aided by interaction with ferromagnetic spin waves has been made by Ilisca.[7]

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[1]R. Gomer and J. R. Schrieffer, to be published.

[2]J. R. Schrieffer, to be published.

[3]S. Doniach, in *Proceedings of the International School of Physics "Enrico Fermi," Course XXXVII,* edited by W. Marshall (Academic, New York, 1967).

[4]The focusing or defocusing of paramagnons near the adatom might change this probability numerically, but it is hard to see how it could change its energy dependence.

[5]J. Kondo, Progr. Theor. Phys. 32, 37 (1967).

[6]E. I. Evzerikhin and G. D. Lyubarskii, in *Scientific Selection of Catalysts,* edited by A. A. Balandin *et al.* (Israel Program for Scientific Research, Jerusalem, Israel, 1968), Vol. XI.

[7]Where nickel-cobalt is ferromagnetic, the spin fluctuations are (a) noncollective with a gap in their spectrum equal to the exchange energy, (b) spin-wave excitations filling this gap. Only the former of these are considered here, and Eqs. (3) and (4) must be modified to allow for the gap. However, spin-wave excitations will likewise contribute to the desorption.

[8]E. Ilisca, Phys. Rev. Lett. 24, 797 (1970).

Localization in Disordered Materials: Existence of Mobility Edges*

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Anderson's theory of localization in disordered systems is extended. It is shown that mobility edges exist, in agreement with the Mott–Cohen-Fritzsche-Ovshinsky model. As the randomness increases, the mobility edges move inwards into the band, and their coincidence is termed Anderson's transition. A criterion is developed restricting the energy regions where mobility edges can be found; explicit results are obtained for a Lorentzian distribution of single-site energies.

Recent models of the electronic structure of disordered materials suppose that there are continuous bands of extended states with tails of localized states.[1,2] Current interpretations of experimental data rest heavily on this notion,[1,2] but no rigorous proof has been given. There seems little doubt of the existence of localized states in the tails,[3] but whether the character of the eigenstates changes abruptly from localized to extended at certain critical energies (termed mobility edges[2]) remains in question. Anderson[4] had demonstrated that for an electron moving in a rigid lattice subject to a Hamiltonian with random matrix elements satisfying certain conditions, the states in the middle of the band are localized, and transport ceases when the randomness in the matrix elements of the Hamiltonian exceeds a certain critical value related to the bandwidth. Mott[1] synthesized Anderson's result with the work on localization in the band tails by arguing for sharp transitions from localized to extended states and back to localized states within the band, for randomness smaller than Anderson's critical value. This model, proposed independently by Cohen, Fritzsche, and Ovshinsky,[2] we refer to as the Mott-CFO model.

We consider the motion of a particle in a three-dimensional periodic lattice[4,5] such that at each site $\vec{n}$ of the lattice the particle can occupy a Wannier state $|\vec{n}\rangle$ of energy $\epsilon_{\vec{n}}$. The Hamiltonian is

$$\langle \vec{l} | H | \vec{m} \rangle = \epsilon_{\vec{m}} \delta_{\vec{l}\vec{m}} + V_{\vec{l}\vec{m}}, \tag{1}$$

where $V_{\vec{l}\vec{m}} = V_{0,\vec{m}-\vec{l}}$ and $V_{\vec{l}\vec{l}} = 0$. The disorder is introduced into the system by allowing the single-site energies $\epsilon_{\vec{m}}$ to be random variables; any two quantities $\epsilon_{\vec{n}}$, $\epsilon_{\vec{l}}$ are taken as statistically independent whenever the distance $r_{\vec{n}\vec{l}}$ is longer than a finite correlation length. This eliminates long-range order from our system. For simplicity we assume that $V_{\vec{l}\vec{m}}$ is a constant, V, for nearest neighbors, and zero otherwise.

Following Anderson we use as a criterion for the existence of localized states overlapping with a given site $\vec{l}=0$ the absence of complete diffusion from this site, i.e., $p_{00} \neq 0$, where p_{00} is the probability of finding the particle in the state $|0\rangle$ at $t=\infty$ if initially ($t=0$) it was in $|0\rangle$. It can be shown that

$$p_{00} = \lim_{s \to 0^+} \frac{s}{\pi} \int_{-\infty}^{\infty} dE\, G_0(E+is) G_0(E-is), \tag{2}$$

where $G_0(E)$ is the 0,0 matrix element of the Green's function $G(E)=(E-H)^{-1}$. Equation (2) can be written as $p_{00}=\int_{-\infty}^{\infty}f_0(E)dE$, where $f_0(E)$ is a positive quantity given by

$$f_0(E)=n_0(E)\lim_{s\to 0^+}\{1-[\Delta_0(E+is)-\Delta_0(E-is)]/2is\}^{-1}. \tag{3}$$

Here $n_0(E)$ is the contribution to the density of states from site 0, and $\Delta_0(E)\equiv E-\epsilon_0-G_0^{-1}(E)$ is the self-energy for site 0. Thus, in order to have $p_{00}\neq 0$, eigenstates of energy E overlapping with the state $|0\rangle$ should exist [i.e., $n_0(E)\neq 0$] and should be localized {i.e., $[1-[\Delta_0(E+is)-\Delta_0(E-is]/2is]^{-1}\neq 0\}$. The latter holds when $\Delta_0(E)$ is analytic across the real axis. Isolated singularities in $\Delta_0(E)$ on the real axis have no importance because $n_0(E)$ simultaneously vanishes. Only a branch cut in $\Delta_0(E)$ on the real axis corresponds to extended states.

It can be shown[6] that the renormalized perturbation series[4] (RPS) for $\Delta_0(E)$, i.e.,

$$\Delta_0(E)=\sum_{\vec{n}\neq 0}V_{0\vec{n}}\frac{1}{E-\epsilon_{\vec{n}}-\Delta_{\vec{n}}^{0}}V_{\vec{n}0}+\sum_{\substack{\vec{n}\neq 0\\ \vec{l}\neq 0,\,\vec{n}}}V_{0\vec{n}}\frac{1}{E-\epsilon_{\vec{n}}-\Delta_{\vec{n}}^{0}}V_{\vec{n}\vec{l}}\frac{1}{E-\epsilon_{\vec{l}}-\Delta_{\vec{l}}^{0,\vec{n}}}V_{\vec{l}0}+\cdots, \tag{4}$$

converges to an analytic function apart from simple poles everywhere on the complex E plane except on those portions of the real axis which correspond to extended states. Thus an eigenstate of energy E overlapping with the state $|0\rangle$ is localized if and only if the RPS (4) converges. In (4) $\Delta_{\vec{n}}^{\vec{r},\vec{l},\cdots}$ is the self-energy corresponding to a Hamiltonian which differs from (1) in that $\epsilon_{\vec{r}}=\epsilon_{\vec{l}}=\cdots=\infty$.

Following Anderson's original suggestion, we have approached the problem of convergence of the RPS (4) probabilistically: For each energy E we find the probability that the series (4) converges (diverges). It can be shown[6] by mathematical and physical arguments that, when there is no long-range statistical correlation among the variables $\{\epsilon_{\vec{m}}\}$, there exist two non-negative functions $L(E)$ and $\chi(E,s)$ such that the magnitude of the Nth-order term of the RPS (4), $|a_N|$, is sharply distributed[7] around the quantity $\chi^N(E,s)$. Moreover when $L(E)\leq 1$, $\chi(E,s)\xrightarrow[s\to 0]{}L(E)$ and when $L(E)\geq 1$, $\chi(E,s)\xrightarrow[s\to 0]{}1$. The quantity $L^N(E)$ is defined as[6]

$$L^N(E)=\sum{}'V_{0\vec{n}_1}\tilde{G}_{\vec{n}_1}{}^{0}V_{\vec{n}_1\vec{n}_2}\tilde{G}_{\vec{n}_2}{}^{0,\vec{n}_1}\cdots V_{\vec{n}_N0}, \tag{5}$$

where

$$\ln\tilde{G}_{\vec{n}_i}{}^{0,\cdots,\vec{n}_{i-1}}=\langle\ln|E-\epsilon_{\vec{n}_i}-\Delta_{\vec{n}_i}{}^{0,\cdots,\vec{n}_{i-1}}|^{-1}\rangle, \tag{6}$$

and $\sum'$ indicates summation over all the indices $\vec{n}_1\cdots\vec{n}_N$ with the restrictions $\vec{n}_1\neq 0$, $\vec{n}_2\neq\vec{n}_1, 0,\cdots,$ $\vec{n}_N=\vec{n}_{N-1},\cdots,0$. Thus the following theorem summarizes our results:

Theorem: Consider the function $L(E)$ defined by (5) and (6). The regions of the energy spectrum for which $L(E)<1$ consist entirely of localized states, those for which $L(E)>1$ consist entirely of extended states, and the solutions of the equation $L(E_c)=1$ give the positions of the mobility edges E_c. $L(E)$ is therefore a localization function.

Suppose that Γ is a measure of the degree of randomness in the system. Then $\Gamma=0$ corresponds to the case of a perfect crystal and, since all the eigenstates of the system are then extended, $L(E)_{\Gamma=0}\geq 1$ for E inside the band, with the equality obtaining at the band edges. On the other hand, when $\Gamma\to\infty$ one can show that $\Delta_0(E)$ approaches zero everywhere and consequently that $L(E)\xrightarrow[\Gamma\to\infty]{}0$. Assuming that $L(E)$ is a continuous function of Γ for each E, we can conclude that for each energy E there is a critical value of Γ, $\Gamma_c(E)$, such that for $\Gamma\geq\Gamma_c(E)$, $L(E)<1$. If we define $\Gamma_c=\max\{\Gamma_c(E)\}$ we see that for $\Gamma>\Gamma_c$, $L(E)<1$ for every E and consequently all states are localized. This is the Anderson transition. For $0<\Gamma<\Gamma_c$ there are mobility edges at energies E_c, satisfying the equation $L(E_c)=1$, which separate regions of localized from regions of extended states, in agreement with the Mott-CFO model. It should be pointed out that Anderson and also Thouless[8] have examined the case $E=0$ and have found qualitatively similar results although not identical with the estimates to be presented here.

One can obtain an order-of-magnitude estimate for the localization function $L(E)$ by neglecting the $\Delta_{\vec{n}_i}{}^{0,\cdots\vec{n}_{i-1}}$ in Eq. (6) and by assuming that the distribution functions for each $\epsilon_{\vec{n}}$ are identical. Then

$$L(E)\approx\alpha KV/\tilde{e}, \tag{7}$$

where $\ln\tilde{e}=\langle\ln|E-\epsilon_i|\rangle$, and α is a correction

factor determined by the condition $L(E_b)_{\Gamma=0}=1$, where E_b is the band edge. K is the percolation constant[9] which is about equal to $2Z/3$, and Z is the number of nearest neighbors. We have obtained explicit results in two specific cases: (a) when the distribution of ϵ_i is a rectangular one with total width W; (b) when the distribution of ϵ_i is a Lorentzian one of half-width Γ. For case (a) the result for $L(E)$ is identical to $Z\times\exp\langle\ln|T|\rangle$ where $\langle\ln|T|\rangle$ is given by Eq. (11) of Ref. 5. In case (b) the result is

$$L(E)\approx ZV/(E^2+\Gamma^2)^{1/2}. \tag{8}$$

Anderson's transition occurs when $W=W_c$ and $\Gamma=\Gamma_c$ for cases (a) and (b), respectively, where

$$W_c\approx 2.7B, \tag{9a}$$

$$\Gamma_c\approx \tfrac{1}{2}B. \tag{9b}$$

In Eqs. (9), $B=2E_b=2ZV$ is the bandwidth. Let us note that Anderson's best estimate for W_c is $4.3B$. Using the correspondence $\frac{1}{4}W\leftrightarrow\Gamma$ [prob$(|\epsilon_i|<\frac{1}{4}W)=\frac{1}{2}$ and prob$(|\epsilon_i|<\Gamma)=\frac{1}{2}$ for the rectangular and Lorentzian distributions, respectively], we see that the estimate (9b) for the Lorentzian is about 25% less than the estimate (9a) for the rectangular. The fact that the Lorentzian gives a lower value for the critical randomness is probably due to its long tails.

A probably better estimate for the quantity $L(E)$ can be obtained if we replace the quantities $\Delta_{\vec{n}_i}{}^{0,\vec{n}_1,\cdots}$ in (6) by $\Delta_{\vec{n}_i}$ and assume that the system is periodic on the average. Then

$$L(E)\approx \beta KV\tilde{G}_0, \tag{10}$$

where β is determined from the condition $L(E_b)_{\Gamma=0}=1$ and $\tilde{G}_0$ is given by Eq. (6).

Estimate (10) however invloves the nontrivial task of evaluating $\tilde{G}_0=\exp\langle\ln|G_0|\rangle$. This evaluation can be done exactly for the case where the ϵ_i are independent random variables with a Lorentzian distribution function. Explicit results will be reported in detail elsewhere.[6]

We conclude this Letter by showing that an upper limit can be found for the quantity $L(E)$ when

$$\tilde{G}_{\vec{n}_i}{}^{0,\vec{n}_1,\cdots}(E)=|\mathcal{G}_{\vec{n}_i}{}^{0,\vec{n}_1,\cdots}[E-\textstyle\sum(E)]|, \tag{11}$$

where $\mathcal{G}_{\vec{n}_i}{}^{0,\vec{n}_1,\cdots}$ is the $\vec{n}_i,\vec{n}_i$ matrix element of the Green's function corresponding to a Hamiltonian of the form (1) with $\epsilon_0=\epsilon_{\vec{n}_1}=\cdots=\infty$ and $\epsilon_{\vec{i}}=\langle\epsilon_{\vec{i}}\rangle=0$ for every $\vec{i}\neq 0,\vec{n}_1,\cdots$. $\sum(E)$ is in general a complex function of E. One can then show that $|\mathcal{G}_{\vec{n}_i}{}^{0,\vec{n}_1,\cdots}[E-\sum(E)]|\leq\mathcal{G}_{\vec{n}_i}{}^{0,\vec{n}_1,\cdots}\times[|E-\sum(E)|]$ if $|E-\sum(E)|\geq ZV$. Thus if we define

$$\mathfrak{L}^N(E)=\textstyle\sum'V_{0\vec{n}_1}\mathcal{G}_{\vec{n}_1}{}^{0}[|E-\sum(E)|]V_{\vec{n}_1\vec{n}_0}\cdots V_{\vec{n}_N0}, \tag{12}$$

it follows that

$$L(E)\leq\mathfrak{L}(E)\text{ for }|E-\textstyle\sum(E)|\geq ZV. \tag{13}$$

However $\mathfrak{L}^N(E)$ as defined in (12) is nothing else than the Nth-order term of the RPS for $\mathfrak{D}_0[|E-\sum(E)|]$, where $\mathfrak{D}_0$ is the self-energy corresponding to the periodic case $\epsilon_{\vec{n}}=\langle\epsilon_{\vec{n}}\rangle=0$ (for every $\vec{n}$). From the theory of periodic systems it is well known that the RPS for $\mathfrak{D}_0(E)$ converges if $|E|>ZV$. Consequently $\mathfrak{L}(E)\leq 1$ for $F(E)\equiv ZV/|E-\sum(E)|\leq 1$. Thus we find that

$$L(E)<1\text{ if }F(E)<1, \tag{14}$$

but that $L(E)\to 1$ as $F(E)\to 1$ only in the limit of zero randomness. Otherwise $L(E)$ remains less than one as $F(E)$ becomes equal to unity.

To summarize, if (11) is true then all the states with eigenenergy E satisfying the relation $F(E)\leq 1$ are localized. In the limit of zero randomness the solutions of the equation $F(E_c')=1$ coincide with the mobility edges E_c. For any finite randomness the mobility edges are always in the region where $F(E)>1$. One can estimate the difference $F(E_c')-L(E_c')=1-L(E_c')$ as being $O\{|\mathrm{Im}\sum(E_c')/[E_c'-\mathrm{Re}\sum(E_c')]|^{1/2}\}$ for small randomness. This can be used for estimating the difference E_c-E_c'.

The practical importance of the preceding results lies in the fact that there are cases where (11) is satisfied either exactly (case of Lorentzian distribution for $\epsilon_{\vec{n}}$) or within the framework of certain approximations [single-site approximations, most notably the coherent potential approximation[10,11] (CPA)]. We consider the Lorentzian case here; the case of a binary alloy has been treated numerically in Ref. 11 via the CPA. In that paper, $L(E)$ was incorrectly assumed to be equal to $F(E)$. However, the results reported remain valid because $F(E)\approx L(E)$ where they pass through unity except for the case of large δ (see Ref. 11 for definition) and for the impurity sub-band, where the mobility edges can be expected from the present analysis to be well within the region designated there as consisting of extended states. This is why the position of the asymptote (Fig. 3 of Ref. 11) as calculated from $F(E)$ differs from the correct one given by percolation theory.

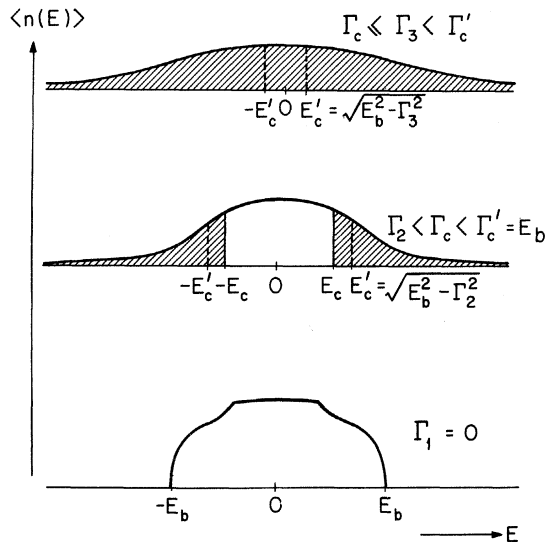

FIG. 1. Sketches of the average density of states per atom $\langle n(E)\rangle$ for three different values of the half-width Γ of the Lorentzian distribution of single-site energies. The mobility edges $\pm E_c$ separate regions of localized states (shaded) from those of extended states, and always lie within the interval $[-E_c', E_c']$. Γ_c is Anderson's critical value of the randomness.

Observing that

$$\ln|G(E)| = \tfrac{1}{2}\lim_{s\to 0^+}[\ln G(E+is) + \ln G(E-is)],$$

and using a trick similar to that of Lloyd,[12] one can prove that (11) holds for the Lorentzian case with $\sum(E) = is(E)\Gamma$, where $s(E)$ is 1 if $\mathrm{Im}E > 0$ and -1 if $\mathrm{Im}E < 0$. Thus in the Lorentzian case $F(E)$ is given by

$$F(E) = E_b/(E^2+\Gamma^2)^{1/2}, \tag{13}$$

and consequently all the eigenstates for $|E| > E_c'$ are localized. $\pm E_c'$ are given by $F(\pm E_c') = 1$, i.e.,

$$E_c' = (E_b^2 - \Gamma^2)^{1/2}. \tag{14}$$

The mobility edges $\pm E_c$ always satisfy the relation $E_c < E_c'$ with $E_c = E_c' - O(\Gamma^{1/2}/E_b^{1/2}) \to E_b$ as $\Gamma \to 0$. As Γ increases, $\pm E_c'$ move inwards into the band (and so do the mobility edges $\pm E_c$), thus broadening the intervals of localized states at the expense of extended states. Anderson's critical value Γ_c is always smaller than Γ_c' calculated from $E_c'(\Gamma = \Gamma_c') = 0$. In other words,

$$\Gamma_c < \Gamma_c' = \tfrac{1}{2}B, \tag{15}$$

and consequently all the states are localized if $\Gamma \geq \frac{1}{2}B$. This discussion is presented pictorially in Fig. 1 through a sketch of the average density of states per atom $\langle n(E)\rangle$ for three different values of the parameter Γ.

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[1]N. F. Mott, Advan. Phys. 16, 49 (1967).

[2]M. H. Cohen, H. Fritzsche, and S. R. Ovshinsky, Phys. Rev. Lett. 22, 1965 (1969).

[3]See, e.g., I. M. Lifshitz, Advan. Phys. 13, 483 (1964); or B. I. Halperin and M. Lax, Phys. Rev. 148, 722 (1966).

[4]P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[5]J. M. Ziman, J. Phys. C: Proc. Phys. Soc., London 2, 1230 (1969).

[6]E. N. Economou and M. H. Cohen, to be published.

[7]In the sense that $\mathrm{prob}[\chi^{N-Nq}(E,s) < |a_N(E+is)| < \chi^{N+Nq}(E,s)] \xrightarrow[N\to\infty]{} 1-e^{-N^{2q-1}}$, where $\frac{1}{2} < q < 1$.

[8]D. J. Thouless, to be published.

[9]S. R. Broadbent and J. M. Hammersley, Proc. Cambridge Phil. Soc. 53, 627 (1957).

[10]B. Velicky, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. 175, 747 (1968).

[11]E. N. Economou, S. Kirkpatrick, M. H. Cohen, and T. P. Eggarter, Phys. Rev. Lett. 25, 520 (1970).

[12]P. Lloyd, J. Phys. C: Proc. Phys. Soc., London 2, 1717 (1969).