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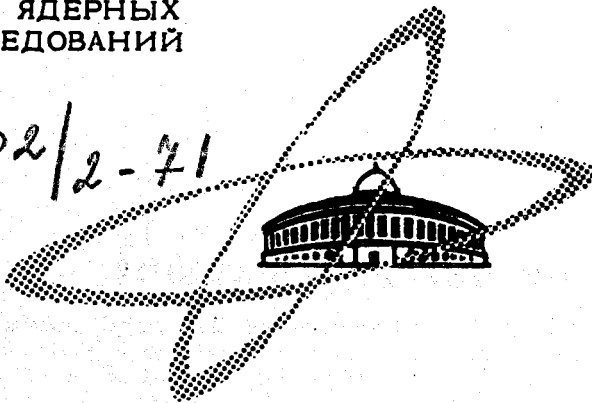
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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

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ENERGY GAPS  
IN DISORDERED ALLOYS

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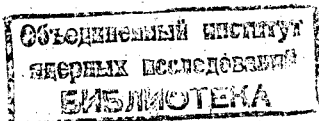
ENERGY GAPS  
IN DISORDERED ALLOYS

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General methods for the calculation of the electronic structure for disordered materials are till now unknown. Therefore the discussion of simple models with the aim to obtain exact conditions for the density of states, especially for the existence of energy gaps, is of great interest. Let us consider a disordered system of muffin-tin-potentials. For such a system Lloyd<sup>1/</sup> has shown, that the integrated density of states  $N(E)$  for any distribution of muffin-tin-potentials, characterized by the phase shifts  $\eta_L^n$  and the positions  $R_n$  can be calculated by

$$N(E) - N^0(E) = -\frac{2}{\pi V} \operatorname{Im} \ln \det \left\| \delta_{nn'} \delta_{LL'} + \frac{1}{\kappa} \operatorname{tg} \eta_L^n G_{LL'}^{nn'} \right\| \quad (1)$$

Recently it has been shown<sup>2/</sup>, that the Lloyd-formula simply follows from a generalized Friedel sum rule. With the generalized phase shifts  $\eta_\lambda$  of the whole system we obtain for (1)

$$N(E) - N^0(E) = \frac{2}{\pi V} \sum_\lambda \eta_\lambda \quad (2)$$

The generalized phase shifts  $\eta_\lambda$  follow from an eigenvalue equation and satisfy the condition<sup>3/</sup>

$$\det \left\| N_{LL'}^{nn'} - \operatorname{ctg} \eta_\lambda J_{LL'}^{nn'} + \operatorname{ctg} \eta_L^n \delta_{LL'} \delta_{nn'} \right\| = 0 \quad (3)$$

From the stationarity of the eigenvalues  $\eta_\lambda$  we obtain the condition<sup>3/</sup>

$$\frac{\partial \eta_\lambda}{\partial \eta_L^n} \geq 0 \quad (4)$$

Therefore from (2) and (4) follows, that the integrated density of states increases (decreases), if the phase shifts of the muffin-tin-potentials are increased (decreased). The same result can be obtained by differentiation of (1) as shown in the Appendix.

As an application let us now consider an alloy, consisting of components  $A$  and  $B$ , which occupy in any distribution a fixed lattice. Let us furthermore assume, that in the considered energy range the phase shifts of the components  $\eta_L^A$  and  $\eta_L^B$  fulfill the condition  $\eta_L^B > \eta_L^A$ . Then for the integrated density of states  $N^{AB}$  of the alloy for any concentration and arrangement of the components follows from (2) and (4) the condition

$$N^B(E) \geq N^{AB}(E) \geq N^A(E), \quad (5)$$

with  $N^A(N^B)$  as the integrated density of states of the pure  $A(B)$  metal. If the pure metals have ranges of forbidden energy in common with the same number of states below the gap (the Brillouin zones containing the states below the gap are the same), then from (5) follows for this range of energy

$$N^B(E) = N^{AB}(E) = N^A(E) \quad (6)$$

Therefore in the alloy persists a gap in the energy range, in which in the metals  $A$  and  $B$  exists a gap in common.

An analogous statement has been obtained by Taylor<sup>/4/</sup> for any ionic potential, which fulfills the condition  $v_A(\vec{r}) \geq v_B(\vec{r})$  in the whole space. Since from  $v_A(\vec{r}) \geq v_B(\vec{r})$  follows  $\eta_L^B \geq \eta_L^A$  for all energies, the Taylor-theorem<sup>/4/</sup> (with muffin-tin-potentials) is a special case of the statement derived above.

The author is grateful to Prof. Dr. P. Ziesche for stimulating discussions.

### Appendix

Starting with a suitable form of the Lloyd-formula (1) (denotation see<sup>/3/</sup>)

$$N(E) - N^0(E) = - \frac{2}{\pi V} \operatorname{Im} \ln \det \| D_{LL'}^{nn'} \|, \quad (A.1)$$

$$D_{LL'}^{nn'} = N_{LL'}^{nn'} - i J_{LL'}^{nn'} + \operatorname{ctg} \eta_L^n \delta_{LL'} \delta_{nn'},$$

we obtain

$$\frac{\partial N(E)}{\partial \eta_L^n} = \frac{2}{\pi V} \frac{1}{\sin^2 \eta_L^n} \operatorname{Im} (D^{-1})_{LL'}^{nn} \geq 0. \quad (A.2)$$

The symmetric matrices  $N_{LL'}^{nn'}$  and  $J_{LL'}^{nn'}$  are real and the matrix  $J_{LL'}^{nn'}$  is positive defined, from which follows  $\operatorname{Im} (D^{-1})_{LL'}^{nn} > 0$ . Therefore the inequality (A.2) is valid.

## Reference

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