

Localization of electrons in disordered systems. The mobility edge and theory of critical phenomena

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It is shown that the most probable spatial behavior of the one-electron Green function in the region of localized states near the mobility edge in the Anderson model coincides with the spatial behavior of the correlation function in the critical region of a second-order phase transition with a zero-component order parameter.

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Ideas about the localization of electrons in a random field lie at the basis of the modern theory of disordered systems.^[1] The most highly developed scheme for treating the problem of localization is the well-known Anderson model^[2-4] describing an electron propagating in a regular lattice with random energy levels at the different sites. Most of the papers on the Anderson model are devoted to proving the localization of electron states when the ratio of the parameter W describing the spread of levels to the amplitude V of an electron transition from site to site is sufficiently large, to determining the critical ratio W_c/V , and also to determining the mobility edges E_c , i. e., the critical electron energies separating the regions of localized and delocalized states in the band.^[1,2,4] It is of great interest to study the character of the electron states near the mobility edge, since the corresponding characteris-

tics essentially determine the kinetics and other electronic properties of disordered systems.^[5] Attempts in this direction have been undertaken in papers by Anderson, Edwards, and Freed.^[3,6,7]

There exist a number of obvious analogies between the problem of the localization of an electron near the mobility edge and the problem of describing the critical phenomena near a second-order phase-transition point. For example, as the electron energy approaches the mobility edge in the region of localized states the localization length of the electron wavefunction diverges, just as the correlation length of fluctuations at a phase-transition point diverges. This prompts the thought that the spatial behavior of electron states near the mobility edge can be described by the (scaling) dependences that are characteristic for the phase-transition problem,

with critical indices determined only by the dimensionality of space and of the corresponding order parameter.^[8]

In the present paper, using the method of Anderson,^[3] we show that the most probable spatial behavior of the one-electron Green function at the mobility edge coincides with the spatial behavior of the correlation function for the problem of critical phenomena with a zero-component order parameter.^[9,10]

The Hamiltonian of the Anderson model has the form^[2,3]

$$H = \sum_j E_j a_j^\dagger a_j + \sum_{ij} V_{ij} a_i^\dagger a_j. \quad (1)$$

Here, a_i^\dagger and a_i are the electron creation and annihilation operators at the lattice site i , and E_j are the random energy levels at the sites, distributed in accordance with the law

$$P(E_j) = \begin{cases} 1/W, & |E_j| < 1/2W \\ 0, & |E_j| > 1/2W \end{cases}. \quad (2)$$

The transition amplitude V_{ij} from site to site is assumed to be nonzero, and equal to a constant V , for transitions between nearest neighbors only.

The character of the electron states is determined by the one-electron Green function

$$G_{ij}(E) = \langle R_i | \frac{1}{E-H} | R_j \rangle, \quad (3)$$

which is the transition amplitude from the site at the point R_j to the site at the point R_i for an electron with energy E . A renormalized perturbation-theory series in V is constructed for this Green function. As Anderson has shown,^[2] the localization problem reduces to investigating the convergence of this series, where, in view of the random character of the quantities E_j , the convergence is understood in the sense of convergence with a certain probability.^[2,4] In the region of localized states the series converges with probability unity, and the condition for convergence determines the critical ratio W_c/V or the position of the localization edge in the band.

The most probable behavior of the Green function can be represented in the form^[2,3]

$$G_{ij}(E)|_{E=0} \sim \sum_{N=0}^{\infty} Z_N(R_i - R_j) \left(\frac{2eV}{W}\right)^N \Psi^N\left(\frac{V}{W}, K\right), \quad (4)$$

where $Z_N(R_i - R_j)$ is the number of paths of N steps, without intersections, linking site j with site i , and Ψ is a slowly varying (logarithmic) function of the ratio V/W and of the so-called connectivity constant K of the lattice.^[2] For simplicity we consider below an Anderson transition in the center of the band (at $E=0$). In the general case, in (4) we must replace $2V/W$ by $2V\rho(E)$, where $\rho(E)$ is the density of electron states.^[3] The critical bandwidth W_c corresponding to the threshold of localization is determined by the equation^[2]

$$1 = \frac{2eV}{W_c} K \Psi\left(\frac{V}{W_c}, K\right). \quad (5)$$

For $E \neq 0$ a condition of the type (5) was discussed in^[1,4].

Thus, the spatial behavior of the Green function is entirely determined by the statistics of nonintersecting paths, through the function $Z_N(R_i - R_j)$. Anderson^[3] and Thouless^[11] used a $Z_N(R)$ obtained as the result of machine experiments. We shall make use of the analytic theory of de Gennes and des Cloizeaux.^[10] Using Wilson's ϵ -expansion method,^[8] de Gennes and des Cloizeaux considered the statistics of random walks without intersections and showed that the function $Z_N(R)$ of interest to us is determined, in a space of d dimensions, by the inverse Laplace transform

$$Z_N(R) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{Ns} G_U(s, R) \quad (6)$$

of the unrenormalized Green function $G_U(s, R)$ of a Euclidian field theory (Landau-Ginzburg phase-transition theory) with Lagrangian of the form

$$\mathcal{L}(x) = \frac{1}{2} \sum_{j=1}^n \{(\nabla\Phi_j)^2 + m_0^2\Phi_j^2\} + \frac{1}{8} g_0 \left(\sum_{j=1}^n \Phi_j^2\right)^2, \quad (7)$$

where n is the number of components of the field Φ and is equal to zero in the problem under consideration. (The condition $n=0$ eliminates the "superfluous" diagrams with loops, which are absent in the nonintersecting random-walk problem.) The dimensionless parameter s is related to the unrenormalized mass: $s = m_0^2 a^2$, where a is a characteristic length of the order of the lattice constant. The phase transition corresponds^[8] to the vanishing of the renormalized mass m of the field theory (7) as $s \rightarrow s_c$:

$$m \sim a^{-\nu}(s - s_c)^{-\nu}, \quad (8)$$

where ν is the critical index of the correlation length.

In (6) we must take $c > s_c$. The parameter s_c is related to the connectivity of the lattice^[9,10,12]:

$$K = \exp(s_c). \quad (9)$$

Using (6) and (3), we obtain

$$\begin{aligned} G_{ij} &\sim \sum_{N=0}^{\infty} \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \exp\{N(s-s_c)\} G_U(s, R_i - R_j) \left(\frac{2eV}{W} K\right)^N \Psi^N\left(\frac{V}{W}, K\right) \\ &\approx \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} G_U(s, R_i - R_j) \sum_{N=0}^{\infty} \exp\{N(s-s_c) + N \ln \frac{W_c}{W}\} \\ &= G_U\left(\ln \frac{W}{W_c} + s_c; R_i - R_j\right) \end{aligned} \quad (10)$$

which is the main result, showing that the most probable spatial behavior of the one-electron Green function of the Anderson model in the region of localized states near the mobility edge ($W \geq W_c$) coincides with the behavior of the correlation function of the phase-transition theory (7) with $n=0$, and $W = W_c$ corresponds to the transition point.

For $W \geq W_c$ the Green function falls off exponentially with distance^[8]:

$$G_{ij} \sim \exp\left\{-\frac{|R|}{R_{loc}}\right\}; \quad |R| = |R_i - R_j| \gg R_{loc}, \quad (11)$$

where

$$R_{loc} \sim m^{-1} \sim a \left| \frac{W - W_c}{W_c} \right|^{-\nu} \quad (12)$$

plays the role of the localization length. Analogously, for $E \neq 0$, but for $E \approx E_c$,

$$R_{loc} \sim a \left| \frac{E - E_c}{E_c} \right|^{-\nu}$$

In the framework of the Wilson ϵ -expansion ($d = 4 - \epsilon$) for $n = 0$, we have

$$\nu \approx \frac{1}{2} \left\{ 1 + \frac{\epsilon}{8} + \frac{15}{256} \epsilon^2 + \dots \right\} \approx 0.592 \quad \text{for } \epsilon = 1, \quad (13)$$

in excellent agreement with Anderson's result $\nu = 0.6$,^[3] obtained from a machine analysis of the statistics of nonintersecting paths.

For $W = W_c$ we have

$$G_{i\infty} \sim |\mathbf{R}|^{-(d-2+n)}, \quad (14)$$

where

$$\eta \approx \frac{\epsilon^2}{64} \left\{ 1 + \frac{17}{16} \epsilon \right\} \approx 0.032 \quad \text{for } \epsilon = 1. \quad (15)$$

The small value of the critical index η implies that the localization assumed by Thouless^[11] (who evidently used unreliable numerical values, obtained in the machine analysis, for the critical indices in the pre-exponential factor in $Z_N(\mathbf{R})$), with a power-law decay of the wavefunctions, is impossible in the given model. In the analog of formula (14) in^[11], the exponent is equal to $17/9$, which falls in the region of possible values (from $\frac{3}{2}$ to $\frac{5}{2}$, according to Thouless) of the localization exponent. In our case, $d - 2 + \eta \approx 1.032$ for $d = 3$.

Naturally, the asymptotic formulas (11) and (14) given above can also be obtained by direct use of the asymptotic formulas for $Z_N(\mathbf{R})$ obtained by des Cloizeaux.^[10]

The analysis carried out is inapplicable in the one-dimensional case, since in the model under consideration, with nearest-neighbor interaction, Anderson's renormalized series for the electron Green function contains only two terms, corresponding to the two possible nonintersecting paths.^[13] The question of localization reduces to an investigation of the convergence of a certain continued fraction, and the statistics of nonintersecting paths do not play a special role. Therefore, a one-dimensional model of a phase transition, of the Landau-Ginzburg type, evidently has no direct relation

to the problem of the localization of electrons in a one-dimensional disordered system. The same conclusion is obtained from other arguments in a recent paper by Thouless.^[14]

In conclusion, we emphasize that the most probable electron Green function near the mobility edge was considered above. In papers by Edwards^[6] and Freed^[7] an analogy has been noted between the problem of nonintersecting random walks and the problem of calculating the one-electron Green function averaged over random configurations of impurities. Starting from this analogy, it is not difficult to convince oneself that the diagrammatic series of Edwards for this Green function,^[15] in the Gaussian approximation for the statistics of the impurities, is generated by the diagrammatic series for $G_U(s)$ of the problem (7) with $n = 0$, after the appropriate analytic continuation in the parameters of the Lagrangian (see also the paper^[14]). The important point here, however, is that the sign of the interaction constant g_0 changes, so that the correspondence with the theory of phase transitions is evidently lost. Physically, this is connected with the fact that random walks without intersections are equivalent to the thermodynamics of a polymer chain with repulsion between the links, whereas the thermodynamics of an electron in a system of impurities is equivalent to the thermodynamics of a polymer with attraction.^[6] The question of the possibility of applying Wilson's ϵ -expansion in this problem remains open.

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