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PERCOLATION LEVEL IN A THREE-DIMENSIONAL RANDOM POTENTIAL

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The ideas of percolation theory have found extensive use recently in the theory of disordered systems, particularly for the description of the electric conductivity of doped crystalline [1, 2] and amorphous semiconductors [3 - 6]. This posed naturally the mathematical problem of percolation in a continuum, the idea of which is related to the previously investigated lattice problems of "nodes" and "bonds," but does not reduce to the latter. This new problem is formulated as follows. Assume that in all space there is specified an arbitrary random function $V(\vec{r})$ with a finite correlation radius (potential energy). Without loss of generality, we assume that the mean value $\langle V \rangle$ is equal to zero. It is required to determine the so-called percolation level ϵ_p , i.e., the minimum value of the energy ϵ at which classically admissible regions, where $\epsilon > V(\vec{r})$, form paths that go off to macroscopic distances.

It is shown in [1, 2] that in a large number of cases the quantity ϵ_p determines the activation energy of the conductivity, which can be measured in experiment with sufficient accuracy.

A method of solving continual percolation problems with a computer was first proposed by us in [8]. The same method was verified there with the aid of a two-dimensional problem for which an exact solution is known. We report here for the first time results concerning the three-dimensional problem.

Our purpose was to explain the extent to which the result depends on various properties of the potential. We were interested mainly in a Gaussian potential V defined by the relation

$$V(\mathbf{r}) = \int K(\mathbf{r} - \mathbf{r}') f(\mathbf{r}') d^3r', \quad (1)$$

where f is a random Gaussian function with a correlator

$$\langle f(\mathbf{r}) f(\mathbf{r}') \rangle = \delta(\mathbf{r} - \mathbf{r}'), \quad (2)$$

and the kernel $K(\vec{r})$ decreases sufficiently rapidly with r beyond the limits of the correlation radius r_0 . The distribution function of the potential is

$$F(V) = \frac{1}{\sqrt{\pi}\gamma} \exp\left(-\frac{V^2}{\gamma^2}\right), \text{ where } \gamma^2 = 2 \int K^2(\mathbf{r}) d^3r. \quad (3)$$

We shall refer henceforth not to the percolation energy ϵ_p , but to the dimensionless quantity v_c - the fraction of space in which $V < \epsilon_p$:

$$v_c = \int_{-\infty}^{\epsilon_p} F(V) dV. \quad (4)$$

We wanted not only to calculate v_c for some concrete form of the function $K(\vec{r})$, but also to verify the extent to which the result is sensitive to its choice. Making the coordinate transformation $x_i' = a_i x_i$, we can easily show that v_c is invariant to the substitution $K(\vec{r}) = K(a_1 x, a_2 y, a_3 z)$, where a_i are arbitrary numbers. We therefore confined ourselves to an investigation of isotropic functions $K(r)$. The calculations were performed with the following functions:

$$K_1(r) = \begin{cases} 1 & r < r_0 \\ 0 & r > r_0 \end{cases}, \quad K_2(r) = \begin{cases} 1 - r/r_0 & r < r_0 \\ 0 & r > r_0 \end{cases} \quad (5)$$

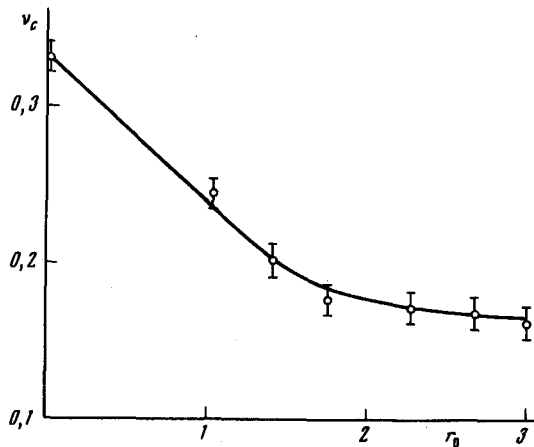
$$K_3(r) = \begin{cases} 1/r & r < r_0 \\ 0 & r > r_0 \end{cases}, \quad K_4(r) = \frac{1}{r} e^{-r/r_0}, \quad K_5(r) = e^{-r/r_0}$$

(the function $K_4(r)$ is needed for the calculation of the activation energy of the hopping conductivity in the case of weak compensation [2]). We found that $v_c = 0.17 \pm 0.01$ and at this accuracy it is independent of the choice of $K(r)$.

We were unable to prove analytically the invariance of v_c to the choice of $K(r)$. In the literature there are many various intuitive estimates of v_c (see [6]).

Our result is closest to the estimate of Zallen and Sher [6]. Putting $v_c = 0.17$ in (4), we obtain $\epsilon_p = -0.68\gamma$.

We note that our result $v_c = 0.17$ pertains to a broader class of potentials. Let us transform the Gaussian potential V with the aid of a function $\phi(V)$ such that $\phi(V) > \phi(\epsilon_p)$ at $V > \epsilon_p$ and $\phi(V) < \phi(\epsilon_p)$ at $V < \epsilon_p$. A particular case of the function $\phi(V)$ may be any function that is monotonic in the interval $(-\infty, \infty)$. The potential ϕ obtained in this manner is generally speaking not Gaussian, but it is easy to verify that the percolation level in it is $\phi(\epsilon_p)$, and the critical fraction of the space v_c turns out to be the same as in a Gaussian potential V . It has turned out that the use of potentials not from this class can change v_c considerably. We have investigated the potentials $V'(\vec{r}) = V^{-1}$ and $V''(\vec{r}) = -|V|$, where V is a Gaussian potential obtained with the aid of the function $K_1(r)$. As a result we obtained $v_c' = 0.27$ and $v_c'' = -0.24$.



The calculations were performed with a BESM-6 computer. The function f was set with a random-number generator at the points of a primitive cubic lattice with unity period, located inside a $20 \times 20 \times 20$ cube. At each point we calculated the potential in accordance with (1). Using the method described in detail in [8], we found the percolation level corresponding to the appearance of paths between opposite faces of the cube. The figure shows the dependence of the fraction of points at which $V < \epsilon_p$ on r_0 at $K(r) = K_1(r)$. Each point was obtained by averaging

approximately over 10 realizations of f . The absolute error in the calculation of the mean value did not exceed 0.01. As $r_0 \rightarrow 0$, the values of the potentials at the points turn out to be entirely uncorrelated, and we obtain the results of the lattice problem of nodes, $v_c = 0.32$ [7]. At $r_0 \gg 1$, v_c ceases to depend on r_0 , corresponding to the transition to the continual problem. The limiting value of v_c is indeed the critical fraction of the volume, which is of interest to us. We obtained similar results for the other potentials mentioned above.

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ROLE OF LINEAR CHAINS IN THE FORMATION OF THE PROPERTIES OF SUPERCONDUCTORS WITH A-15 STRUCTURE

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It is shown that the elastic properties of superconductors with β -W structure follow from the assumption that the α -electron energy spectrum is almost flat.

Superconductors of the A_3B type have an interesting property in that the transition to the superconducting state is a structural transition at a temperature T_m close to T_c , and if there is no transition obtained, a tendency to this transition is observed, manifest in a softening of the corresponding elastic moduli [1, 2]. In all the known cases, T_m differs from T_c by not more than a factor of two, whereas the temperature dependences that anticipate the transition extend to temperatures 300 - 400°K.

It was noted in [3] that owing to the small overlap of the shells, an important role in the structure of β -W can be played by three systems of linear chains of transition-element atoms. The approximation of strong coupling of the d-electrons in the chain was involved to one degree or another in all the subsequent studies [4 - 6], in which an anomalously large density of states $v(\epsilon_F)$ was assumed, owing to the singular behavior $v(\epsilon) \sim \epsilon^{-1/2}$ at the edge of the one-dimensional band.

It is shown below that the main properties of this group of compounds can be understood within the framework of the concrete symmetry of the A-15 structure on the basis of the concepts of the Fermi-liquid theory, with allowance for the changes introduced by the one-dimensional character of the filaments. Indeed, in a one-dimensional metal the Cooper pairing is connected with the Peierls doubling of the period [7]. It will be made clear below that it is also connected with the tetragonal deformation in the β -W structure. The literature contains discussions both of the non-phonon superconductivity mechanisms in these compounds and of the role of the structure instability in the increase of