Scaling Theory of Localization: Absence of Quantum Diffusion in Two Dimensions

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Arguments are presented that the $T=0$ conductance G of a disordered electronic system depends on its length scale L in a universal manner. Asymptotic forms are obtained for the scaling function $\beta(G)=d\ln G/d\ln L$, valid for both $G \ll G_c \simeq e^2/\hbar$ and $G \gg G_c$. In three dimensions, G_c is an unstable fixed point. In two dimensions, there is no true metallic behavior; the conductance crosses over smoothly from logarithmic or slower to exponential decrease with L.

Scaling theories of localization have been discussed by Thouless and co-authors[1-3] and by Wegner.[4] Recently Schuster,[5] using methods related to those of Aharony and Imry,[6] has proposed a close relationship of the localization problem to a dirty XY model of the same dimensionality. Wegner has proposed a scaling for dimensionality $d \neq 2$ of the conductivity

$$\sigma \sim (E - E_c)^{(d-2)\nu}, \tag{1}$$

while Schuster identifies ν as the correlation-length exponent of the XY model $= \frac{1}{2}$ at $d>4$. The latter proposes a universal jump of conductivity for $d=2$ given by $e^2/\hbar\pi^2$. This is not inconsistent with the results of Wegner[4] and is in rough agreement with the early calculations of Ref. 2. It has not been clear how (1) could be reconciled with the physical ideas of Mott[7] as related to the beginning of a scaling theory by Thouless.[3] We here develop a renormalization-group scheme based on the Mott-Thouless arguments, which in many essential ways agrees with Wegner's results, and in other ways severely disagrees. In particular, we recover (1) for $d>2$, where ν is the localization-length exponent below E_c. This is in clear contradiction to Mott,[7] who argues that in all cases the conductivity jumps to zero at E_c. At $d=2$, we find no jump in σ but a steep crossover from exponential to very slow dependence on size. There is *no* true metallic conductivity. These results were presaged by Thouless and coworkers[8,9] to some extent, with Ref. 8 indicating a transition region for three dimensions, and Ref. 9 a size-dependent minimum metallic conductivity.

Our ideas are based on the relationship[1] between conductance as determined by the Kubo-Greenwood formula and the response to perturbation of boundary conditions in a finite sample described by Thouless and co-workers[3]

$$\frac{\text{“}V\text{”}}{W} = \frac{\Delta E}{dE/dN} = \frac{2\hbar}{e^2} C = \frac{2\hbar}{e^2} \sigma L^{d-2}. \tag{2}$$

Here G is the conductance (*not* conductivity σ) of a hypercube of size L^d [here $L \gg L_0$ (L_0 = microscopic size)], dE/dN is the mean spacing of its energy levels, and ΔE is the geometric mean of the fluctuation in energy levels caused by replacing periodic by antiperiodic boundary conditions. Actually, when “V/W” is relatively large, it is hard to match the energy levels and, in fact, ΔE is defined using the curvature for small χ when we replace periodic $\psi(n+1)=\psi(1)$ by $\psi(n+1)=e^{i\chi} \times \psi(1)$ boundary conditions. This procedure is valid throughout the range of interest.[3] We will comment on the validity of (2) in a fuller paper, but here we add the following remarks. The equivalence of the Kubo-Greenwood formula and the breadth ν of the distribution of ΔE as described in Ref. 3a is not quite precisely provable but does not depend as stated in that reference on independence of momentum matrix elements $p_{\alpha\beta}$ and energy difference $E_\alpha - E_\beta$ between two states, only on a uniform distribution of those $E_\alpha - E_\beta$ which have large $p_{\alpha\beta}$.

Our scaling theory depends on the following ideas.

(I) We define a generalized dimensionless conductance which we call the “Thouless number” as a function of scale L:

$$g(L) = \frac{\Delta E(L)}{dE(L)/dN} \left(= \frac{G(L)}{e^2/2\hbar} \right), \tag{3}$$

where we now contemplate a small *finite* hypercube of size L. In the case $L \gg l$, the mean free path, we may use (2) to define a conductance $G(L)$ which is not related directly to the macroscopic conductivity but is a function of L, and is

defined by (3) from the average of the Thouless energy-level differences at scale L. When $L<l$, there is phase coherence on a scale L and g is no longer given by (3) but it can be shown that $(e^2/\hbar)g=G$ can be defined as the conductance of a hypercube imbedded in a perfect crystal.

(II) We remark that $g(L)$ is the relevant dimensionless ratio which determines the change of energy levels when two hypercubes are fitted together. This is the hypothesis of Thouless and can be justified in several ways on physical grounds. For instance, once $L>$ mean free path, the phase relationships for an arbitrary integration of the wave equation across the cube are as random from one side to another as those between wave functions on different cubes. This could be shown to be related to Wegner's "neglect of eigenvalues far from E_F" by a scaling argument. In this limit $g(L)$ represents [as indicated in (2)] the "V/W" of an equivalent many-level Anderson model where each block has $(L/L_0)^d$ energy levels and a width of spectrum

$$W=(dE/dN)(L/L_0)^d.$$

We cannot see how any statistical feature of the energy levels other than this coupling/granularity ratio can be relevant.

(III) We then contemplate combining b^d cubes into blocks of side bL and computing the new $\Delta E'/(dE/dN)'$ at the resulting scale bL. The result will be

$$g(bL)=f(b,g(L)), \tag{4}$$

or in continuous terms

$$d\ln g(L)/d\ln L=\beta(g(L)). \tag{5}$$

The scaling trajectory has only one parameter, g.

(IV) At large and small g we can get the asymptotics of β from general physical arguments. For large g, macroscopic transport theory is correct and, as in (2),

$$G(L)=\sigma L^{d-2},$$

so that

$$\lim_{g\to\infty}\beta_d(g)=d-2. \tag{6}$$

For small g $(V/W\ll 1)$, exponential localization is surely valid and therefore g falls off exponentially:

$$g=g_a e^{-\alpha L}.$$

Thence

$$\lim_{g\to\infty}\beta_d(g)=\ln[g/g_a(d)]. \tag{7}$$

Here g_a is a dimensionless ratio of order unity.

From the asymptotics (6) and (7), we may sketch the universal curve $\beta_d(g)$ in $d=1,2,3$ dimensions (Fig. 1). The central assumption of Fig. 1 is continuity: Since β represents the blocking of finite groups of sites, it can have no built-in singularity, and hence it would be unreasonable for it to have the cusp indicated by the dashed line: This is the curve which would be required to give the Mott-Schuster jump in conductivity for $d=2$. The only singularities then, must be fixed points $\beta=0$. Physically, it is also certain that β is monotonic in g, since smaller V/W surely always means more localization.

In constructing Fig. 1, we have used perturbation theory in V/W which shows that the first deviation of β from $\ln(g/g_a)$ is *positive*, with

$$\beta=\ln(g/g_a)[1+\alpha g+\sim g^2+\ldots], \tag{8}$$

since this is essentially just the "locator" perturbation series first discussed by Anderson.[10] The steepening of the slope of β given by (8) makes $\nu\lesssim 1$, as we shall see, for $d=3$ or greater.

For large g, we suppose that β may be calculated as a perturbation series in $W/V=g^{-1}$:

$$dg/d\ln L=g(d-2-a/g+\ldots). \tag{9}$$

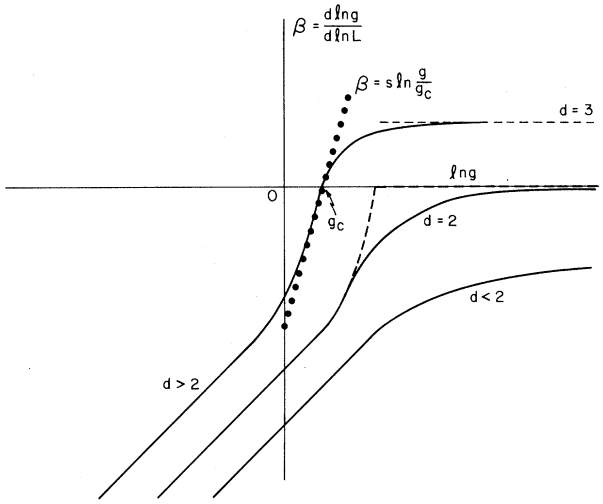

FIG. 1. Plot of $\beta(g)$ vs $\ln g$ for $d>2$, $d=2$, $d<2$. $g(L)$ is the normalized "local conductance." The approximation $\beta=s\ln(g/g_c)$ is shown for $g>2$ as the solid-circled line; this unphysical behavior necessary for a conductance jump in $d=2$ is shown dashed.

The first correction term in this series may be estimated in perturbation theory by considering backscattering processes of the sort first discussed by Langer and Neal[11] in their analysis of the dependence of resistivity on impurity concentration.

The use of Langer and Neal involves a rather subtle question. Converting the calculation of Langer and Neal to dimensionality 2 in particular, one obtains

$$g(L) = g_0 - g_1 \ln\Lambda ,$$

where Λ is a length cutoff for a certain divergent integral of second order in the density of scatterers. Langer and Neal assume this cutoff is l, the mean free path; for scales $L < l$, it should, of course, be L and we obtain just the result expected from (9), $d\ln g/d\ln L \sim -g^{-1}$. On the other hand, our universality argument seems to require $L > l$. We have restudied the cutoff question and will show in a fuller paper that their cutoff is not correct.

On the other hand, we have been unable to show definitively that the mean free path does *not* represent a relevant scale for the problem, since once $L > l$, we find, for example, that the coefficient of $\ln L$ depends on l. We must rely rather on our general arguments from continuity and regularity, and an intuition that only g is relevant, to suppose that a series development of β in g^{-1} should exist, once $L \gg l$.

The consequences of Fig. 1 and Eqs. (8) and (9) are as follows: For $d > 2$, the β function has a zero at g_c of order unity. It is an unstable fixed point which signals the mobility edge. The critical behavior can be estimated by integrating β starting from a microscopic L_0 and with g_0 near g_c. We use the linear approximation

$$\beta = s \ln(g/g_c) , \tag{10}$$

where $s > 1$, since $\alpha > 0$ in (8). For $g_0 > g_c$, we obtain

$$\sigma = A\frac{e^2}{\hbar}\frac{g_c}{L_0^{d-2}}\left(\ln\frac{g_0}{g_c}\right)^{(d-2)/s} , \tag{11}$$

where A is of order unity. The distance to the mobility edge is measured by

$$\epsilon = \ln(g_0/g_c) \approx (g_0 - g_c)/g_c , \tag{12}$$

and the factor $Ae^2/\hbar L_0^{d-2}$ in (11) is the Mott conductivity which here appears in the scaling form proposed by Wegner.

In the localized regime ($g_0 < g_c$), we get

$$g \approx g_c \exp(-A|\epsilon|^{1/s} L/L_0) , \tag{13}$$

so that the exponent of the localization length is the inverse slope of β at g_c,

$$\nu = 1/s . \tag{14}$$

These results again agree with those of Wegner.

In two dimensions, we have a strikingly different picture (see Fig. 1). Instead of a sharp mobility edge there is *no* critical g_c where $\beta(g_c) = 0$, but β is *always negative* so that in all cases $g(L \to \infty) = 0$. Instead of a sharp universal minimum metallic conductivity, there is a universal crossover from logarithmic to exponential behavior which for many experimental purposes may resemble a sharp mobility edge fairly closely. If we extrapolate the form we would deduce from Langer's perturbation-theory calculation, on the "extended" side of the crossover

$$g \simeq g_0 - A g_c \ln(L/L_0) \tag{15}$$

the conductivity decreases logarithmically with scale until $g = g_c$ at the scale L_l, where

$$\frac{L_l}{L_0} = \exp\left[\frac{1}{A}\left(\frac{g_0}{g_c} - 1\right)\right] . \tag{16}$$

From this point on g decreases exponentially with L, the localization length being of order L_l as given by (16). This type of behavior was already anticipated from computer studies,[9] but the nature of the actual solution is surprising to say the least, as well as the fact that it appears to have been anticipated in terms of a divergence of perturbation theory in the weak-coupling limit by Langer and Neal.[11]

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Theory for the Acoustic-Wave-Induced Electric Field Gradient in Transition Metals

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For transition metals I report the dependence of the acoustic-wave–induced electric field gradient (EFG) on $N(0)$, the electronic density of states at the Fermi-energy ϵ_F. It is shown that the EFG due to linear volume deformation of the unit cells of the crystal is proportional to $N_s(0)$, the s-electron density of states at ϵ_F, but does not correlate with $N(0)$ which is in general largely due to d electrons. However, the EFG due to long-wavelength shear waves correlates linearly with $N_d(0)$, the d-electron density of states at ϵ_F.

Recently, the electronic contribution to the electric-field-gradient (EFG) tensor in Mo, Nb, and Ta caused by acoustic waves was determined by nuclear acoustic resonance (NAR).[1,2] The results are shown in Fig. 1. Most remarkable is the fact that the change, Δq, in EFG is insensitive to $N(0)$, the electronic density of states at the Fermi energy ϵ_F, if the acoustic wave causing Δq only gives rise to linear dilatations of the unit cells of the crystal. However, Δq seems to be proportional to $N(0)$ if the acoustic wave giving rise to Δq causes shear dilatations of the unit cells. With the assumption that the observed electronic change in EFG results from the electron-lattice coupling, it then becomes immediately obvious that these results of the NAR experiments are of interest in understanding the coupling of shear modes and volume deformations to electrons, in particular d electrons, in transition metals.

In the following simple physical arguments and a simple theory are presented to explain the dependence on $N(0)$ of the acoustically induced EFG. First, one expects on general physical grounds that in transition metals long-wavelength volume deformations couple essentially only to s electrons since, because of different screening of the electron redistribution, the "compression" and "expansion" of d-electron bonds caused by d-electron response to volume deformations cost much more energy than is the case for s-electron response.[4] Therefore, the electronic change, Δq, in EFG should essentially result from the coupling of the s electrons to the acoustic wave and thus should correlate to $N_S(0)$, the s-electron density of states at ϵ_F, but not to the total density of states $N(0)$ which is in general largely determined by the d-electron density of states,

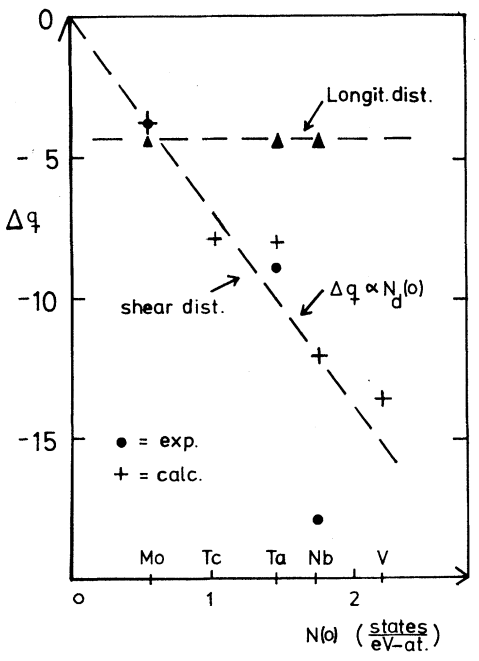

FIG. 1. Dependence on $N(0)$ of the change, Δq, of EFG due to an acoustic wave (Refs. 1,2). The parameter η is discussed in Ref. 3. We put $\Delta q(\mathrm{Mo}) = \Delta q_{\mathrm{expt}}$.