CONDUCTOR TO INSULATOR PHASE TRANSITION IN DISORDERED SOLIDS

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An outline is given of the current theoretical understanding of the conductor-insulator (Anderson) transition in disordered solids. The emphasis is put on the presentation of the approach employing kinetic equations. The numerical experiments performed on the Anderson model are also discussed.

I. Introduction

The discussion of transport and optical properties of metals and semiconductors is usually based on the Bloch states, which are electron eigenstates in an ideal lattice. The influence of statical disorder as caused by impurities, topological irregularities etc. is reflected in a decrease of a phase coherence of wavefunctions. Bloch states are not eigenstates any more and are smeared out on an energy interval $\Delta E = \hbar/\tau$ which is related to the time τ between subsequent collisions with impurities. Consequently, the same τ determines also transport properties, e.g. the dc conductivity is given by $\sigma_0 \propto \tau$.

The essential requirement for the validity of standard transport theories for the solid state is the extended nature of eigenstates. In 1958, P. Anderson$^{1)}$ was the first who realized that the usual picture could be qualitatively wrong for the cases of strong statical disorder, namely eigenstates could become strictly localized. In the region of localized states the electron cannot exhibit diffusion and does not contribute to dc conductivity. Anderson postulated also the existence of a sharp transition between the extended and the localized regime which could be achieved by varying the disorder strength. Later he also recognized that the localization phenomenon contradicts the ergodic hypothesis, namely a non-diffusing electron does not travel through the whole phase space which would be in principle allowed, i.e. accessible without violation of obvious conservation laws as the conservation of energy etc. Anderson transition is thus an example of a transition between the ergodic and the nonergodic behaviour.

Largest effects of statical disorder are expected at low temperatures by materials with partly filled electron bands, i.e. metals, impurity bands in semiconductors. Temperatures should be low to exclude activation processes via phonons etc. The influence of electron—electron interaction on localization is not yet clarified, hence we shall not discuss it. Still there are indications that this interaction does not eliminate localization but rather reinforces it. Mott$^{2)}$ introduced a notion of mobility edges (see Fig. 1) since the conductor—insulator transition can be reached also at fixed disorder by varying the Fermi energy E_F. On the conducting side he postulated the existence of the minimum metallic conductivity[2], which proved to be specially suited for experimental verification of the theory.

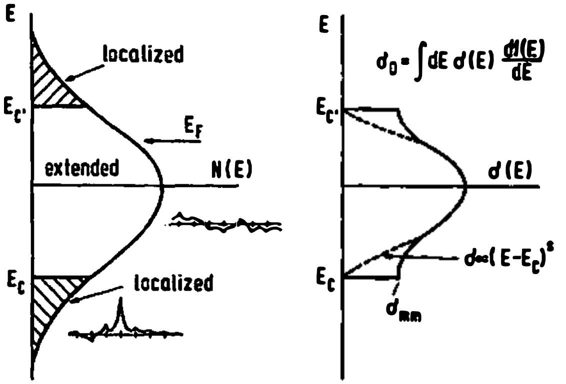

Fig. 1. Mobility edge model: In the band two energies E_c, E_c, separate the regions of localized and extended states. Shown is also the dc conductivity (at T = 0) $\sigma(E)$ as a function of the Fermi energy E with proposals of discontinuous and continuous variation near mobility edges.

In favor of the sharp transition are also experimental results[3], i.e. conductivity measurement results for mixed crystals $La_{1-x}Sr_xVO_3$, $Gd_{1-x}Sr_xVO_3$ and for two-dimensional systems as the inversion layers on the Si – SiO_2 [3] interface and thin metallic films[4] of Au, Cu, Al etc. In the above examples one could by changing parameters reach the transition between the region of temperature independent (residual) conductivity, characteristic for conductors, and the insulating regime where the dc conductance is possible only via activation processes.

In recent years also the evidence has accumulated that the Anderson transition has characteristics of a continuous phase transition with the scaling behaviour in the vicinity of mobility edges[5,6].

II. Anderson model and numerical experiments

In theoretical investigations of disordered solids the most frequently studied model was that of Anderson[1]. It describes noninteracting electrons within the tight binding approximation

$$H = \sum_i u_i c_i^+ c_i + \sum_{i,j} V_{ij} c_i^+ c_j , \qquad (1)$$

where $c_i^+ (c_i)$ are creation (annihilation) operators for an electron on lattice site i. The lattice is still regular, whereas the disorder is within local energies u_i, u_i being random and independent variables which are for simplicity assumed as uniformly distributed within the interval $-W/2 < u_i < W/2$. Transfer matrix elements still have translational symmetry, i.e. $V_{ij} = V$ for nearest neighbours and $V_{ij} = 0$ elsewhere. Despite the simplicity of the model there are only very few exact results available. One of them is the case of Lorentz distribution of u_i, where one can evaluate exactly one–particle Green's functions and the density of states ρ_E. Results show that ρ_E as well as the one-particle Green's functions do not reveal anomalies at the transition, hence they are not critical quantities.

Due to the lack of analytical results an important contribution to the understanding of localization phenomena has been obtained by numerical experiments performed on various disorder models, mainly on the Anderson model. Methods could be generally divided into: approaches employing a direct diagonalization[7] of the Hamiltonian[1] and approaches simulating the time–evolution of wavefunctions[8,9]. Diagonalization results confirmed the existence of a sharp transition between the extended and localized regime[7]. Both methods have been used for the calculation of the phase diagram, i.e. mobility edges $E_c(W)$ for few examples of two and three-dimensional lattices[7,8]. On the insulating side $W>W_c$ near the transition results confirmed the steady increase of the localization length r_L of eigenfunctions ψ_i $\psi_i \propto \exp(-r_{0i}/r_L)$. As a very useful criterion for the transition the participation ratio P has been introduced

$$P^{-1} = \sum_i |\psi_i|^4/(\sum_i |\psi_i|^2)^2 . \qquad (2)$$

P represents an effective number of states, on which the eigenfunction is localized, i.e. P is finite for $W > W_c$ and $P = \infty$ for $W < W_c$. On the conducting side the most interesting quantity is the dc conductivity σ_0. Mott[2] argued, that just below the transition eigenfunctions are entirely stochastic, and on the basis of this conjecture proposed there the value σ_{mm} (minimum metallic conductivity), consequently a discontinuous behaviour of σ_0 at the transition (see Fig. 1)

$$\sigma_{mm} = 0.12\ e^2/\hbar , \quad d = 2 , \qquad (3a)$$

$$\sigma_{mm} = \gamma\, e^2/\hbar a_0 , \ \gamma = 0.025 - 0.1 , \ d = 3 . \qquad (3b)$$

Note that in $d = 2$ σ_{mm} is a universal constant, whereas in $d = 3$ σ_{mm} still depends on the lattice spacing a_0. In disagreement with conductivity measurements, numerical experiments[9] do not agree (see Fig. 2) upon the proposed behaviour. They seem to be more compatible with the critical behaviour, as one could expect from the analogy with phase transitions

$$W < W_c : \ \sigma_0 \propto |W - W_c|^s , \quad P^{-1} \approx r_L^{-1} = 0 , \qquad (4a)$$

$$W > W_c : \ \sigma_0 = 0 \quad , \ P^{-1} \propto r_L^{-2} \propto |W - W_c|^{2\nu} . \qquad (4b)$$

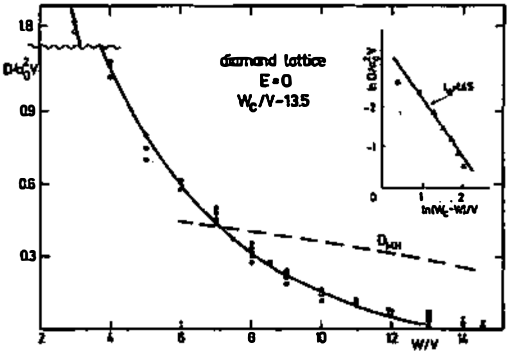

Fig. 2.
Diffusion constant D proportional to the dc conductivity $\sigma_0 = e^2 \rho_E D$, as a function of disorder strength W/V for the Anderson model on the diamond lattice, obtained by simulation[9]. In the vicinity of W_c D is well below D_{MH}, i.e. the value as proposed by Mott (3b).

III. Theory: method of kinetic equations.

In recent years the renormalization group method has been applied to the problem in order to clarify the situation in the vicinity of the Anderson transition and to find the values for the critical exponents s, ν. Results[10] indicate that d = 2 is the lower critical dimensionality of the problem, namely for $d \leqslant 2$ states are always localized and $W_c = 0$. For lattices with $d > 2$ there is still no agreement on the values s and ν in the literature[5].

In the following we shall describe an alternative method employing the kinetic equations and present some results which it yields. The method has been introduced by Götze [11] for the study of the electron gas in a three–dimensional parabolic band with the diagonal disorder. The method has been later generalized to d = 2 [11] and to the case of the Anderson model[12]. The novelty and also the advantage of this approach is in the fact that within it one calculates directly quantities which are supposed to be critical. The aim is thus to find meaningful approximations for the density relaxation function

$$\phi(q,z) = \langle(\rho(q)|(z-\mathcal{L})^{-1}\rho(q))\rangle_c , \tag{5a}$$

$$\rho(q) = \sum_i \exp(i\vec{q}.\vec{r}_i)\, c_i^+ c_i , \tag{5b}$$

where $\rho(q)$ is the electron density operator and $\langle\ \rangle_c$ denotes the average over all random configurations of u_i. When we employ kinetic equations for $\rho(q)$ and introduce an approximation which replaces the matrix of memory functions with just one function m(q,z), we can express $\phi(q,z)$ for general q and z as

$$\phi(q,z) = [\phi^o(q,z-m(q,z))^{-1} + \zeta(q)\, m(q,z)]^{-1} , \tag{6}$$

where $\zeta(q) = (\rho(q)|\rho(q))^{-1}$ and $\phi^o(q,z)$ denotes the unperturbed (W = 0) Lindhard relaxation function which could be calculated exactly[12]. Since we have properly taken into account the particle number conservation, $\phi(q,z)$ as given by expression (6) reproduces for small $qa_0 \ll 1$ a characteristic diffusion form

$$\phi(q,z) = \rho_E/(z + iq^2 D(q,z)) \,. \tag{7}$$

The function $D(q,z)$ represents the generalized diffusion constant. From equations (6) and (7) now the expressions for the ac conductivity $\sigma(z)$ and the dynamical polarizability $\chi(z)$ follow

$$\sigma(z) = e^2 \rho_E D(0,z) = \frac{i e^2 n_E a_0^2}{z - m(0,z)} \tag{8a}$$

$$\chi(z) = \frac{i}{z}\sigma(z) = \frac{-e^2 n_E a_0^2}{z^2 - z\, m(0,z)} \,, \tag{8b}$$

where n_E is the electron density. In the conducting regime $\sigma_0 = \sigma(0) > 0$, hence we can define the relaxation time $\tau = 1/m''(0,0) > 0$. On the insulator side the dc electric field does not induce current but rather static polarization, therefore the statical polarizability should be finite $\chi(0) = e^2 \rho_E r_L^2 > 0$ and $\sigma_0 = 0$. Then, it follows from (8b) $\lim_{z \to 0} [z\, m(0,z)] = \eta > 0$. Consequently, memory function has an anomalous nonergodic behaviour at low frequencies, i.e. $m(0,z) = \eta/z$. The phase transition is thus fixed by the instability of the insulator $\eta \to 0$ or the blocking of the conductor $\tau^{-1} = m''(0,0) \to \infty$.

From the above discussion one can conclude that the function $m(q,z)$ is essential for the description of the Anderson transition. Next step in the theory is devoted to the choice of an appropriate approximation for $m(q,z)$. We employ the analogy with mode coupling theories of critical dynamics and decouple the stochastic fluctuations of energies u_q and the density $\rho(q)$. Then, it is possible to express $m(q,z)$ with the $\phi(q,z)$

$$m(q,z) = \frac{1}{n_E m^*} \sum_{q'} \langle |u_{q-q'}|^2 \rangle_c \left| (\vec{q} - \vec{q}\,') \cdot \frac{\vec{q}}{q} \right|^2 \phi(q',z) \,, \tag{9}$$

where m^* denotes the effective mass of the electron. Approximation (9) is an generalization of the usual golden–rule formula for the inverse relaxation time $1/\tau$, where in the latter case the unperturbed function $\phi^0(q',z)$ enters expression (9) instead of $\phi(q',z)$. The essential difference is in the fact that $\phi(q',z)$ contains also slow diffusion processes, what leads to an important feedback mechanism. Namely, $m(0,z)$ determines through equation (8a) the diffusion coefficient $D(0,0)$ etc. Together with known statical quantities as n_E, ρ_E equations (6) and (9) form a closed set. From (9) also a simple q dependence follows $m(q,z) = M(z) + q^2 N(z)$.

Finally, let us summarize essential results obtained by the described method :
a) At the condition for the phase transition $M''(0)$, $N''(0) = \infty$, the set of equations gives nontrivial results for mobility edges $W_c(E) > 0$, when the lattice dimensionality is $d > 2$. For the cases $d = 2$ and $d = 1$ only the trivial solution $W_c = 0$ is possible due to the divergence of q integrals, hence states are localized and the system

behaves always as an insulator.

b) In the conducting regime $W < W_c$ we obtain $\tau = 1/M''(0) > 0$. From the expansion around $W \sim W_c$ we can fix the critical exponent $s = 1$, what is valid for $d > 2$. Thus the theory predicts a continuous drop of σ_0 near the transition, in contrast to the notion of the minimum metallic conductivity (3a,b). Of interest is also the frequency dependence $\sigma(\omega)$, namely it reveals a marked deviations from the usual Drude–type behaviour

$$\mathrm{Re}\,\sigma(\omega) = \sigma_0/(1 + \omega^2\tau^2)\,. \tag{10}$$

While equation (10) predicts a maximum at $\omega = 0$, in reality (see Fig. 3) it moves to larger frequency with increasing disorder W.

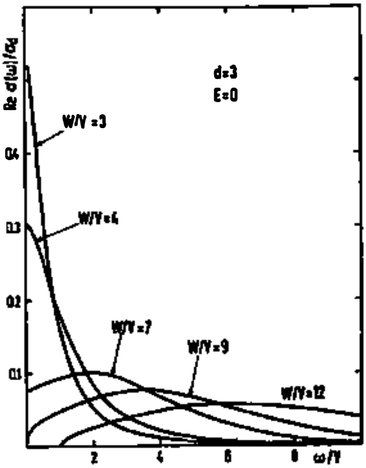

Fig. 3.
ac conductivity for the Anderson model on the simple cubic lattice for various parameters W/V, obtained with the method of kinetic equations[12].

c) In the insulating regime $W > W_c$ the system of equations is solvable at small frequencies only if M and N obey the analytic behaviour $M(z) = \eta/z$ and $N(z) = \zeta/z$, functions have thus one pole at $z = 0$, what is consistent with the nonergodic behaviour. Static polarizability $\chi(0)$ is finite and in the vicinity of the transition we obtain via expansion the result $\nu = 1/(d-2)$, when $2 < d \lesssim 4$. $\sigma_0 = 0$ in this regime, nevertheless $\mathrm{Re}\,\sigma(\omega)$ increases for larger ω. As we see from Fig. 3, one can fix the transition from $\sigma(\omega)$ curves only at low ω, whereas at larger frequencies an insulator cannot be resolved from an conductor.

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