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SOME PROBLEMS OF THE THEORY OF ELECTRON ENERGY SPECTRUM OF A DISORDERED SEMICONDUCTOR

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Abstract. - The paper consists of two parts. In the first one we consider the localisation problem at d=2. Assertion of all states to be localised is shown to depend upon some dynamic properties of the system - contrary to the d=1 and d=3 cases where just the geometrical considerations are known to be sufficient. The second part contains an attempt to understand what is in fact measured when one studies light absorption by the spatially inhomogeneous films (of the a Si:H type).

§ 1. Localisation problem. - According to [1 - 4] all electron states are expected to be localised in a two-dimensional disordered semiconductor with a random field present. However the calculations presented in [5, 6] suggest that the result might be in fact model-dependent - that is dependent upon some particular dynamical properties of the system [x]. The reason seems to lie in the fact that at d=2 small L-dependent corrections to the dimensionless conductance g are important (L is the length of the sample). Hence it seems worthwhile to reconsider the case d=2 somewhat taking account of some points which were not previously considered.

According to [1, 2] at small values of g (virtually in a discrete spectrum) the leading term at the temperature T=0 is $g = g_a \exp(-2\alpha L)$, where g_a is a constant and α^{-1} is the typical localisation radius (we slightly change the notation). This eq. seems almost obvious: due to the level repulsion effect the isoenergetic levels should belong to the most distant localisation centers [xx]. However the so-called discrete levels near and above the Fermi-level F have in fact a natural width δ. Hence finite length hops become possible with no activation needed provided the hopping distance exceeds the correlation length R_0 entering the two-level correlation function. Using the well-known Mott reasoning one obtains [xxx]

$$2\alpha R_0 = \ln(|F|/\delta). \qquad (1)$$

x) The same statement is true for the problem of the minimum metallic conductivity at d=3 [7].

xx) Thus we abandon the particular definition of g for finite samples adopted in [1, 2] in favour of what seems to us a more direct one. However both definitions seem to lead to identical results (in a non-correlated case this is veryfiable immediately).

xxx) Analogous results may be obtained using a more sophisticated two-level correlation function found in ref. [8]. The r.h.s. of eq. (1) should be replaced then by $2{,}6 \ln(4{,}3|F|/\delta)$ with $\alpha = \sqrt{6|F|}$ ($\hbar = m = 1$).

The possibility of "isoenergetic" hopping over the length $R > R_0$ is proportional to the $\exp(-2\alpha R)$. This reduces to the previously used form, $\exp(-2\alpha L)$, if $L \sim R_0$; the same holds for g (at $L < R_0$ such hops are obviously impossible - $\sigma = g = 0$ at T=0 under equilibrium conditions). On the other hand if $L \gg R_0$ the hops seem to proceed mostly over the distance R which is small compared to L and is determined by the percolative arguments. The conductance then becomes independent of L - up to the exponentially small terms coming from the rare cases of extremely long hops. Thus at $L \gg R_0$

$$g = g_\infty + g_1 \exp(-2\alpha L). \qquad (2)$$

To make a rough estimate of R_0 we put $\alpha = 10^5 \mathrm{cm}^{-1}$, $\tau = \hbar/\delta = 10^{-4}$s (this is probably an overestimate), $|F| = 1{,}4$ ev. Then $R_0 \approx 10^{-4}$cm. This seems to be big enough to make sensible the concept of a continuous spectrum, if any, the self-averaging property of g seems to be preserved as well since all the discrete levels are expected to occur within the sample. At the same time, the length R_0 is small enough to force us to take account of yet another length present - the correlation length γ^{-1} entering the binary correlation function of random field fluctuations. This length enters the corrections to g when the latter is big enough (virtually in a continuous spectrum). In the case of a charged impurity scattering [x] we obtain (d=2, g_∞ corresponds to $L \to \infty$):

$$g = g_\infty \left[1 - 12\pi^{-1/2} (\gamma L)^{-5/2} \exp(-\gamma L) \right]. \qquad (3)$$

Yet another correction, $-a/g$, where $a > 0$ is a constant, is to be included in the r.h.s. of (3) [1, 2] - provided the correction [5, 6] is unimportant. (The latter case is formally obtained by putting a=0).

In presence of new lengths, γ^{-1} and R_0, the function g(bL) obtained by forming a hypercube of b^2 cubes should generally be written in the form $g(bL) = f\left[b, g(L), \gamma L, LR_0^{-1}\right]$ and a certain ingredient of the renormalisation group philosophy is generally lost. Yet some analogue of the renormalisation group equation may still be obtained using the method of [1, 2] :

$$\frac{d \ln g}{d \ln L'} = \beta\left[g(L'), \gamma L', L' R_0^{-1}\right] ; \quad \beta = g^{-1}(L') \frac{d f}{d b}\Big|_{b=1}. \qquad (4)$$

Here L' ($\leq L$) is a variable parameter to be identified with L after the calculation is over. Now this eq. is generally nonautonomous, since β may depend explicitly upon $\gamma L'$ and $L' R_0^{-1}$. This however does not change the essence of the argument based upon studying the sign of β. For our purposes it is sufficient to consider two limiting cases.

a) "Short" samples: $L \lesssim R_0$. Here the hops are over almost all of the sample; the function β is given by

$$\beta = \begin{cases} -\alpha L, & g \ll 1, \quad (a) \\ 12\pi^{-1/2} (\gamma L)^{-3/2} \exp(-\gamma L) - a/g_\infty, & g \gg 1 \quad (b) \end{cases} \qquad (5)$$

Since the first term in the r.h.s. of (5.b) is small but finite the

x) Analogous result is obtained when the scattering is due to a smooth random field.

sign of β is defined here by the details of the dynamics. Thus we obtain either a complete localisation or a mobility edge.

b) "Long" samples: $L \gg R$. The exponentials of the type $\exp(-2\gamma L)$ should now be neglected wherever possible and we have

$$\beta = \begin{cases} -\frac{g_1}{g_0} 2\alpha L \exp(-2\alpha L) \to -0, \quad g \ll 1, & \text{(a)} \\ -a/g_\infty, \quad g \gg 1. & \text{(b)} \end{cases} \qquad (6)$$

In this case the results of [1, 2] seem to be formally confirmed (provided $a \neq 0$).

§ 2. Optical absorption. - We consider the films of the columnar-like structure containing for example, the "true" a-Si:H ("columns") and the intermediate "tissue" [9-11]. The essence of the problem may be seen by considering the cylindrical columns of radius R passing through the film perpendicular to the illuminated surface (which is a plane z=0). Let the distance between the columns be high enough; then the film is in fact just a system of independent "waveguides" separated by a tissue. In contrast to the conventional waveguides these are filled by an absorbing material and the "walls" formed by a tissue are anything but metallic. All this however does not change the mathematics too much. Let ε_1, σ_1 and ε_2, σ_2 be the real parts of the dielectric permeability and high frequency conductivity of the column material and tissue respectively and let the absorption in the tissue be much higher than in the column material. Then the electric field of the plane polarised wave in the film, $\bar{E}\exp(-i\omega t)$, is approximately given by

$$\bar{E} = \sum_{n \geq 1} \exp\left(i\varphi + i\alpha_n z - \beta_n z\right)\left\{\bar{E}_{i,n}(\rho)\,\theta(R-\rho) + \bar{E}_{e,n}(\rho)\,\theta(\rho-R)\right\}. \qquad (7)$$

This eq. holds everywhere except the thin layer near the illuminated surface. Here ρ and φ are the cylindrical coordinates, the axis coinciding with that of a column, θ is the usual step-function, while the vector-functions $\bar{E}_{i,n}$ and $\bar{E}_{e,n}$ are expressed respectively in terms of the cylindrical functions $J_1(\varkappa_n^{(1)}\rho)$ and $H_1^{(1)}(\varkappa_n^{(2)}\rho)$, n is the number of the root of a certain transcendental equation for $\varkappa_n^{(1)}R$; at $(2\pi\sigma_2 R/c\sqrt{\varepsilon_2}) \gg 1$ this equation is just $J_1(\varkappa_n^{(1)}R) \cdot J_1'(\varkappa_n^{(1)}R) = 0$. The complex wave-number $\alpha_n + i\beta_n$ is easily obtained in terms of σ_1, ε_1 and $\varkappa_n^{(1)}R$; by definition $\beta_n > 0$. The r.h.s. of (7) is a sum of terms with various complex propagation constants. If the film is thick enough, then just one of the terms survives. However even in this case the absorption coefficient measured in a transmission experiment differs from that obtained for a homogeneous material. The surviving term corresponds to

$$\beta_1 \equiv \beta = \frac{2\pi\sigma_1}{c\sqrt{\varepsilon_1}}\left(1 - 0{,}086\,\lambda^2/R^2\right)^{-1/2}, \qquad (8)$$

where c is the light velocity in a free space, $\lambda = 2\pi c/\omega$ is the light wave length; eq. (8) is valid provided $\lambda/\sqrt{\varepsilon_1}\pi R < 1$, but this is not necessarily a strong inequality. Since λ might well be of the order of R, the correction might in fact be quite noticeable. More important however is the fact that in the case typical for a thin film many terms may survive (especially in the optical tail re-

gion). In this case the usual concept of a single absorption coefficient might become quite misleading. The apparent absorption coefficient obtained from a transmission experiment becomes dependent upon the thickness of the film.

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