diffusion propagator. The proof is restricted to momentum independent interaction and an arbitrarily large, but finite number of interaction lines, i.e. diagrams with more than one diffusion propagator are generally excluded.

In addition to the pure diffusion pole singularities, which are caused by particle number conservation and thus have a classical analogue, there exists a second type of singularity which is of pure quantum nature: the particle-particle propagator is singular for small ω, $\vec{Q}$, where $\vec{Q}$ is the total momentum of the two particles [3,24]. This singularity, the so-called Cooper pole or $2k_F$ pole, arises from a subtle quantum interference effect, which only exists if the system is time reversal invariant. It is easily seen that the singularity is exactly the diffusion pole, with a different momentum variable. For a time reversal invariant system the exact energy eigenfunctions $\varphi_n(r)$ may be chosen real, and hence the exact Green's function obeys $G^R(\vec{p},\vec{p}',E) = G^R(-\vec{p}',-\vec{p},E)$. From this one obtains, together with (2b)

$$\phi_{\vec{p}\vec{p}'}(\vec{q},\omega) = \phi_{(\vec{p}-\vec{p}+\vec{q})/2,\ (\vec{p}'-\vec{p}+\vec{q})/2}(\vec{p}+\vec{p}',\omega)\ . \tag{21}$$

Equation (21) is demonstrated diagrammatically in Fig. 3.

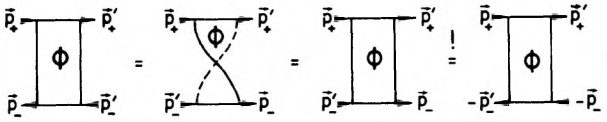

Fig. 3 Diagrammatic demonstration of the crossing symmetry for $\phi_{\vec{p}\vec{p}'}(\vec{q},\omega)$ in the case of time reversal invariance; see eq. (21)

The singularity in the particle-hole propagator at $\vec{p}+\vec{p}'=0$ is obtained in lowest order by summing the maximally crossed diagrams [24] as shown in Fig. 4, with the result

$$\Lambda^{\circ}_{\vec{p}\vec{p}'}(\vec{q},\omega) = \frac{2\,U_\circ\gamma}{-i\omega+D_\circ(\vec{p}+\vec{p}')^2}\ . \tag{22}$$

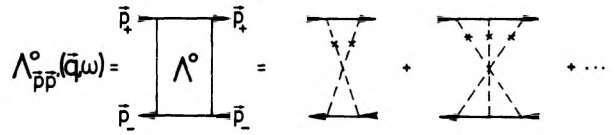

Fig. 4 Maximally crossed diagrams

Any diagram containing $\Lambda^{\circ}_{\vec{p}\vec{p}'}(\vec{q},\omega)$ contributes mainly for momenta $\vec{p} \simeq -\vec{p}'$, thus connecting the left and right hand side of Λ°. For instance, substituting $\Lambda^{\circ}_{\vec{p}\vec{p}'}(\vec{q},\omega)$ in (12), and putting $\vec{p}' = -\vec{p}$ in $\Delta G_{\vec{p}}(\vec{p}\cdot\vec{q})$, one finds

$$K^{2k_F}(\vec{q},\omega) = [\pi N(E_F)]^{-1} \sum_{\vec{Q}}{}' \frac{1}{-i\omega+D_o Q^2} \quad , \tag{23}$$

where we have introduced $\vec{Q} = \vec{p}+\vec{p}'$. Note that the additional factor of k^2 in (20) originates from the angular integration on $\vec{p}$ and $\vec{p}'$, which requires factors of $\vec{p}.\vec{k}$ and $\vec{p}'\cdot\vec{k}$, by expanding Green's functions $G^R_{\vec{p}+\vec{k}}$, etc, to yield a finite result. The most important diagrams are therefore those, where a Λ° block is crossing diagonally, thus connecting the two external momenta $\vec{p}$ and $\vec{p}'$. We may then classify the diagrams contributing to the total vertex Γ (and therefore to ϕ) in the way depicted in Fig. 5.

In Fig. 5 a wavy line represents Λ°. The vertex Γ is defined as the sum of all diagrams with no interaction line diagonally connecting the end points.

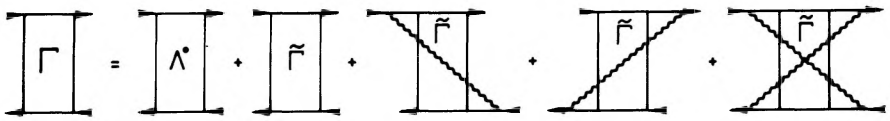

Fig. 5 Exact classification of the total vertex Γ using Cooper-poles (see text)

Observe that only the second diagram of Fig. 5 contains reducible diagrams. Therefore U, the irreducible vertex, is also given by the diagrams of Fig. 5 where, however, $\tilde{\Gamma}$ is replaced by the irreducible part $\tilde{\Gamma}_i$ in the second diagram. The last diagram in Fig. 5 consists of the set of "superdivergent" diagrams [16] containing a Q-integral over $(\Lambda^{\circ})^2$ and hence over the diffusion pole squared. Such an irreducible contribution and similar ones giving arbitrary powers of Λ° would give rise to much stronger infrared divergent terms for K and therefore may be expected to be cancelled. The cancellation may be demonstrated by employing the time reversal symmetry relation (21), which may be represented diagrammatically as shown in Fig. 3. By this operation the diagrams of Fig. 5 are untwisted and Λ° is transformed into a sum of particle-hole ladder diagrams. Defining the central part of the last diagram in Fig. 5 as

$$T(\vec{Q},\omega) = \sum_{\vec{p}_1,\vec{p}_2}{}' G^R_{\vec{p}_{1+}} G^A_{\vec{p}_{1-}} \tilde{\Gamma}_{\vec{p}_1\vec{p}_2}(\vec{Q},\omega) G^R_{\vec{p}_{2+}} G^A_{\vec{p}_{2-}} \quad , \tag{24}$$

where $\vec{Q} = \vec{p}+\vec{p}'$ and $\vec{p}_{i\pm} = \vec{p}_i \pm \vec{Q}/2$, it is seen that T consists of all diagrams contributing to the density-relaxation function $\phi(\vec{Q},\omega)$, excluding those with parallel interaction lines (part of a ladder) at the ends. Hence $T(\vec{Q},\omega)$ obeys

$$T = \phi - \phi_o - R_o\Gamma_o T - T\Gamma_o R_o - R_o\Gamma_o T\Gamma_o R_o \tag{25}$$

with $R_o(\vec{Q},\omega) = \sum_{\vec{p}}{}' G^R_{\vec{p}+} G^A_{\vec{p}-}$ and $(-2\pi i)\,\phi_o = (R_o/U_o)\,\Gamma_o = R_o/(1-R_oU_o)$.

Solving (25) for T and substituting the small $\omega,\vec{q}$ expression $R_o = U_o^{-1}[1 - \frac{-i\omega+D_oQ^2}{2\gamma}]$ one finds

$$T(\vec{Q},\omega) = (2\gamma)^{-2}(-i\omega + D_oQ^2)^2 \; [\; \phi(\vec{Q},\omega) - \phi_o(\vec{Q},\omega)\;]. \qquad (26)$$

It is clear that the quadratically divergent term $\Lambda_o^2(\vec{Q},\omega)$ is cancelled.

Substituting (26) and (22) into the diagrams of Fig. 5 one arrives at the following exact expression for the relaxation kernel:

$$K(\vec{q},\omega) = 1 + [2\pi N^2(E_F)]^{-1} \sum_{\vec{Q}} \phi(\vec{Q},\omega) + K_1 + K_2 \; , \qquad (27)$$

where

$$K_1(\vec{q},\omega) = \text{const.} \sum_{\vec{Q}} \gamma^{-1}(-i\omega+D_oQ^2)\; [\phi(\vec{Q},\omega)-\phi_o(\vec{Q},\omega)]$$

and

$$K_2(\vec{q},\omega) = -i\tau \sum_{\vec{Q}} (\vec{p}\cdot\vec{q})(G^R-G^A)\; \tilde{\Gamma}_i\; (G^R-G^A)\; (\vec{p}'\cdot\vec{q}) \; .$$

The term K_1 is obviously smaller than the first term and may be safely neglected. The term K_2 is also less divergent, because by construction, it does not contain diagrams in which the left and right vertex are connected by a Cooper pole. Hence all diffusion poles $\Gamma_i(\vec{Q},\omega)$ that may occur in K_2 are multiplied by factors Q^2, originating from terms $(\vec{p}_i\cdot\vec{Q})$ necessary to render finite angular integrals. We may therefore neglect K_2 as well.

The remaining term in (27) is independent of the external momentum $\vec{q}$. More precisely, in deriving (27) we have already neglected terms of the order of $(q\ell)^2$, where $\ell = v_F\tau$ is the mean free path.

4. Self-consistent theory: Dynamical conductivity

Taking the $\vec{Q}$-sum over $\phi(\vec{Q},\omega)$ (the $2k_F$-pole) in (27) as the dominant divergent contribution to $K(\vec{q},\omega)$, one has the following self-consistent equation for $D(\omega)$ and hence the conductivity $\sigma(\omega)$:

$$\frac{D_o}{D(\omega)} = 1 + \frac{k_F^{2-d}}{\pi m} \int_0^{k_o} dk\; \frac{k^{d-1}}{-i\omega+ D(\omega)k^2} \; . \qquad (28)$$

It is useful to introduce a dimensionless coupling parameter λ by

$$\lambda = (2\pi\; E_F\; \tau)^{-1},$$

whence $D_o = (\pi dm\lambda)^{-1}$.

In equation (28) a momentum cutoff of the order of the inverse mean free path $k_o \sim 1/\ell = \pi\lambda k_F$ is used. Equation (28) may be written in the following form

$$\frac{D(\omega)}{D_o} = 1 - d\lambda k_F^{2-d} \int_0^{k_o} dk\; \frac{k^{d-1}}{[-i\omega/D(\omega)]+k^2} \; . \qquad (29)$$

In the localized regime we expect $\lim_{\omega\to\infty} [-i\omega/D(\omega)] = \xi^{-2}$, where ξ is the localization length. Indeed the density relaxation function in this regime takes the form [12]

$$\phi(\vec{q},\omega) = \frac{-N_F}{\omega} \frac{1}{1+q^2\xi^2} \tag{30}$$

describing exponential localization with characteristic length ξ. Since in the localized regime $D(\omega=0) = 0$, (29) immediately yields a transcendental equation for ξ,

$$1 = d\lambda\ (k_F\xi)^{2-d} \int_0^{k_o\xi} dy\ \frac{y^{d-1}}{1+y^2} \ . \tag{31}$$

Let us now discuss the solution of (29) and (31). For low dimensions, $d < 2$, the solution of (29) is necessarily of the form $D(\omega) \propto i\omega$, i.e. the particles are localized even for arbitrarily small disorder.

The localization length for $1<d<2$ is obtained from (31) in the limit of small coupling λ as

$$\xi = k_F^{-1} \left[\frac{d}{2}\lambda\ \Gamma(\tfrac{d}{2})\ \Gamma(1-\tfrac{d}{2})\right]^{\frac{1}{d-2}} \ . \tag{32}$$

For $d = 1$, $k_o\xi \sim 1$ and therefore one obtains $\xi = 4v_F\tau$ which agrees with the exact results [25,26].
For $d = 2$ one finds exponentially weak localization,

$$\xi = k_o^{-1} \exp\left(\frac{1}{2\lambda}\right) \ . \tag{33}$$

The localization length is seen to grow so rapidly with decreasing λ that below $\lambda \sim 0.02$ the localization property does not have practical consequences for laboratory systems.

The static electric polarizability is obtained from the localization length via $\alpha(0) = e^2(\sigma_o/D_o)\xi^2$.

The leading term of the frequency dependent conductivity is calculated from (29) as

$$\mathrm{Re}\ \sigma(\omega) = \sigma_o\ \omega^2\tau^2\ b_d \ , \tag{34}$$

where

$$b_1 = 512 \ , \qquad d = 1$$

$$b_2 = \frac{1}{4\lambda} e^{2/\lambda} \ , \qquad d = 2 \ .$$

The level repulsion effect, which leads to a $\omega^2(\ell n\omega)^{d+1}$ dependence in $\mathrm{Re}\sigma(\omega)$ is not obtained in the present theory. This may not be surprising as it only shows up in higher order in ω as compared to the leading $\sigma(\omega) \propto -i\omega$ dependence.

For dimensions $d > 2$ the self-consistent equation (29) has a solution $D(\omega=0) \neq 0$ for coupling strength less than a critical value λ_c.

Rewriting (29) in the form

$$\frac{D(\omega)}{D_o} = 1 - \frac{d\lambda}{d-2}\left(\frac{k_o}{k_F}\right)^{d-2} + d\lambda\left(\frac{Dk_F^2}{-i\omega}\right)^{\frac{2-d}{2}} \int_0^{b(\omega)} dy \frac{y^{d-3}}{1+y^2} \tag{35}$$

where $b(\omega) = [D(\omega)/(-i\omega\tau\, D_o)]^{1/2}$, one finds

$$\frac{D(0)}{D_o} = 1 - \frac{\lambda}{\lambda_c} \quad , \text{ for } \quad \lambda < \lambda_c, \tag{36}$$

where

$$\lambda_c = \frac{d-2}{d}\left(\frac{k_o}{k_F}\right)^{2-d} \quad , \quad d \geq 2 \tag{37}$$

or substituting $k_o = \pi\lambda k_F$,

$$\lambda_c = \left[\frac{d-2}{d}\, \pi^{2-d}\right]^{1/(d-1)} . \tag{38}$$

The d.c. conductivity $\sigma(0)$ is seen to vanish at the Anderson transition as $\sigma(0) \propto \lambda_c - \lambda$ for any $d > 2$, i.e. the critical exponent of the conductivity is $s = 1$ [17,18,19]. The result (36) implies that

$$\sigma(0) = \sigma_o - e^2 \frac{1}{d} c_d k_F^{d-2} \quad , \tag{39}$$

i.e. a disorder independent term is subtracted from the weak coupling conductivity expression $\sigma_o = (e^2 n\tau/m)$ ($c_d = \frac{2}{\pi} S_d (2\pi)^{-d}$, with S_d the surface of the d-dimensional unit sphere).

In the localized regime ($\lambda > \lambda_c$) (35) has the general solution for small ω

$$\frac{D_o}{D(\omega)} = D_o \xi^{-2}/(-i\omega) + O(\omega^o) \tag{40}$$

for any dimension d. Expanding the r.h.s. of (35) in powers of ξ^{-1},

$$1 = d\lambda (k_F\xi)^{2-d} \left[\frac{(k_o\xi)^{d-2}}{d-2} - \int_0^\infty dy \frac{y^{d-3}}{1+y^2} + O((k_o\xi)^{d-4})\right] ,$$

for $2 < d < 4$

and

$$1 = d\lambda (k_F\xi)^{2-d} \left[\frac{(k_o\xi)^{d-2}}{d-2} - \frac{(k_o\xi)^{d-4}}{d-4} + \int_0^\infty dy \frac{y^{d-5}}{1+y^2} + O((k_o\xi)^{d-6})\right]$$

for $d > 4$

one obtains for $2 < d < 4$ that near the transition ξ diverges as

$$\xi = k_F^{-1} \left[\frac{d-2}{dp_d\lambda} \left|1 - \frac{\lambda}{\lambda_c}\right|\right]^{-1/(d-2)} , \quad 2 < d < 4 \tag{41}$$

where $p_d = \Gamma(\frac{d}{2})\ \Gamma(2-\frac{d}{2})$, i.e. the localization length ξ diverges with the critical exponent $\nu = \frac{1}{d-2}$ [17,19]. For $d > 4$ the critical exponent of the localization length is $\nu = 1/2$ [17,19], independent of dimension, and

$$\xi = k_o^{-1}\left[\frac{d-4}{d-2}\ \frac{\lambda_c}{\lambda}\ \left|1 - \frac{\lambda_c}{\lambda}\right|\right]^{-1/2}\ , \qquad d > 4 \qquad (42)$$

At the upper critical dimension $d = 4$ one obtains logarithmic corrections to the classical behavior;

$$\xi = k_o^{-1}\ \left|1 - \frac{\lambda}{\lambda_c}\right|^{-1/2}\ \ell n\ \left|1 - \frac{\lambda}{\lambda_c}\right|^{-1/2}\ . \qquad (43)$$

For $2 < d < 4$ the critical exponents s and ν obey the relation $s=(d-2)\nu$ first derived by WEGNER [6]. The particular values $s=1$ and $\nu = \frac{1}{d-2}$ have been found in ε expansion around $d = 2$ for the nonlinear σ-model of interacting matrices with orthogonal symmetry [9,10,27], which is thought to describe the critical properties of the nonmagnetic impurity Anderson localization problem. By a plausible assumption about the vanishing of all higher order coefficients in the β-function (see below) HIKAMI [28] has recently extended the field-theoretical analysis to the full range $2 < d < 4$. Results for s and ν consistent with ours have also been found by 1/n-expansion for a n-orbital-per-site model [7,8].

In the conducting regime ($\lambda < \lambda_c$) for $\omega\tau \ll 1-\lambda/\lambda_c$ and in the insulating regime close to the transition ($\lambda \geq \lambda_c$) the upper limit of the k-integral in (35) is $b(\omega) \gg 1$ and may then be taken to infinity. One finds for the frequency dependent conductivity $\sigma(\omega)$

$$\frac{\sigma(\omega)}{\sigma_o} = 1 - \frac{\lambda}{\lambda_c} + p_d\ \frac{\lambda}{\lambda_c}\ \left[\frac{-i\omega\tau}{\sigma(\omega)/\sigma_o}\right]^{\frac{d-2}{2}} \qquad (44)$$

An essentially identical equation has been derived recently from the nonlinear σ-model of orthogonal symmetry [28]. It follows from (44) that $\sigma(\omega)$ has the scaling form [29]

$$\frac{\sigma(\omega)}{\sigma_o} = (-i\omega\tau)^{\frac{d-2}{d}}\ F_d\ (\omega/\omega_c)\ , \qquad (45)$$

with the limiting values for $\omega \ll \omega_c$

$$\begin{aligned} F\ (\tfrac{\omega}{\omega_c}) &\propto (-i\omega/\omega_c)^{2/d}\ , && \lambda > \lambda_c \\ F\ (\tfrac{\omega}{\omega_c}) &\propto (-i\omega/\omega_c)^{\frac{2-d}{d}}\ , && \lambda < \lambda_c \end{aligned} \qquad (46)$$

and for $\omega \gg \omega_c$

$$F\ (\tfrac{\omega}{\omega_c}) = \text{const.}\ , \qquad \lambda \lesseqgtr \lambda_c\ .$$

The latter case ($\omega \gg \omega_c$) describes the scaling region, where $\sigma(\omega) \propto (-i\omega)^{\frac{d-2}{d}}$. The cross-over frequency ω_c scales with the localization length as $\omega_c \propto \xi^{-d}$. Similar scaling forms for $\sigma(\omega)$ have been found by WEGNER [6], GÖTZE [12] (for d = 3), HIKAMI [28] and SHAPIRO and ABRAHAMS [30].

In d = 3 dimensions (44) may be solved explicitly with the result

$$\frac{\sigma(\omega)}{\sigma_o} = \left(\frac{\pi^2}{12}\right)^{1/3} (-i\omega\tau)^{1/3} \{[(1+i\frac{\omega_c}{\omega})^{1/2} - 1]^{2/3} + [(1+i\frac{\omega_c}{\omega})^{1/2} + 1]^{2/3} - 2(i\frac{\omega_c}{\omega})^{1/3}\} , \tag{47}$$

where

$$\omega_c\tau = \frac{4}{9\pi^2} \left(\frac{\lambda}{\lambda_c} - 1\right)^3 . \tag{48}$$

For larger frequencies $\sigma(\omega)$ merges into the well-known Drude behavior $\sigma(\omega)/\sigma_o = (1-i\omega\tau)^{-1}$.

5. Self-consistent theory: Length-dependent conductance

The scaling properties of the self-consistent theory are most clearly exhibited by the conductance as a function of sample size L. This is also the natural quantity to make contact with the scaling theory [3] and the field-theoretical treatments [6-11,27,28]. Starting from the equation (29) for the frequency dependent diffusion coefficient, we first observe that in a sample of length L (volume L^d) the wave number of any diffusion mode is greater than 1/L. On the other hand, for given disorder the states of the finite sample are localized whenever the states of the infinite system are localized. This is expressed by replacing $-i\omega/D(\omega)$ in the integral of (29) by ξ^{-2}, where ξ is the localization length of the infinite system. The L-dependent diffusion coefficient is then obtained as

$$\frac{D(L)}{D_o} = 1 - d\lambda\xi^2 k_F^{2-d} \int_{1/L}^{k_o} dk \, \frac{k^{d-1}}{1+k^2\xi^2} , \tag{49}$$

or, taking into account the equation (31) for ξ,

$$\frac{D(L)}{D_o} = d\lambda \, (k_F\xi)^{2-d} \int_0^{\xi/L} dy \, \frac{y^{d-1}}{1+y^2} . \tag{50}$$

The calculation of the current density J flowing in a sample of finite length L under the influence of an applied electric field E is nontrivial due to the nonlocal character of the density response of localized electrons. We may determine the electric current by requiring that it be equal and opposite to the diffusion current under open circuit conditions. At the end of the sample (x = L) the current density is then given by $J = eD(L)\,d(\delta\rho)/dx\big|_{x=L}$ where $\delta\rho(x)$ is the density change induced by the electric potential $U(x) = eE(L-x)$, given by $\delta\rho(x) = \int_o^L dx' \, \chi(x-x') \, U(x')\big|_{x=L}$.

Here $\chi(x)$ is the static density response function, obtained by Fourier transforming (30), $\chi(x) = N_F\,[\delta(x)-(2\xi)^{-1}e^{-|x|/\xi}]$. The dimensionless conductance $g(L) = \frac{\hbar}{e^2} L^{d-2} J/E$ is finally obtained as

$$g(L) = c_d\; x^{d-2}\,(1+x)\,e^{-x}\,I_d(x)\;, \tag{51}$$

where $I_d(x) = \int_0^{1/x} dy\,\frac{y^{d-1}}{1+y^2}$ and we defined $x = L/\xi$.

It is seen that $g(L)$ depends on the coupling constant λ only via the scaled length of the sample, $L/\xi(\lambda)$, and therefore is a scaling function. This is in agreement with the assumptions of the scaling theory of ABRAHAMS et al. [3], as well as the renormalization group treatments of field-theoretical models [6-11,27,28]. The integral in (51) may be performed with the results $I_1(x) = \tan^{-1}(1/x)$, $I_2(x) = (1/2)\,\ell n\,[1 + 1/x^2]$ and the relations $I_d(x) = x^{2-d}/(d-2) - I_{d-2}(x)$ for $d > 2$. Thus for $d = 1$ and $d = 2$ one finds explicitly

$$\begin{aligned} g(L) &= \frac{2}{\pi^2}\;(\xi/L)\,\tan^{-1}(\xi/L)\,(1 + L/\xi)e^{-L/\xi}, \quad d = 1 \\ g(L) &= \frac{1}{2\pi^2}\;\ell n\,[1 + (\xi/L)^2]\,(1 + L/\xi)e^{-L/\xi}, \quad d = 2\;. \end{aligned} \tag{52}$$

In the conducting regime (for $d > 2$ and $\lambda < \lambda_c$) we find from (50) by letting $\xi \to 0$

$$g(L) = c_d\,(d-2)^{-1}\;\;[1 + p_d(L/\xi')^{d-2}], \qquad 2 < d < 4 \tag{53}$$

where the correlation length ξ' is given by (41) for $\lambda < \lambda_c$. Note that $g(L)$ approaches the coupling independent constant $c_d/(d-2)$ for $(L/\xi) \to 0$.

The crucial quantity of the field-theoretical approach is the β-function. It is interesting to calculate $\beta[g(L)]$ from our explicit $g(L)$ and to compare with available results.

From the general result (51) we find

$$\beta\;[g(L)] \;\equiv\; \frac{d\ell ng}{d\ell nL} = d - 2 - \frac{c_d}{g}\,\frac{(1 + x)e^{-x}}{1+x^2} - \frac{x^2}{1+x}\;, \tag{54}$$

where $x = L(g)/\xi$ and $L(g)$ is the inverse function of $g(L)$.

The exponential dependence of $g(L)$ for large L/ξ leads to

$$\beta(g) = \ell ng + 0\;[\ell n\;(\ell n\,\frac{1}{g}\,)] \quad , \quad g \ll 1. \tag{55}$$

for all dimensions. On the other hand, for large g and correspondingly small x one finds

$$\beta = d - 2 - \frac{c_d}{g} - x^2\,(1 - \frac{3}{2}\,\frac{c_d}{g}\,) + 0\;(x^3)\,. \tag{56}$$

For $d \leq 2$ we find $\beta(g) < 0$ for any finite g, implying localization. For $d = 1$ one calculates $x = (\pi g)^{-1}$ and hence β apparently may be expanded in a power series in $1/g$. However, for $d = 2$ one finds $x = e^{-\pi^2 g}$ and hence the correction terms to the leading term $-\frac{c_d}{g}$ are nonanalytic for $\frac{1}{g} \to 0$. This is consistent with the finding of field-theoretical calculations [9,10,27] that the coefficients of g^{-n} for $n = 2,3,4$ are zero, and the conjecture that all higher coefficients are zero, too [28].

For $d > 2$ the β-function crosses zero at $g = g_c = c_d/(d-2)$. In the regime $g > g_c$, where g scales as L^{d-2} for large L, β is given by (56) with $x = 0$, since the localization length is infinite in the conducting regime. The slope of β at g_c is continuous and equal to

$$\frac{d\beta}{d\ell n g}\Big|_{g_c} = \frac{1}{\nu} \quad , \qquad d > 2$$

as expected from the scaling theory [3], where $\nu = (d-2)^{-1}$ for $2 < d < 4$ and $\nu = 1/2$ for $d > 4$.

In Fig. 6 we have plotted the scaling function $\beta(g)$ versus $\ell n g$ for dimensions $d = 1, 2, 3, 4$.

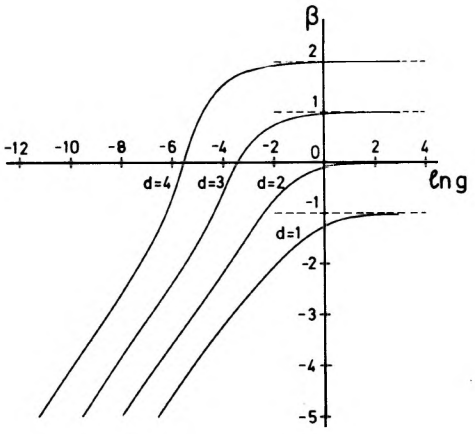

Fig. 6 The β-function for the length dependent conductance g(L), $\beta[g(L)] = d\ell n g/d\ell n L$, for dimensions d=1,2,3,4

One may define a frequency dependent conductance $g(\omega)$ in a volume ξ^d - in analogy to g(L) - by

$$g(\omega) = (e^2/\hbar)^{-1}\, \sigma(\omega)\xi^{d-2} \quad . \tag{57}$$

It follows from (44), however, that $g(\omega)$ is not a proper scaling parameter because it goes as $\omega^{(d-2)/d}$ for $\omega \gg \omega_c$, i.e. in the scaling regime. Therefore one has to introduce a modified scaling parameter $G(\omega) = (-i\omega/\omega_c)^{(2-d)/d}\, g(\omega)$ so that for $\omega \gg \omega_c$ $G(\omega)$ is constant. Eq. (44) then takes the form

$$\frac{d-2}{c_d p_d}\, G = \pm\, z^{(2-d)/d} + G^{(2-d)/2}, \quad d < 4 \tag{58}$$

where $z = -i\omega/\omega_c$ and

$$\omega_c = \frac{e^2}{\hbar} \frac{D_o}{\sigma_o} \xi^{-d} \tag{59}$$

and the upper (lower) sign corresponds to the conducting (insulating) regime. It is obvious that G is a scaling function with respect to frequency. The corresponding β-function can easily be calculated. For $d < 4$ one obtains

$$\beta[g(\omega)] = \frac{d\ell nG}{d\ell n\omega} = \frac{2}{d} \frac{(2-d)G^{d/2}+c_d p_d}{2G^{d/2}+c_d p_d} . \tag{60}$$

Observe, that for $d \leq 2$ the β-function does not change sign, corresponding to the absence of an Anderson transition, while for $d > 2$ β goes through zero at $G_c = [c_d p_d/(d-2)]^{2/d}$. Also note, that for $d = 2$ $\beta[G(\omega)]=(1+2\pi^2 G)^{-1}$ is an analytic function of G in contrast to $\beta[G(L)]$.

6. Conclusion

In this article we have presented a self-consistent theory of the Anderson localization problem with particular emphasis on the critical regime. We find a lower critical dimensionality $d = 2$ and an Anderson transition for $d > 2$, with the static conductivity vanishing continuously as a linear function of the disorder parameter. The localization length ξ diverges at the transitions with the critical exponent $\nu = 1/(d-2)$ for $2 < d < 4$ and $\nu = 1/2$ for $d > 4$. The dimensionless frequency dependent conductance (in volume ξ^d) as well as the length dependent conductance (in volume L^d) vary with disorder only via a scaled frequency ω/ω_c (where $\omega_c \propto \xi^{-d}$) and a scaled length L/ξ. The scaling functions are given explicitly. The corresponding β-functions agree with renormalization group calculations where comparison is possible. For $\omega \gg \omega_c$ (and $\omega\tau \ll 1$), i.e. in the scaling regime, and $d > 2$, the conductivity in the localized and extended regimes varies as $\sigma(\omega) \propto (-i\omega)^{(d-2)/d}$. For $\omega \ll \omega_c$ in the localized regime, the real part of the conductivity is obtained as $Re\sigma(\omega) \propto \omega^2$. This is in disagreement with the generally accepted result $Re\sigma(\omega) \propto \omega^2[\ell n\omega]^{d+1}$, where the logarithm is due to a level repulsion effect for pairs of impurities [31]. Such an effect might be included by formulating the theory in terms of localized states.

The q-dependence of the diffusion coefficient is not understood yet within the present theory: whereas from scaling arguments [3,32] one expects $D(\vec{q},\omega) \propto q^{d-2}$ for $q\xi \gg 1$, we have not found any q-dependence on this scale from the diagrammatic calculation of $D^{-1}(\vec{q},\omega)$ in terms of the irreducible vertex function. Also the behavior at still larger wave-vectors and frequencies has not been considered. The cutoff in the wave-vector at the inverse mean free path, which is sufficient in the critical regime, should be replaced by a more realistic description of the density relaxation function $\phi(\vec{q},\omega)$ for larger q and ω values, as e.g. in [12].

A problem of considerable interest is the influence of symmetry-breaking fields on the Anderson transition. The quantum scattering interference

effect causing the "Cooper"-pole contribution to the diffusion coefficient, which is ultimately responsible for localization in the theory presented here, is destroyed by time reversal invariance breaking fields, like a magnetic field [33,34] or magnetic impurities [34,35]. In this event, localization can only be caused by particle-hole diffusion pole divergencies. For the case of magnetic impurities we are able to show that infrared divergencies in K from a single diffusion pole are again cancelled in the way discussed in section 3. Such contributions from diagrams containing two and more diffusion poles have been claimed to cancel by KHMELNITSKII [36] and EFETOV et al. [11]. This would imply the existence of an Anderson transition in d = 2 and d = 1. This is in disagreement with results by HIKAMI [19,28] and OPPERMANN [37], who find a lower critical dimension of d = 2, implying that infrared divergent terms exist in $d \leq 2$. Given the leading infrared divergent contribution to $K(\vec{q},\omega)$, if it exists, one might again try to derive a self-consistent equation. In the case of an external magnetic field, a self-consistent theory along the lines of the present work has been proposed [38].

Finally, the effect of Coulomb interactions between the particles is expected to be important for a metal-insulator transition. It is hoped that a self-consistent theory of this more complicated problem may be developed on the basis of the present work.

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