LOCAL MOMENTS AND LOCALIZED STATES

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by
PHILIP W. ANDERSON
Bell Telephone Laboratories, Inc, Murray Hill, New Jersey, and Princeton University, Princeton, New Jersey, USA

I was cited for work both. in the field of magnetism and in that of disordered systems, and I would like to describe here one development in each held which was specifically mentioned in that citation. The two theories I will discuss differed sharply in some ways. The theory of local moments in metals was, in a sense, easy: it was the condensation into a simple mathematical model of ideas which. were very much in the air at the time, and it had rapid and permanent acceptance because of its timeliness and its relative simplicity. What mathematical difficulty it contained has been almost fully- cleared up within the past few years.

Localization was a different matter: very few believed it at the time, and even fewer saw its importance; among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it. Only now, and through primarily Sir Nevill Mott's efforts, is it beginning to gain general acceptance.

Yet these two finally successful brainchildren have also much in common: first, they flew in the face of the overwhelming ascendancy. at the time of the band theory of solids, in emphasizing *locality* : how a magnetic moment, or an eigenstate, could be permanently pinned down in a given region. It is this fascination with the local and with the failures, not successes, of band theory, which the three of us here seem to have in common. Second, the two ideas were born in response to a clear experimental signal which contradicted the assumptions of the time; third, they intertwine my work with that of my two great colleagues with whom I have been jointly honored; and fourth, both subjects are still extremely active in 1977.

I. The "Anderson Model": Local Moments in Metals

To see the source of the essential elements of the model I set up for local moments in metals, it will help to present the historical framework. Just two years before, I had written a paper on "superexchange" (1) discussing the source and the interactions of the moments in insulating magnetic crystals such as MnO, $CuSO_4$. $5H_2O$, etc. I had described these substances as what we should now call "Mott insulators" on the insulating side of the Mott transition, which unfortunately Sir Nevill says he will not describe. Briefly, following a suggestion of Peierls, he developed the idea that these magnetic insulating salts were so because to create an ionized electronic excitation would require an additional excitation energy U, the energy necessary to change the configurations of two distant atoms from $d^n + d^n$ to $d^{n-1} + d^{n+1}$. This energy *U*

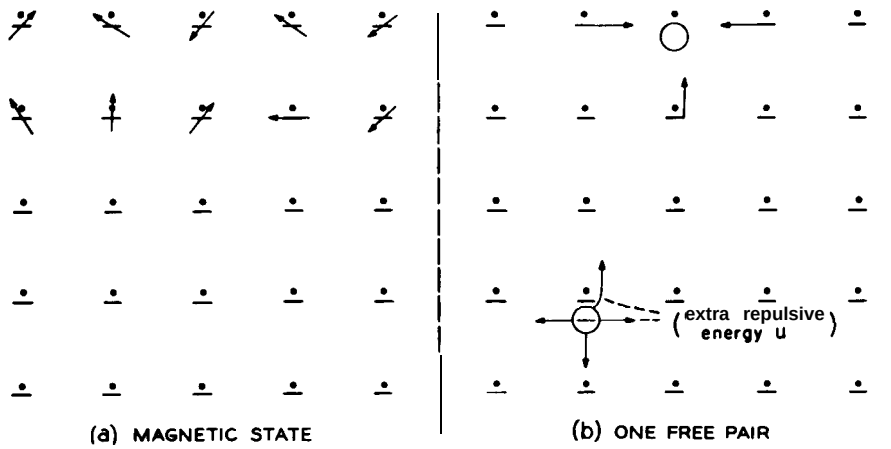


Fig. 1. Mott-Peierls mechanism for magnetic state. State with free pair has extra repulsive energy "U" of two electrons on same site.

is essentially the Coulomb repulsive energy between two electrons on the same site, and can be quite large (see Fig. 1). To describe such a situation, I set up a model Hamiltonian (now called the "Hubbard" Hamiltonian).

$$H = \sum_{i,j,\sigma} b_{ij}\, c_{i\sigma}\, c_{j\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow} \tag{1}$$

Here b_{ij} represents the amplitude for the electron to "hop" from site to site—such hops as shown in Fig. 1, right half—and U the repulsion energy between two opposite spin electrons on the same site (parallel, of course, being excluded). With (1)—appropriately generalized—it was possible to understand the predominantly antiferromagnetic interactions of the spins in these Mott insulators, which include the ancient "lodestone" or magnetite, as well as the technically important garnets and ferrites. These interactions are caused by the virtual hopping of electrons from a site to its neighbor and return, which is only

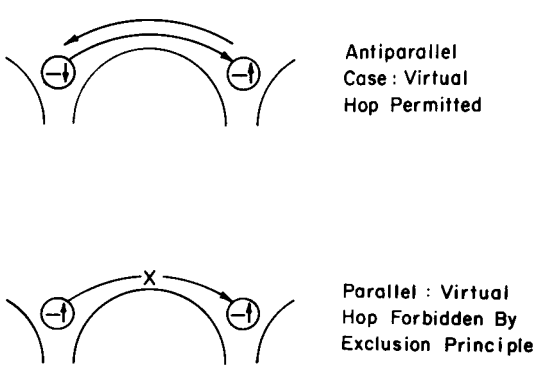


Fig. 2. Virtual hopping as the origin of superexchange.

possible for antiferromagnetism, where the requisite orbital is empty. From simple perturbation theory, using this idea,

$$\mathcal{J}_{ij} = \frac{-2b^2_{ij}}{U} \tag{2}$$

where b represents the tendency of electrons to hop from site to site and form a band. (The provenance of (2) is made obvious in Fig. 2.) In fact, I showed later in detail (2) how to explain the known empirical rules describing such interactions, and how to estimate parameters b and U from empirical data.

The implications for magnetism in metals - as opposed to insulators - of this on-site Coulomb interaction U were first suggested by Van Vleck and elaborated in Hurwitz' thesis (3) during the war, and later in a seminal paper which. I heard in 1951, published in 1953 (4). Also, very influential for me was a small conference on magnetism in metals convened at Brasenose College, Oxford, September 1959, by the Oxford-Harwell group, where I presented some very qualitative ideas on how magnetism in the iron group might come about. More important was my first exposure to Friedel's and Blandin's ideas on resonant or virtual states (5, 6) at that conference. The essence of Friedel's ideas were 1) that impurities in metals were often best described not by atomic orbitals but by scattering phase shifts for the band electrons, which would in many cases be of resonant form; 2) that spins in the case of magnetic impurities might be described by spin-dependent scattering phase shifts.

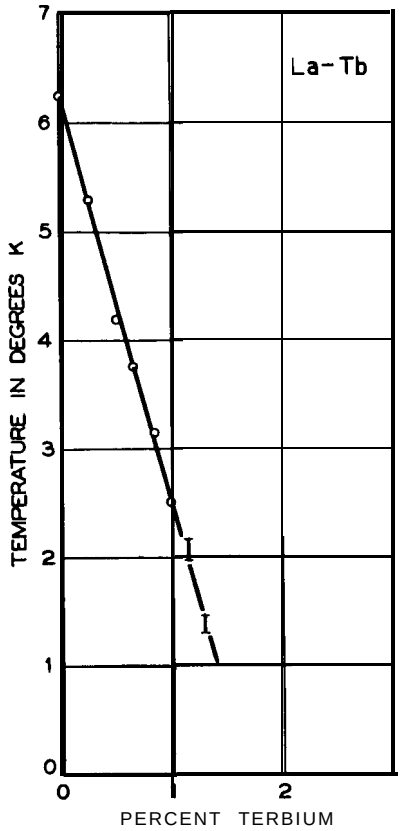
Matthias and Suhl, at Bell, were at that time much involved in experiments and theory on the effect of magnetic scatterers on superconductivity (7). For many rare earth atoms, the decrease in T_c due to adding magnetic impurities is clear and very steep; (see Fig. 3a), and even steeper for most transition metal impurities. For instance, Fe at the 10^{-5} level completely wipes out superconductivity in Mo. But in many other cases, e.g., Fe in Ti, a nominally magnetic atom had no effect, or raised T_c (as in Fig. 3b). A systematic study of the occurrence of moments was carried out by Clogston *et al* (8). As yet, no real thought (except see Ref. (6)) had been given to what a magnetic moment in a metal *meant:* the extensive investigations of Owen *et al* (9) and of Zimmermann (10), for instance, on Mn in Cu, and the Yosida calculation (11), essentially postulated a local atomic spin given by God and called S, connected to the free electrons by an empirical exchange integral J; precisely what we now call the "Kondo Hamiltonian":

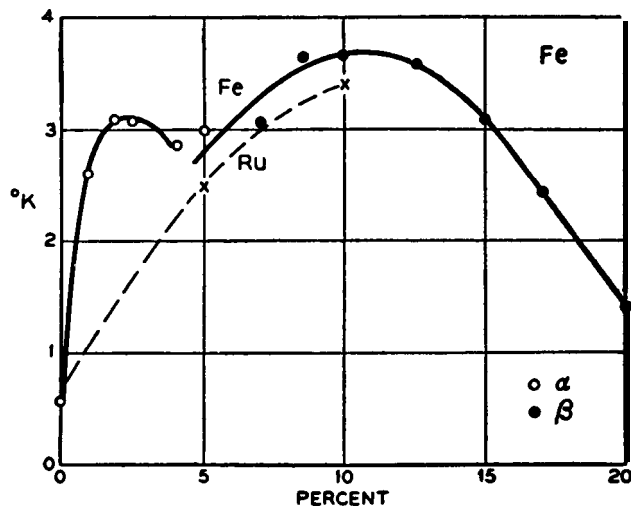
$$H = \sum_{k\sigma} \varepsilon_k \, n_{k\sigma} + \mathcal{J} \, \vec{S} \cdot \vec{s} \tag{3}$$

$$\text{where } s = \sum c^{+}_{k\sigma} \, \vec{\sigma}_{\sigma\sigma'} \, c_{k'\sigma'}$$

is the local spin density of free electrons at the impurity.

The "Anderson model" (12) is the simplest one which provides an electronic mechanism for the existence of such a moment. We insert the vital on-site exchange term U, and we characterize the impurity atom by an additional orbital φ_d, with occupancy $n_{d\sigma}$ and creation operator $c^{+}_{d\sigma}$, over and above





Superconducting transition temperatures of iron or ruthenium solid solutions in titanium.

Fig. 3. Effect of magnetic impurities on T_c of a superconductor (a); when nonmagnetic T_c goes up (b).

the free electron states near the Fermi surface of the metal (the obvious over-completeness problem is no real difficulty, as I showed later (13). The physics should be clear by reference to Fig. 4. The Hamiltonian is

$$H = \sum_{k\sigma} \varepsilon_k \, n_{k\sigma} + U n_{d\uparrow} n_{d\downarrow} + E_d \, (n_{d\uparrow} + n_{d\downarrow}) \tag{4}$$

$$+ \sum_{k\sigma} V_{dk} \, (c_{d\sigma} c_{k\sigma} + cc)$$

where in addition to free electrons and the magnetic term U, we have a d-to-k tunneling term V_{dk} representing tunneling through the centrifugal barrier which converts the local orbital φ_d into one of Friedel's resonances. The resonance would have a width

$$\Delta = \pi < V^2_{dk} > \varrho(E_d) \tag{5}$$

and in the absence of U would be centered at E_d, the energy of the d resonance (if the density of states ϱ is sufficiently constant—see Fig. 4 again).

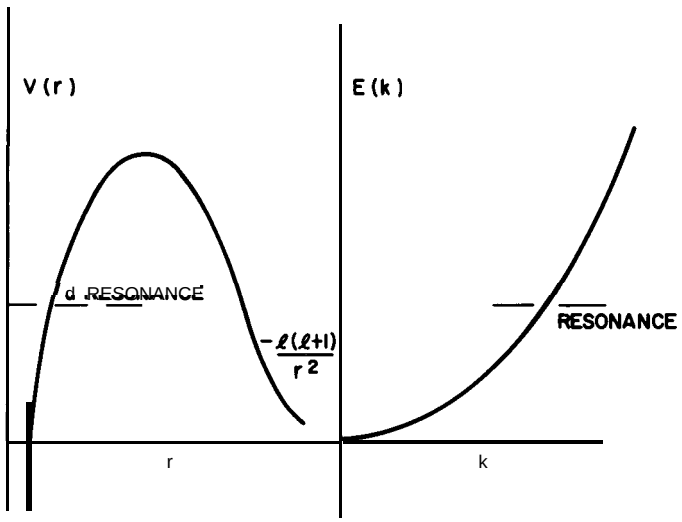


Fig. 4. d-Resonance due to tunneling through the centrifugal barrier.

A simple Hartree-Fock solution of this Hamiltonian showed that if E_d is somewhat below E_F, and if $\Delta/U < \pi$, the resonance will split as shown in Fig. 5 (from the original paper). One has two resonances; one for each sign of spin, a mostly occupied one below the Fermi level and a mostly empty one above. This leads to a pair of equivalent magnetically polarized solutions, one for each direction of spin. In these solutions, the local state φ_d is mixed into scattered free-electron states: there are no local bound electronic states, but there is a local moment. Again, in Hartree-Fock theory, the magnetic region is shown in Fig. 6. The parameters could be estimated from chemical data or from first principles, and it was very reasonable that Mn or Fe in

polyelectronic metals should be non-magnetic as was observed, but magnetic in, for instance, Cu.

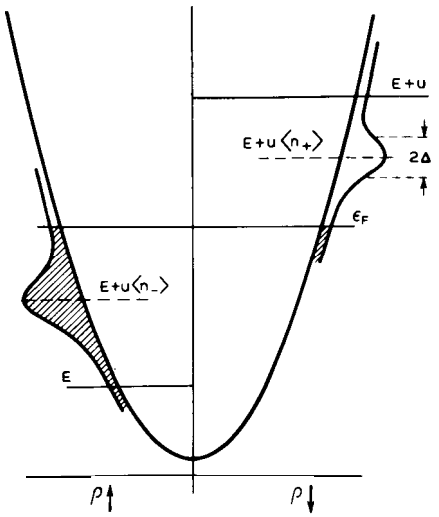


Fig. 5. Spin-split energy levels in the magnetic case.

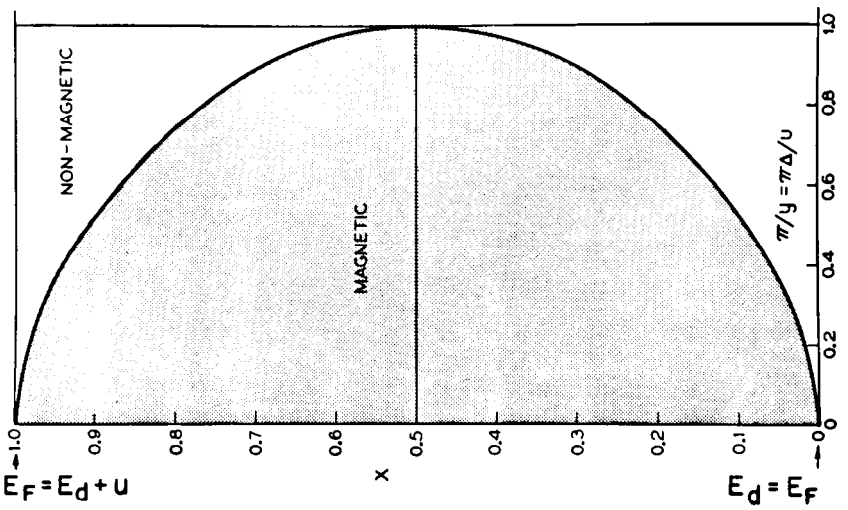


Fig. 6. Magnetic region of parameter space in the "Anderson Model".

This seems and is a delightfully simple explanation of a simple effect. The mathematics is shamelessly elaborated (or simplified) from nuclear physics (Friedel's improvements on Wigner's theory of resonances) and similar things occur in nuclear physics called "analog resonances". Nonetheless, it has led to an extraordinary and still active ramification of interesting physics.

Before discussing some of these branchings, let me say a bit about the model's simplicity, which is to an extent more apparent than real. The art of

model-building is the exclusion of real but irrelevant parts of the problem, and entails hazards for the builder and the reader. The builder may leave out something genuinely relevant; the reader, armed with too sophisticated an experimental probe or too accurate a computation, may take literally a schematized model whose main aim is to be a demonstration of possibility. In this case, I have left out (1) the crystal structure and in fact the atomic nature of the background metal, which is mostly irrelevant indeed. (2) The degeneracy of the *d* level, which leads to some important physics explored in an Appendix of the paper and later and much better by Caroli and Blandin (14). In the Appendix I showed that if the resonance was sufficiently broad compared to other internal interactions of the electrons in the *d* orbitals, the different *d* orbitals would be equally occupied as is usually observed for transition metal impurities; in the opposite case the orbital degrees of freedom will be "unquenched", as is almost always the case for rare earth atoms. (3) Left out are all correlation effects except *U;* this relies on the basic "Fermi liquid" idea that metallic electrons behave as if free, but detaches all parameters from their values calculated naively: they are *renormalized,* not "bare" parameters. This is the biggest trap for the unwary, and relies heavily on certain fundamental ideas of Friedel on scattering phase shifts and Landau on Fermi liquids. I have also left out a number of real possibilities some of which we will soon explore.

One of my strongest stylistic prejudices in science is that many of the facts Nature confronts us with are so implausible given the simplicities of nonrelativistic quantum mechanics and statistical mechanics, that the mere demonstration of a reasonable mechanism leaves no doubt of the correct explanation. This is so especially if it also correctly predicts unexpected facts such as the correlation of the existence of moment with low density of states, the quenching of orbital moment for all *d*-level impurities as just described, and the reversed free-electron exchange polarization which we shall soon discuss. Very often such, a simplified model throws more light on the real workings of nature than any number of "ab initio" calculations of individual situations, which even where correct often contain so much detail as to conceal rather than reveal reality. It can be a disadvantage rather than an advantage to be able to compute or to measure too accurately, since often what one measures or computes is irrelevant in terms of mechanism. After all, the perfect computation simply reproduces Nature, does not explain her.

To return to the question of further developments from the model : I should like to have had space to lead you along several of them. Unfortunately, I shall not, and instead, I shall show you a Table of the main lines, and then follow one far enough to show you an equation and a picture from the recent literature.

The one of these lines I would like to take time to follow out a bit is the "model" aspect I. This started as a very physical question: what is the sign and magnitude of the spin-free electron interaction? Already in '59 *before* the model appeared, I made at the Oxford Discussion a notorious bet of one pound with (now Sir) Walter Marshall that the free-electron polarization caused by the spins in metals would be negative, for much the same reason as in

Table 1 : Ramifications of the Anderson Model

I.	AM as an exact field-theoretic model-see text: a) AM = Kondo; Anderson, Clogston, Wolff, Schrieffer b) Fundamental difficulties of both: Alexander, Schrieffer, Kondo, Suhl, Nagaoka, Abrikosov c) Solution of Kondo: PWA, Yuval, Hamann, Yosida, Wilson, Nozieres, etc. d) Solution of AM: Hamann, Wilson, Krishna-Murthy, Wilkins, Haldane, Yoshida, etc.
II.	"Microcosmic" view of magnetism in metals; interacting AM's and rules for alloy exchange interactions, Alexander, PWA (15), Moriya (16)
III.	Applications to Other Systems a) Adatoms and molecules on surfaces, Grimley (17), Newns (18), etc. b) Magnetic impurities in semiconductors, Haldane (19) c) With screening+phonons, - U: mixed valence, surface centers, etc., Haldane (20) The sky seems to be the limit.

superexchange: the occupied spin state *below* the Fermi level is repulsive, that above is attractive because it can be occupied by the free electrons of the same spin. Clogston and I published this for the Anderson model (21). This was formalized by Peter Wolff, and published later with. Schrieffer (22), into a perturbative equivalence of "Kondo" and "Anderson" models with the exchange integral $\mathcal{J}$ of (3) being

$$\mathcal{J} = \frac{2\Delta}{\pi}\left(\frac{1}{E_d} - \frac{1}{E_d+U}\right) \tag{6}$$

$$(\Delta = \pi < |V_{dk}|^2 > \varrho(E_F))$$

Soon, however, it came to be realized that neither Kondo nor Anderson models behaved reasonably at low temperatures (Kondo (23), Suhl (24), Schrieffer (25), etc.), but exhibited nasty divergences at low temperatures which seemed to signal disappearance of the local moment. The best physical description of what happens (for a more extensive review for nonspecialists perhaps my series of papers in Comments on Solid State Physics will suffice) is that at high temperatures or on high energy (short time) scales, the Hartree-Fock theory given above is correct, and there is a free spin. But as the energy scale is lowered, the effective antiferromagnetic coupling between this spin and the free-electron gas "bootstraps" itself up to a very large value, eventually becoming strong enough to bind an antiparallel electron to it and become non-magnetic. This is a very precise analog of the process of continuous "confinement" of the color degrees of freedom of modern quark theories (26) and is a delightful example of the continuing flow of ideas and techniques back and forth between many-body physics and quantum field theory.

In the past few years extensive investigations via renormalization group theory (which, in a nearly modern form, was first applied to this problem (27)) have led to the essential solution of this "Kondo problem". A very succinct way of describing that solution is the computation of the scaling of the susceptibility as a function of temperature by Wilson (28) (Fig. 7). For comparison, and to show the remarkable precision of the Schrieffer-Wolff transformation,

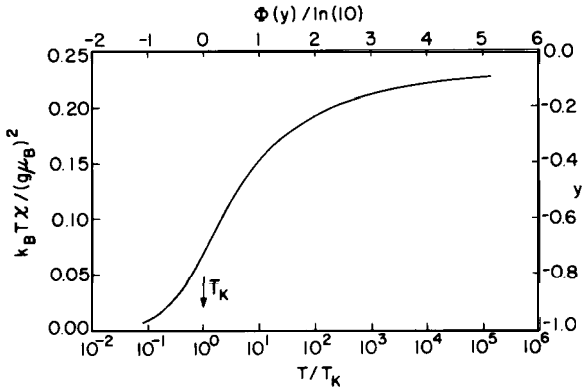


Fig. 7. Susceptibility of the Kondo Model as calculated by Wilson.

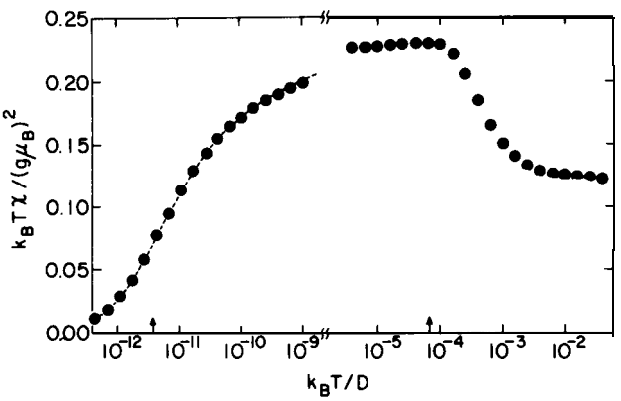


Fig. 8. Susceptibility of the "Anderson Model" showing equivalence to Kondo. (from Krishna-Murthy et al (29))

we give as the last figure of this subject Krishna-Murthys' corresponding calculation (29) for the Anderson model (Fig. 8) and one equation: Haldane's precise equivalencing of the parameters of the two models, from his thesis (20) :

$$T_K = \frac{1}{2\pi}\left(\frac{2\Delta U}{\pi}\right)^{1/2} \exp\left[\frac{E_d(E_d+U)}{2\Delta U}\right] \tag{7}$$

which may be used to find the properties of one model from the other: e.g.,

$$X(t\rightarrow 0) = \cdot\frac{103}{T_K} \text{ etc.}$$

I am indebted to a London Times article about Idi Amin for learning that in Swahili "Kondoism" means "robbery with violence." This is not a bad description of this mathematical wilderness of models; H. Suhl has been heard to say that no Hamiltonian so incredibly simple has ever previously done such violence to the literature and to national science budgets.

II. The Origins of Localization Theory

In early 1956, a new theoretical department was organized at the Bell Laboratories, primarily by P. A. Wolff, C. Herring and myself. Our charter was unusual in an industrial laboratory at the time: we were to operate in an academic mode, with postdoctoral fellows, informal and democratic leadership, and with an active visitor program, and that first summer we were fortunate in having a large group of visitors of whom two of those germane to this story were David Pines and Elihu Abrahams.*

The three of us took as our subject magnetic relaxation effects in the beautiful series of paramagnetic resonance experiments on donors in Si begun by Bob Fletcher and then being carried on by George Feher. Feher was studying (primarily) paramagnetic resonance at liquid He temperatures of the system of donor impurities (e.g., P, As, etc.) in very pure Si, in the concentration range 10^{15}-10^{18} impurities/cc encompassing the point of "impurity band" formation around 6×10^{17}. At such temperatures most of the donors were neutral (except those emptied by compensating "acceptor" impurities such as B, Al or Ga), having four valences occupied by bonds, leaving a hydrogenic orbital for the last electron which, because of dielectric screening and effective mass, has an effective Bohr radius of order 20 Å (Fig. 9). The free spin of

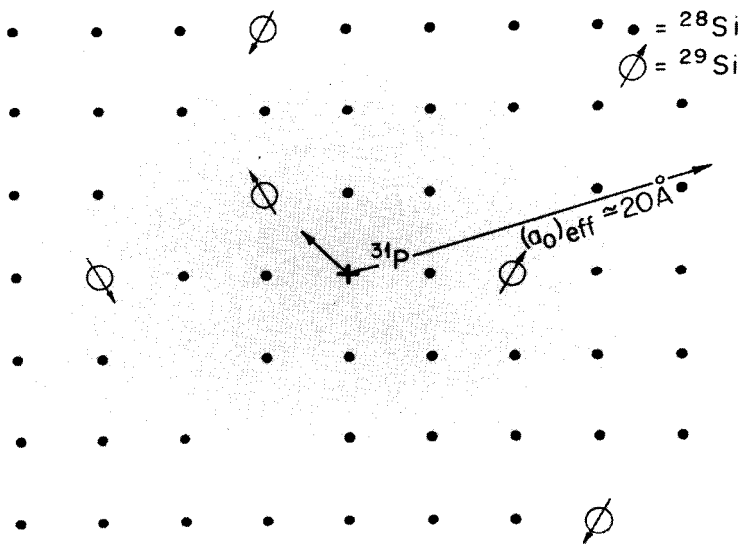


Fig. 9. Donor wave functions in Si and Si_{29} nuclei: schematic.

* It may be of interest to note that theorists permanently or temporarily employed at Bell Labs that summer were at least the following: a) (permanent or semipermanent) P. W. Anderson, C. Herring, M. Lax, H. W. Lewis, G. H. Wannier, P. A. Wolff, J. C. Phillips; b) (temporary) E. Abrahams, K. Huang, J. M. Luttinger, W. Kohn, D. Pines, J. R. Schrieffer, P. Nozieres; c) (permanent but not in theory group) : L. R. Walker. H. Suhl, W. Shockley.

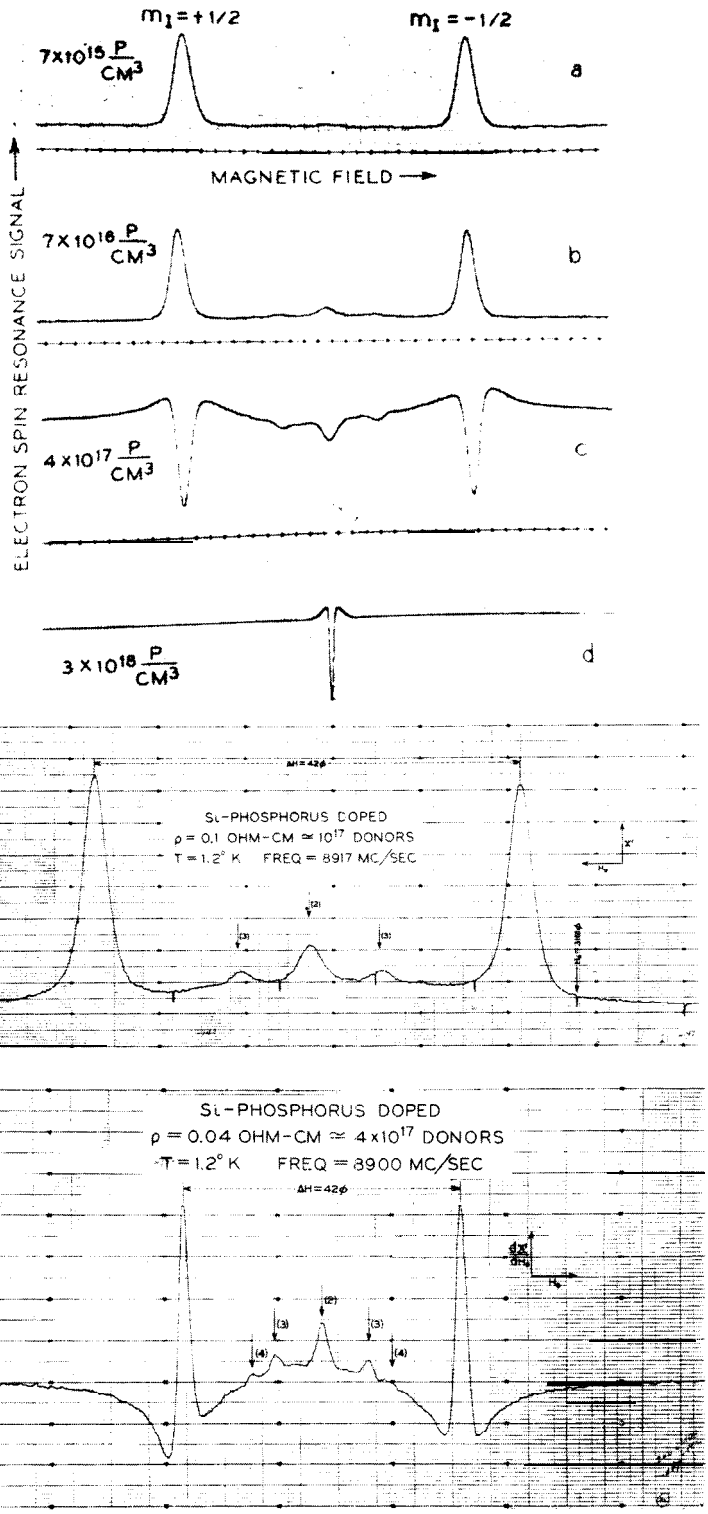
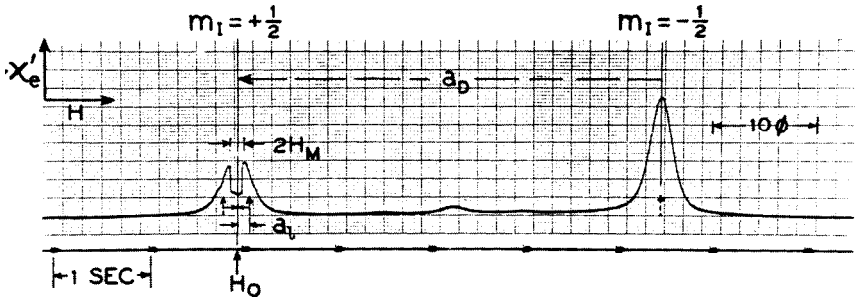


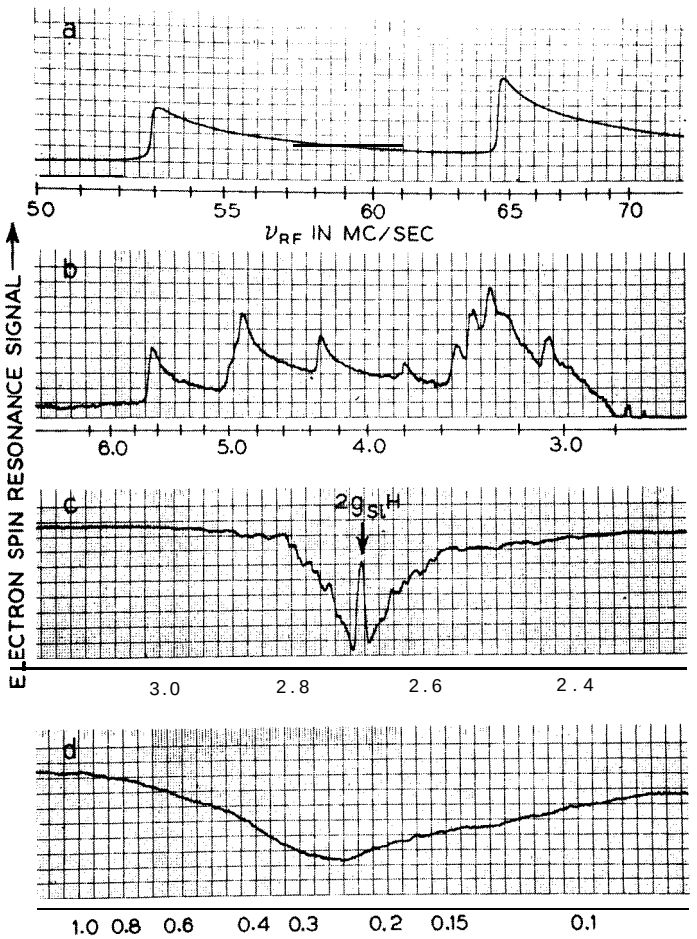
Fig. 10. a) Hyperfine structures of donor EPR at increasing donor (P) concentrations the Mott-Anderson metal-insulator transition. b) Example of well-developed cluster lines.

this extra donor orbital has a hyperfine interaction with the donor nucleus (^{31}P or As, for instance) leading to the clean hfs (30) shown in Fig. 10. In addition, isotopic substitution proved that most of the residual breadth of the lines is also caused by hfs interactions, of the very extended electronic orbital with the random atmosphere of ~ 5 % of Si_{29} nuclei in natural Si, and for reasonably low donor densities of ~ 10^{16}/cc the actual spin-spin and spin-lattice relaxation times were many seconds. That is, the lines were "inhomogeneously broadened", so that many very detailed experimental techniques were available. Feher and Fletcher (31) had already probed what we would now call the Mott-Anderson transition in these materials (Fig. 10a) . As the concentration was raised, first lines with fractional hfs appeared, signifying clusters of 2, 3, 4, or more spins in which the exchange integrals between donors overweighed the hf splitting and the electron spins saw fractionally each of the donor nuclei in the cluster. (A good example is shown in Fig. 10b.) Finally, at ~ 6 x 10^{17}, came a sudden transition to a homogeneously broadened free-electron line: the electrons went into an "impurity band" at that point. Pines, Bardeen and Slichter (33) had developed a theory of spin-lattice relaxation for donors, and it was our naive expectation that we would soon learn how to apply this to Feher's results. In fact, no theoretical discussion of the relaxation phenomena observed by Feher was ever forthcoming, only a description of the experiments (34). What the three of us soon realized was that we were confronted with a most complex situation little of which we understood. In particular, we could not understand at all the mere fact of the extremely sharp and well-defined "spin-packets" evinced by such experiments as "hole digging" and later the beautiful "ENDOR" effect (32, 34). (In the ENDOR experiment Feher would select a spin packet by saturating the line at a specific frequency ("digging a hole", Fig. 1 la) and monitor the nmr frequencies of ^{29}Si nuclei in contact with packet spins by exciting with the appropriate radio frequency and watching the desaturation of the packet (Fig. 1 lb). In this figure, the many seconds recovery time after passing the ENDOR line is actually an underestimate of the packet T_2 because the system is driven.) Thus every individual *P* electron had its own frequency and kept it for seconds or minutes at a time.

We assumed from the start the basic ideas of Mott with regard to actual electron motion: that since there were few compensating acceptors, Coulomb repulsion kept most of the donors singly-occupied leaving us with the paramagnetic spin system we observed. W. Kohn seems to have suggested that even the empty donors would be pinned down by staying close to their compensating negatively charged acceptors because of Coulomb attraction (see Fig. 12). Thus there was little actual electron motion, and we noticed only some speeding up of the relaxation times as we approached what now would be called the "Mott-Anderson" transition. Stretching our gullibility a bit, we could believe that nothing spectacular was *necessarily* required to prevent mobility of the actual charged electron excitations. (It was, however, at this time that I suggested to Geballe the study of dielectric relaxation in these materials to probe this motion, which led to the discovery of the now well-



DEMONSTRATION OF THE INHOMOGENEOUS BROADENING IN P-DOPED SILICON ($\rho = 0.25\ \Omega$ CM, T = 1.2° K, $H_O = 3000\ \phi$) IN THE ENDOR TECHNIQUE SPIN PACKETS ARE FLIPPED AS INDICATED BY ARROWS



DOUBLE RESONANCE SPECTRUM IN P-DOPED Si.
$\approx 2 \times 10^{16}$ P/CM^3, T=1.3° K, $\nu_e \approx 9000$ MC/SEC

Fig. 11. a) "Hole-digging" and ENDOR spectrum. While saturating a specific frequency (11a) an rf signal of variable frequency is applied (11b). Note slow refilling of hole (exponential recoveries) in Fig. 11b: sweep time is several minutes. This is the Si^{29} spin-lattice relaxation, enhanced by the rf power applied.

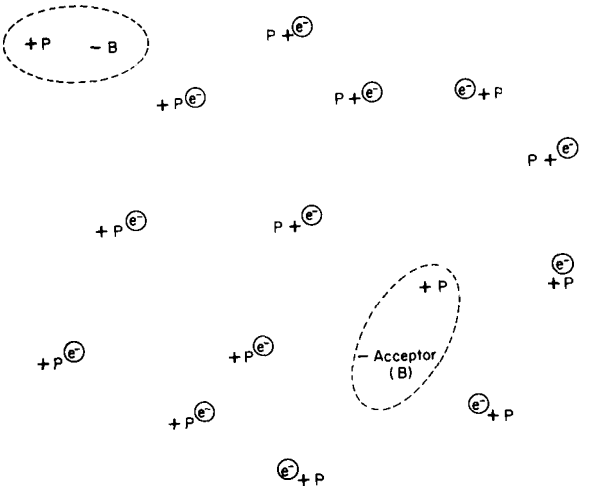


Fig. 12. Hypothetical binding of charged donors to acceptors.

known Pollak-Geballe "$\omega^{0,8}$" conductivity (34). I felt that the absence of conduction in the impurity band was also a serious question, in this as in many other systems.)

No arguments using Coulomb interaction saved us from a second dilemma: the absence of spin diffusion. Bloembergen, in 1949 (36), had proposed the idea of spin diffusion in nuclear spin systems, which has since had much experimental verification. His idea was that the dipolar interactions caused mutual precessions which, in the high temperature paramagnetic state of a spin system, could by diffusion equilibrate the spin temperature in space, thereby giving a means - for example - for nuclear spins to relax by diffusing to the neighborhood of an electronic spin impurity. To calculate the process he used a simple estimate from the Golden Rule plus random walk theory.

Portis (37), in 1953, introduced the idea of random "inhomogeneous broadening" where complete equilibration within a spectral line is impeded, and instead one speaks of "spin packets" of spins having a definite resonance frequency within the line (Fig. 13). (Such packets are spatially random, of

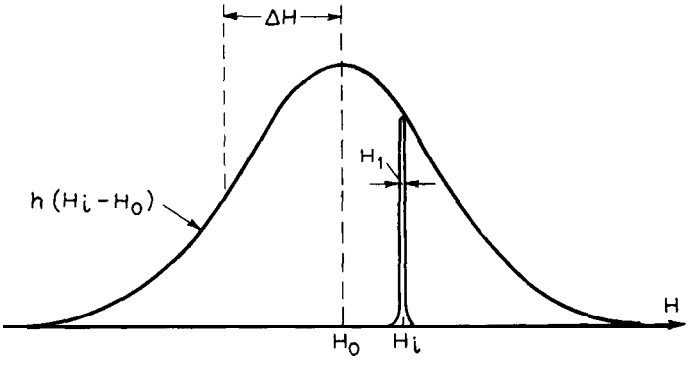


Fig. 13. "Spin packets" and spectral diffusion.

course; in macroscopically inhomogeneous systems the same phenomena had been seen much earlier.) Portis estimated that if the interaction of neighboring spins was $\mathcal{J}_{ij}$, the lifetime of a spin packet (38) should be of order

$$\hbar/\tau \simeq \pi|\mathcal{J}_{ij}|^2 \times \frac{z}{W} \tag{8}$$

W being the width of the line and z the number of neighbors: this is apparently obvious by the Golden Rule. But when Elihu Abrahams estimated $\mathcal{J}_{ij}$ for our system, he found that according to (8), τ should have varied from .1 to 10^{-6}s, whereas Feher's spin packets stayed saturated for 10-100 s in a typical ENDOR experiment. His estimates were checked by the "cluster" phenomenon of Fig. 10.

I find in my notes a reference on 6/20/56 to a discussion with Pines where I suggested an "All or Nothing" theorem to explain this. Later, on 10/31/56, comes an optimistically claimed "proof" of "Anderson's Theorem", much like an unsophisticated version of my final paper which even so is hardly a "proof" ; such. does not yet really exist. I also seem to have spoken to an uninterested audience at the Seattle International Theoretical Physics Symposium. But the actual work was not completed until shortly before I talked about it to much the same group of residents and visitors on July 10th. and 17th, 1957. By that time, I had clearly been a nuisance to everyone with "my" theorem: Peter Wolff had given me a short course in perturbation theory, Conyers Herring had found useful preprints from Broadbent and Hammersley on the new subject of percolation theory, Larry Walker had made a suggestion and Gregory Wannier posed a vital question, etc. But my recollection is that, on the whole, the attitude was one of humoring me.

Let me now give you the basics of the argument I then presented (39) but in much more modern terminology (the mathematics is the same, essentially). I don't think this is the only or final way to do it; a discussion which is more useful in many ways, for instance, can be based on Mott's idea of minimum metallic conductivity as used by Thouless and co-workers and as he will touch upon; but I think this way brings out the essential nature of this surprising nonergodic behavior most clearly. I apologize for this brief excursion into mathematics, but please be assured that I include the least amount possible.

The first problem was to create a model which contained only essentials. This was simple enough: a linearized, random "tight-binding" model of non-interacting particles:

$$H = \sum_i E_i n_i + \sum_{ij} V_{ij}\, c_i^{+} c_j \tag{9}$$

in which the "hopping" integrals V_{ij} were taken to be nonrandom functions of r_{ij} (the sites i can sit on a lattice if we like) but E_i was chosen from a random probability distribution of width W (Fig. 14). The objects c_i could be harmonic oscillator (phonon) coodinates, electron operators, or spinors for which $V_{ij} \simeq \mathcal{J}_{ij}$ and we neglect the $\mathcal{J}_{ij} S_i^z S_i^z$ interactions of the spin flips. The essential thing is that (9) leads to the linear equation of motion

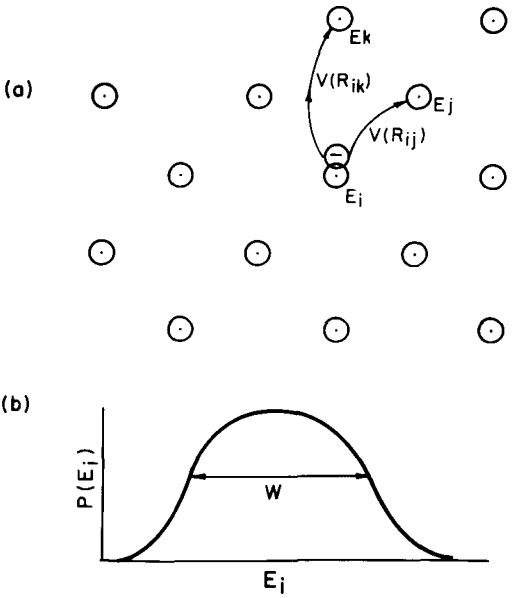


Fig. 14. Model for diffusion in a random lattice
a) sites and hopping integrals
b) probability distribution of E_i

$$ihc_i = E_i c_i + \sum V_{ij} c_j \qquad (10)$$

If W is zero and all E_i the same (say 0), (10) describes a band of Bloch states of width about $\sum \bar{V}_{ji}$. For $W \ll \bar{V}_{ij} = V$, the theories of transport recently developed by Van Hove and Luttinger (40) clearly would describe resistive impurity scattering of free waves (say, electrons, for simplicity). If, on the other hand, $W \gg V$, that would describe our system of local hf fields large compared to $\mathcal{J}_{ij}$; or of random Coulomb and strain energies large compared to the hopping integrals for the electrons from donor to donor.

What is clearly called for is to use W as a perturbation in the one case, and V_{ij} in the other; but what is not so obvious is that the behavior of perturbation theory is absolutely different in the two cases. For definiteness, let us talk in terms of the "resolvent" or "Greenian" operator which describes all the exact wavefunctions φ_a and their energies E_a:

$$G = \frac{1}{\mathrm{E}-\mathrm{H}}; \text{ i.e. } G(r, r') = \sum_a \varphi_a(r) \frac{1}{E - E_a} \varphi_a(r') \qquad (11)$$

where the φ_a and E_a are the exact eigenfunctions of the Hamiltonian (9). In the conventional, "transport" case, we start our perturbation theory with plane-wave-like states

$$\varphi_k^0 = \frac{1}{\sqrt{N}} \sum_i e^{ik \cdot R_i} \varphi_i$$

with energy

$$E_k = \sum_{(i-j)} V_{ij} \cos k \cdot (R_i - R_j)$$

which we assume are only weakly perturbed by the scattering caused by randomly fluctuating E_i's. The E_k's are a continuum in the limit of a large system and we take advantage of this to rearrange perturbation theory and get

$$G_{kk} = \frac{1}{E - E_k - \sum(k, E)} \tag{12}$$

where $\sum$, the "self-energy", is itself a perturbation series (Fig. 15a)

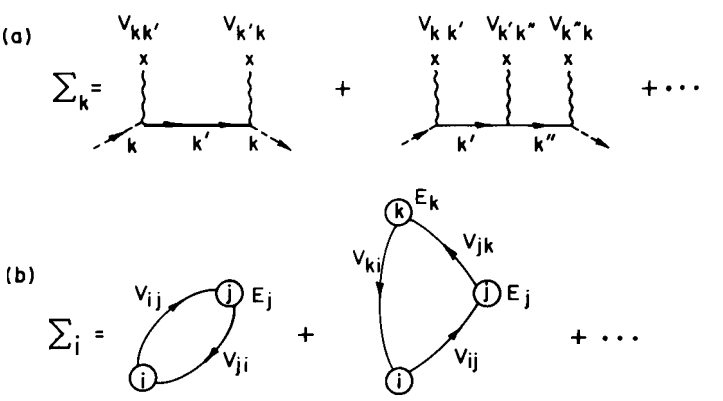


Fig. 15. a) Self-energy diagrams in conventional "propagator" theory.
b) Self-energy diagrams in "locator" theory.

$$\sum = \sum_{k' \neq k} (V_{kk'})^2 \frac{1}{E - E_{k'}} + \sum_{k'', k' \neq k} \frac{V_{kk''} V_{k''k'} V_{k'k}}{(E - E_{k'})(E - E_{k''})} + \ldots \tag{13}$$

which, since E_k is a continuum, has a finite imaginary part as E approaches the real axis

$$\lim_{\mathrm{Im}E \to \pm 0} \mathrm{Im} \sum = \pm \pi \int |V_{kk'}|^2 \delta(E_{k'} - E) + \ldots \tag{14}$$

Note that $V_{kk'}$ in this case comes from the width "W" not V_{ij}.)

This equation means that E_k has a finite width. in energy, and ImG, the density of states, is a finite, continuous function of E (Fig. 16).

$$\lim_{s \to \pm 0} G_k(E + is) = \frac{1}{E - E_k - R_e \sum \mp i\Delta(E)} \tag{15}$$

G has a genuine *cut* on the real axis, and there is a continuum of energy states at every site, of every energy in the band: the states are what we now call "extended". That is, the definition (11) of G basically tells us

$$\mathrm{Im}G(i, i; E) = \pi \sum_a |\varphi_a(r_i)|^2 \delta(E - E_a). \tag{16}$$

Transforming (15) to find G_{ii}, we find that the $|\varphi_a(r_i)|^2$ are each infinitesimal

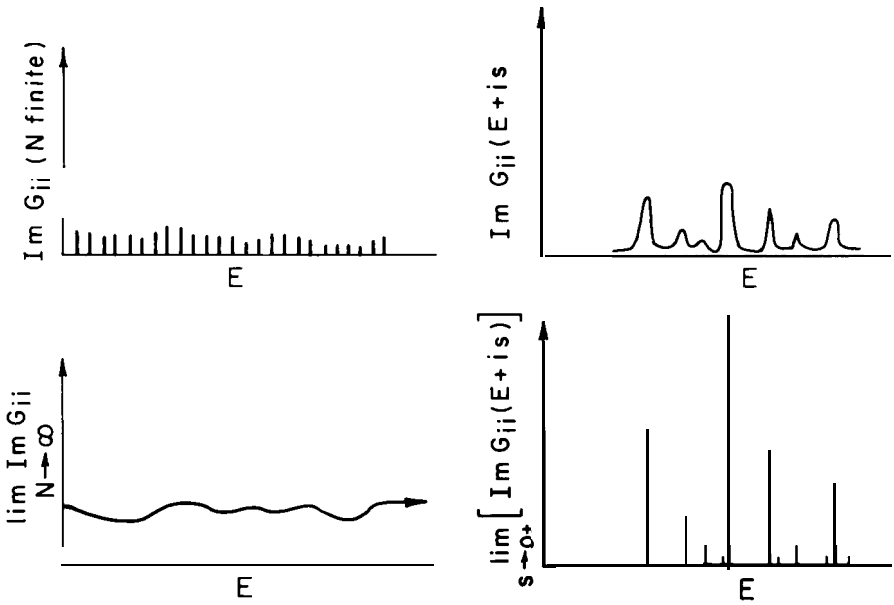


Fig. 16. a) Im G_{ii} in extended case
b) Im G_{ii} in localized case

of order $\frac{1}{\sqrt{N}}$, forming in the limit $N \to 0$ a true continuum of states of every energy at site i. Of course, there are sum rules stating that every state is somewhere and that no states get lost:

$$\sum_i |q_a(i)|^2 = \sum_a |q_a(i)|^2 = 1 \tag{17}$$

and these are satisfied by $q_a(i) \sim (\sqrt{N})^{-1}$, where N is the total number both of *a's* and *i's*.

My contribution was just to show that this is not the only possible case, other than just an empty band of energies, or a set of discrete states as one may have near a single attractive potential like a hydrogen atom. What I showed is that one may have a continuum in energy but not in *space*. This is immediately made plausible just by doing perturbation theory in the opposite order.

In this case one takes E_i as the big term, and the starting eigenfunctions and eigen-energies are just

$$\varphi_i^0 = \varphi_i,\ E_i^0 = E_i \tag{18}$$

and V_{ij} is the perturbation. In this case, (which Larry Walker suggested I call "cisport") we use a "locator" instead of a "propagator" series, for the "locator" G_{ii} not the "propagator" G_{kk}:

$$G_{ii}(E+is) = \frac{1}{E+is-E_i-\sum_i(E+is)} \tag{19}$$

where now the self-energy $\sum$ is a superficially similar series to (13) (Fig. 15b)

$$\sum_i = \sum_{j \neq i} \frac{(V_{ij})^2}{E - E_j} + \sum \frac{V_{ij}\, V_{jk}\, V_{ki}}{(E-E_j)(E-E_k)} + \cdots \tag{20}$$

If at this point we make one tiny mistake, we immediately arrive back at Portis' answer (8) : namely if we *average* in any way, we get

$$\mathrm{Ave}\left\{ \lim_{s \to 0+} \left(\mathrm{Im} \sum_{j,\, k \neq i} (E + is) \right) \right\} \simeq \frac{\langle V_{ij}^2 \rangle}{W} \tag{21}$$

But there is a very important fundamental truth about random systems we must always keep in mind *: no real atom is an average atom, nor is an experiment ever done on an ensemble of samples* . What we really need to know is the *probability distribution* of $\mathrm{Im}\sum$, *not* its average, because it's only each specific instance we are interested in. I would like to emphasize that this is the important, and deeply new, step taken here: the willingness to deal with *distributions,* not averages. Most of the recent progress in the fundamental physics of amorphous materials involves this same kind of step, which implies that a random system is to be treated not as just a dirty regular one, but in a fundamentally different way.

Having taken this point of view, it is sufficient to study only the first term of (20), it turns out. Let us first pick a finite s, and then take the limit as s → o. With a finite s,

$$\mathrm{Im}\left(\frac{\sum}{s} \right) = \sum_j \frac{|V_{ij}|^2}{(E-E_j)^2 + s^2}$$

The condition that E_j appear as a peak of Im $\frac{\sum}{s}$ is that E_j be within s of E, and that $V_{ij} >$ s. To assess the probability that V_{ij} is large enough, use the physically realistic assumption of exponential wavefunctions:

$$V(R) = V_0\, \mathrm{e}^{-R/R_0}.$$

In the energy interval of size s, there will be ns/W energies E_j per unit volume ($\mathcal{N}$ is the site density per unit volume), while $V >$ s implies

$$V > s : R < R_0 \ln \frac{s}{V_0}$$

and the probability that both V > s and $E\text{-}E_j < s$ is

$$P(V > s,\, |E - E_j| < s) = \mathcal{N} \cdot \frac{4\pi R_0^3}{3} \left(\frac{s}{W} \right) \left(\ln \frac{s}{V_0} \right)^3$$

$$P(s \to \mathrm{o}) = 0$$

It is easy to formalize this: one may show that the probability distribution of $\mathrm{Im}\sum$ is essentially

$$\lim_{s \to 0} P\left(\mathrm{Im}\left(\frac{\sum}{s} \right) = X \right) \mathrm{d}X = \frac{\mathrm{d}X}{X^{3/2}}\, \mathrm{e}^{-\frac{s}{X}} \tag{22}$$

which indeed has a divergent average as it should, but is finite nonetheless, so that $\mathrm{Im}\sum \propto s$ and there is not a finite cut at the real axis.

When we stop and think about what this means, it turns out to be very simple. It is just that we satisfy the sum rules (17) not by each $\varphi_a(i)$ being infinitesimal, but by a discrete series of finite values: the biggest φ_a^i is of order 1, the next of order l/2, etc., etc., (see Fig. 16b). Thus, $\mathrm{Im}G_{ii}$ is a sum of a discrete infinite series of &functions with convergent coefficients. This is the *localized* case.

That is more than enough mathematics, and is all that we will need. The rest boils down simply to the question of when this lowest-order treatment is justified, and how it breaks down.

The bulk of the original paper was concerned with how to deal with the higher terms of the series and show that they don't change things qualitatively : what they do, actually, is just to *renormalize* V_{ij} and the *Ej's* so that even if V_{ij} is short-range initially, it becomes effectively exponential; and, of course, the $V_{ij's}$ broaden the spectrum. If this is the case, one then realizes that the extended case can only occur because of a breakdown of perturbation theory. This comes about as the higher terms of perturbation theory "renormalize" $V(R_j)$ and stretch it out to longer and longer range, so that the exponentially localized function become less so and finally one reaches a "mobility edge" or "Anderson transition".

Here we begin to tie in to some of the ideas which Professor Mott will describe. First, it is evident that the self-energy series is a function of E-i.e., of where we are on the real energy axis - so it will cease to converge first at one particular energy *E,* the "mobility edge." For a given model, it is reasonable - in fact usual - to have the localized case for some energies, the extended one for others, separated by a "mobility edge". The significance of this fact was realized by Mott.

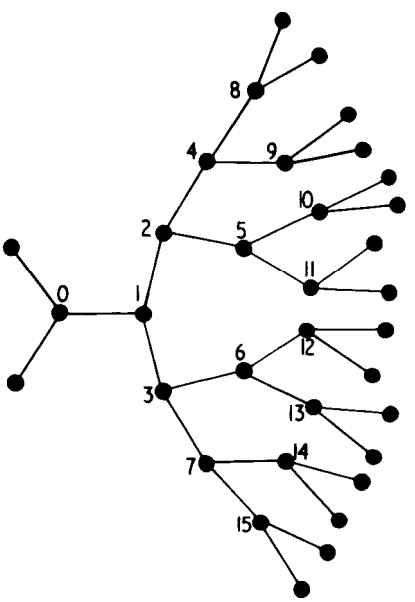


Fig. 17. "Cayley Tree" on which localization theory is exact.

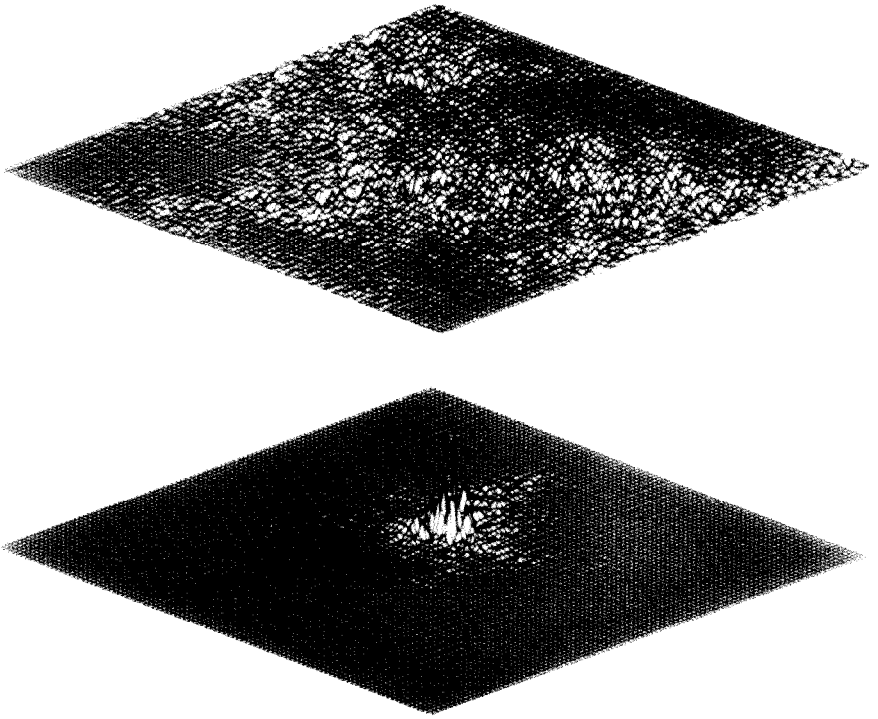


Fig. 18. Computer demonstration of localization (courtesy of Yoshino and Okazaki).
a) W/V = 5.5
b) W/V = 8.0

The actual calculation of this divergence or "Anderson transition" was carried out by me using conservative approximations in the original paper, but it was only much later realized (41) that that calculation was exact on a "Cayley tree" or Bethe Lattice (Fig. 17). Much earlier, Borland (42) and Mott and Twose (43) had shown that localization always occurs in one dimension (also a Cayley tree case, with K = 1). Since it is easy to convince oneself that the Cayley tree is a lattice of infinite dimensionality *d* (though finite neighbor number) it is likely that delocalization first occurs at some lower critical dimensionality d_c, which we now suspect to be 2, from Thouless' scaling theory (44). This dimensionality argument (or equivalent ones of Thouless) first put to rest my earliest worry that my diagram approximations were inexact : in fact, they *under* estimate localization, rather than otherwise. A second reason why I felt discouraged in the early days was that I couldn't fathom how to reinsert interactions, and was afraid they, too, would delocalize. The realization that, of course, the Mott insulator localizes without randomness, because of interactions, was my liberation on this: one can see easily that the Mott and Anderson effects supplement, not destroy, each other, as I noted in some remarks on the "Fermi Glass" (45) which more or less marked my re-entry into this problem. The present excitement of the field

for me is that I feel a theory of localization with interactions is beginning to appear, in work within my group as well as what Professor Mott will describe. It is remarkable that in almost all cases interactions play a vital role, yet many results are not changed too seriously by them.

I will close, then, and leave the story to be completed by Professor Mott. I would like, however, to add two things: first, a set of figures of a beautiful computer simulation by Yoshino and Okazaki (46), which should convince the most skeptical that localization does occur. The change in W between these two figures is a factor 1.5, which changed the amplitudes of a typical wave function as you see, from extended to extraordinarily well localized. (see Fig. 18).

Finally, you will have noted that we have gone to extraordinary lengths just to make our magnetic moments - in the one case - or our electrons - in the other - stay in one place. This is a situation which was foreshadowed in the works of an eminent 19th century mathematician named Dodson, as shown in the last figure (Fig. 19). "Now here, you see, it takes all the running you can do, to keep in the same place."

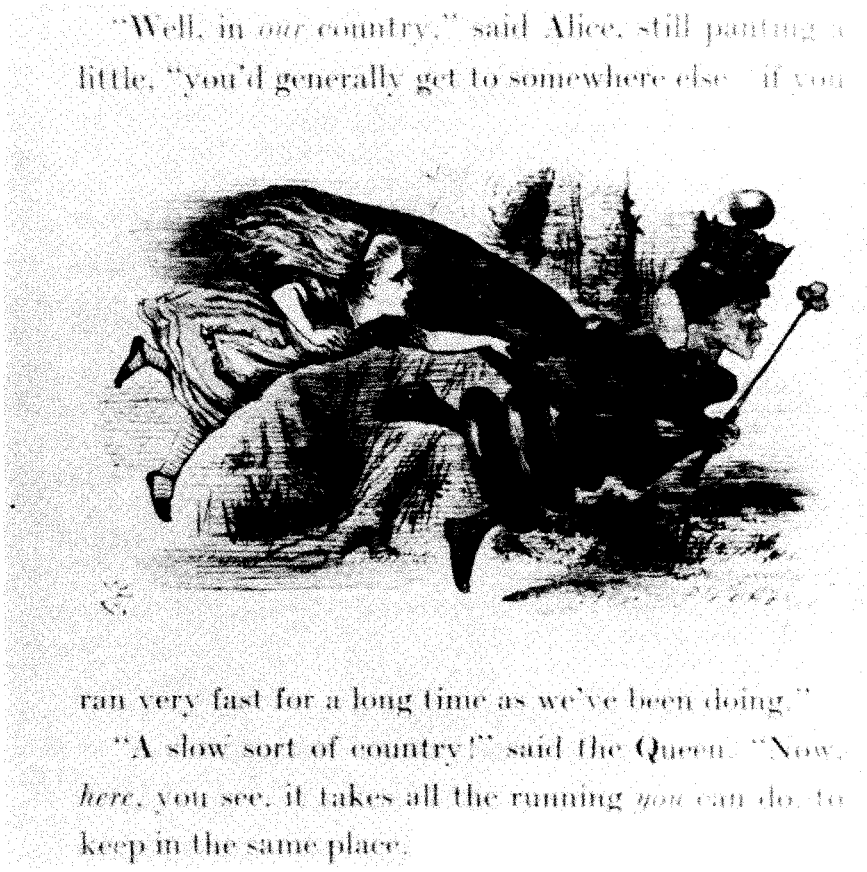


Fig. 19. Efforts to avoid localization (Dodson).

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