Urbach's rule and the Lifshits singularity in the spectrum of electronic states of a disordered medium

A. A. Klochikhin and S. G. Ogloblin

Leningrad Institute of Nuclear Physics

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We obtain the energy dependence of the exponential in the density of localized states of a crystal whose lattice sites are randomly occupied by two kinds of atoms within the energy interval from the mobility edge to the Lifshits boundary, using the framework of the single-instanton approach and a single-band Hamiltonian with diagonal disorder. We show that in the region below the mobility edge there is an energy interval of considerable extent over which the energy dependence of the density of states follows Urbach's rule with high accuracy. Although we investigate the three-dimensional case in this paper, the same phenomenon will also occur for $d = 1$ and 2 as well as for multicomponent systems, provided that there is a Lifshits singularity in the spectrum of localized states. For $d = 3$ we find an exact and an approximate expression for the Urbach parameter E_u and its dependence on the parameters of the problem. We show that observed values of E_u can be explained for various disordered systems using realistic values of the parameters of the Hamiltonian.

INTRODUCTION

The disordering of crystals leads to washing-out of the edges of their electron bands and to the appearance of "tails" in the density of (localized) states extending deep into the forbidden region. It is a firmly established experimental fact that the decay of the density of localized states follows Urbach rule for energies that are far from the mobility edge E_g, i.e., $\rho(\omega) \propto \exp([-E_g - \omega]/E_u)$ for $\omega < E_g$. The value of the Urbach parameter E_u varies from one system to another over a range from several eV down to a few tens of meV. A great variety of systems exhibit Urbach's-rule behavior in their densities of states: amorphous silicon,[1,2] glass,[3] superionic crystals,[4] and solid solutions;[2,5] in these systems the density of states can change by three to four orders of magnitude. Data on solid solutions of $A_{II}B_{VI}$ compounds[5] show that the Urbach parameter $E_u(c)$ is a function of the solute concentration c over a wide range of variation of the latter. However, up to now no one has found a theoretical explanation for the Urbach law.

As first shown by I. M. Lifshits, the tail of localized states is finite in width.[6] The interval of values of ω where localized states occur is bounded on one side by the mobility edge E_g, above which an electron is spread out through the entire volume of the crystal, and on the other side by the Lifshits boundary E_L below which it is impossible for such a state to appear. The behavior of the density of localized states near the Lifshits boundary is singular, and the character of the singularity depends only of the dimensions of the crystal. For three-dimensional systems the behavior of the density as $\omega \to E_L$ is described by the expression

$$\rho(\omega) \propto \exp\left(-\frac{4\pi^4}{3}\ln\frac{1}{c}\left[\frac{E_0}{(\omega - E_L)}\right]^{3/2}\right), \tag{1}$$

where E_0 is an energy whose scale is determined by the size of an attractive center and by the mass of the carrier (its precise definition will be given below), while c is the concentration of attractive centers.

In the literature there exist strict mathematical proofs of the singular character of the dependence of the density of states near a Lifshits boundary, and also calculations of $\rho(\omega)$ in the single-instanton approximation in the neighborhood of E_L based on simple physical models.[9-12] The case that has been investigated most completely is the Lorentz model, i.e., the case of an extremely small concentration of impurity centers with a repulsive potential (in our notation this corresponds to the limit $1 - c \ll 1$). Experimental observation of localized states in the neighborhood of E_L appears to be unlikely at this time, due to the extremely small value of the density in this region. The experimentally-accessible interval of observation $E_g - \omega$ is considerably smaller than the distance to the Lifshits boundary $E_g - E_L$. Therefore, there is considerable interest in investigating the character of the dependence of the density of states over the entire region of frequencies $E_g > \omega > E_L$, where the density of states is already rather small, in order to confirm the single-instanton approach.

In this paper we investigate the problem for a single-band model of the binary alloy A_cB_{1-c} with diagonal disorder, i.e., the Anderson model. In this case, the Lifshits boundary coincides with the position of the bottom of the band of crystal A. We obtain a density of localized states whose decay follows Urbach's rule over a wide range of frequencies extending up to the mobility edge, although this region is considerably smaller than the energy region which separates the mobility edge from the Lifshits boundary.

HAMILTONIAN AND GREEN'S FUNCTION

In this model, we assume that a macroscopic volume V of solid solution consisting of N sites of a crystal lattice is occupied in a random way by atoms of two types, A and B. The average numbers of A and B atoms equal $\overline{N}_A = cN$ and $\overline{N}_B = (1-c)N$, respectively, where c is the concentration of A atoms. The single-band Hamiltonian for this system can be written in the form

$$H = -\sum_{\mathbf{n},\mathbf{m}} \psi_{\mathbf{n}} w_{\mathbf{m}} (\psi_{\mathbf{n}+\mathbf{m}} - \psi_{\mathbf{n}}) + \sum_{\mathbf{n}} E_{\mathbf{n}} \psi_{\mathbf{n}}^2, \tag{2}$$

in which we will assume that ψ_n is real. The diagonal matrix

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element E_n is equal to E_A if a site is occupied by an A atom and E_B in the opposite case.

For the limiting cases $c = 0$ and $c = 1$, the Hamiltonian (2) reduces to the Hamiltonians of pure (ordered) B or A crystals, respectively. In these cases, all the E_n are replaced by $E_\alpha = E_A$ or E_B. In the plane-wave representation, the matrix elements of the Hamiltonian take the form

$$H_{\mathbf{q}}{}^{\alpha}=\varepsilon_{\mathbf{q}}+E_\alpha, \tag{3}$$

where

$$\varepsilon_{\mathbf{q}}=w_0-w_{\mathbf{q}}. \tag{4}$$

The Green's function is written as

$$G_{\mathbf{nm}}{}^{\alpha}(\omega)=\{\omega-H^\alpha\}_{\mathbf{nm}}^{-1}=\frac{1}{N}\sum_{\mathbf{q}}\frac{\exp[i\mathbf{q}(\mathbf{R}_n-\mathbf{R}_m)]}{\omega-\varepsilon_{\mathbf{q}}-E_\alpha} \tag{5}$$

where $\mathbf{R}_n$ is the radius vector to the lattice site $\mathbf{n}$.

For the case of random occupation of sites by atoms of the two kinds, the Green's function for each realization depends on the composition and placement of the atoms

$$G_{\mathbf{nm}}(\omega;\ \mathbf{R}_1,\ldots,\ \mathbf{R}_N)=\{\omega-H(\mathbf{R}_1,\ldots,\ \mathbf{R}_N)\}_{\mathbf{nm}}{}^{-1}. \tag{6}$$

Let us write (6) in the form of a functional integral, assuming that the normalizing integral is eliminated by using the replica representation[13-15] or by introducing anticommuting variables.[6] We will omit the details of this procedure, since we will limit ourselves to calculating the exponent of the averaged Green's function in what follows.

Thus,

$$G_{\mathbf{nm}}(\omega;\mathbf{R}_1,\ldots,\mathbf{R}_N)=\int D[\psi]\psi_{\mathbf{n}}\psi_{\mathbf{m}}\exp\{-A[\psi]\}, \tag{7}$$

where

$$A[\psi]=\frac{1}{2}\sum_{\mathbf{n},\mathbf{m}}\psi_{\mathbf{n}}(H_{\mathbf{nm}}-\omega\delta_{\mathbf{nm}})\psi_{\mathbf{m}},$$
$$H_{\mathbf{nm}}=-w_{\mathbf{m}-\mathbf{n}}+\delta_{\mathbf{nm}}\Big(\sum_{\mathbf{l}}w_{\mathbf{l}}+E_{\mathbf{n}}\Big) \tag{8}$$

and δ_{nm} is the Kronecker symbol.

The physically interesting quantity is the Green's function averaged over all possible configurations of site occupation:

$$\bar{G}_{\mathbf{nm}}(\omega)=\int D[\psi]\psi_{\mathbf{n}}\psi_{\mathbf{m}}\langle\exp\{-A[\psi]\}\rangle. \tag{9}$$

It is clear from (8) and (9) that the averaged value is a function of

$$\exp\Big\{-\frac{1}{2}\sum_{\mathbf{n}}E_{\mathbf{n}}\psi_{\mathbf{n}}{}^2\Big\}. \tag{10}$$

Let us measure ω and E_n from the average value of E_n at a lattice site:

$$\bar{E}=cE_A+(1-c)E_B. \tag{11}$$

The quantity E coincides with the position of the bottom of the band of the solid solution in the virtual-crystal approximation, and in this approximation is the mobility edge $E_g \equiv E_g^{vc}(c) = \bar{E}$. Making the change of variables

$$\varepsilon=\omega-E_g,\quad \Delta_{\mathbf{n}}=E_{\mathbf{n}}-E_g, \tag{12}$$

we will represent the action $A[\psi]$ in the form of two terms:

$$A[\psi]=A_{vc}[\psi]+\Delta A[\psi], \tag{13}$$

where

$$A_{vc}[\psi]=\frac{1}{2}\sum_{\mathbf{n},\mathbf{m}}\psi_{\mathbf{n}}(H_{\mathbf{nm}}-\varepsilon\delta_{\mathbf{nm}})\psi_{\mathbf{m}}, \tag{14}$$

$$\Delta A[\psi]=\frac{1}{2}\sum_{\mathbf{n}}\Delta_{\mathbf{n}}\psi_{\mathbf{n}}{}^2. \tag{15}$$

The fluctuation-induced term $\Delta A[\psi]$ in the action depends on the method of filling the sites. For random occupation, an A atom will occur with probability c and a B atom with probability $1 - c$ at each site. Keeping in mind that the averaged exponential separates into a product of exponentials, each of which is averaged independently, we obtain

$$\langle\exp\{-\Delta A[\psi]\}\rangle=\Big\langle\exp\Big\{-\sum_{\mathbf{n}}\frac{\Delta_{\mathbf{n}}}{2}\psi_{\mathbf{n}}{}^2\Big\}\Big\rangle$$
$$=\prod_{n=1}^{N}\Big\{c\exp\Big(-\frac{\Delta_A}{2}\psi_{\mathbf{n}}{}^2\Big)+(1-c)\exp\Big(-\frac{\Delta_B}{2}\psi_{\mathbf{n}}{}^2\Big)\Big\}, \tag{16}$$

$$\Delta_A=E_A-E_g=-(1-c)\Delta,\quad \Delta=E_B-E_A>0,$$
$$\Delta_B=E_B-E_g=c\Delta. \tag{17}$$

eventually, the averaged Green's function can be written in the form

$$\bar{G}_{\mathbf{nm}}(\omega)=\int D[\psi]\psi_{\mathbf{n}}\psi_{\mathbf{m}}\exp\{-\tilde{A}[\psi]\}, \tag{18}$$

where

$$\tilde{A}[\psi]=A_{vc}[\psi]-\ln\langle\exp\{-\Delta A[\psi]\}\rangle. \tag{19}$$

These expressions are applicable for any values of c; in the two limiting cases $c = 0$ and $c = 1$, G reduces to G^α, where $\alpha = \mathrm{B}$ and A, respectively. Without including the fluctuation-induced part, the action (18) reduces to the Green's function in the virtual-crystal approximation

$$G^{vc}_{\mathbf{nm}}(\varepsilon)=\frac{1}{N}\sum_{\mathbf{q}}\frac{\exp[i\mathbf{q}(\mathbf{R}_{\mathbf{n}}-\mathbf{R}_{\mathbf{m}})]}{\varepsilon-\varepsilon_{\mathbf{q}}}. \tag{20}$$

The expansion of (18) in a perturbation-theory series in powers of Δ_A and Δ_B can be represented in the form of Feynmann diagrams;[17] a feature of this series is automatic exclusion of the possibility of multiple occupation of a site due to the appearance of subtractions, as first described in Ref. 18.

FLUCTUATION-INDUCED BOUND STATES

Bound states appear below the mobility edge, and cannot be described by perturbation theory. We will use the one-instanton approach[19] (see also Refs. 5,11,12,14, and 15), which in the present case implies that the number of bound states and the total volume they occupy are small compared to the crystal volume so that wave functions of different bound states do not overlap.

The equation for the bound states is found from the condition that the action be an extremum

$$\frac{\delta\tilde{A}[\psi]}{\delta\psi_{\mathbf{n}}}=0, \tag{21}$$

i.e.,

$$\sum_{\mathbf{m}}[H_{\mathbf{nm}}-\varepsilon\delta_{\mathbf{nm}}]\psi_{\mathbf{m}}+u_{\mathbf{nn}}[\psi]\psi_{\mathbf{n}}=0, \tag{22}$$

where the effective potential energy depends nonlinearly on ψ_{n}^2

$$u_{\mathbf{nn}}[\psi]=-(E_g-E_{\mathrm{A}})\left[1-\frac{\exp(-{}^1/_2\Delta\psi_{\mathbf{n}}^2)}{c+(1-c)\exp(-{}^1/_2\Delta\psi_{\mathbf{n}}^2)}\right]. \tag{23}$$

We note that $\varepsilon<0$ in the energy range of interest to us. In this case, the sign of $u_{\mathrm{nn}}[\psi]$ corresponds to attraction, and its value is bounded by the inequality

$$0<|u_{\mathbf{nn}}[\psi]|<(E_g-E_L),\quad E_L\equiv E_{\mathrm{A}}. \tag{24}$$

Introducing the notation $\psi_{\mathrm{cl}}(n)$ for the solution to Eq. (22), and carrying out the replacement $\Phi_{\mathrm{cl}}^2(\mathbf{n})=(\Delta/2)\psi_{\mathrm{cl}}^2(\mathbf{n})$, we can write Eq. (22) in matrix form

$$\{I-G^{vc}(\varepsilon)u[\Phi_{cl}]\}\Phi_{cl}=0, \tag{25}$$

where I is the unit matrix. The criterion for the appearance of a localized state with energy $\varepsilon=0$ is[20]

$$\sum_{\mathbf{n}}G_{0\mathbf{n}}^{vc}(0)u_{\mathbf{nn}}[\Phi_{cl}]\geqslant 1 \tag{26}$$

which can always be fulfilled by choosing an appropriate value of the magnitude of Φ_{cl}. On the other hand, for sufficiently large values of this quantity we obtain a bound state with an energy that is arbitrarily close to the maximum depth of the potential well (23), i.e., to the Lifshits boundary.

In the region below the mobility edge, the density of states $\rho(\omega)$ is given up to a preexponential factor by

$$\rho(\omega)\propto\exp\{-\tilde{A}[\Phi_{cl}]\}, \tag{27}$$

where, taking (22) into account,

$$\tilde{A}[\Phi_{cl}]=-\sum_{\mathbf{n}}(F-F'_{\Phi_{cl}^2}\Phi_{cl}^2)_{\mathbf{n}},$$
$$F=\ln[c+(1-c)\exp(-\Phi_{cl}^2(\mathbf{n}))]. \tag{28}$$

The expression $F-F'_{\Phi_{\mathrm{cl}}^2}\Phi_{\mathrm{cl}}^2$ has the form of a step function: in the region of large values of Φ_{cl}^2, it equals $\ln c$, while in the region of small Φ_{cl}^2 it is proportional to Φ_{cl}^4. Thus, we can estimate that $\tilde{A}[\Phi_{\mathrm{cl}}]$ equals $n_0\ln c$, where n_0 is the number of lattice sites within a radius of the fluctuation-induced bound state. In what follows, we will show that $\tilde{A}[\Phi_{\mathrm{cl}}]$ leads both to Urbach behavior below the mobility edge and to a Lifshits singularity as $\varepsilon\to E_L-E_g$. The lattice formulation for the equations for the fluctuation-induced bound states (22), (25) is necessary for those large value of Δ that exceed the critical perturbation energy at a site $G_{00}^{-1}(0)$ by an appreciable amount, for which a bound state forms even for a single attractive center. This form of the equation is also convenient for investigating quantum fluctuations, which are necessary in order to calculate the preexponential factor, because it rids the theory of ultraviolet divergences. In what follows, we will consider a continuum analogue of this equation, assuming that the quantity Δ does not exceed the critical value, and limit ourselves to calculating only the exponent

CONTINUUM LIMIT

The continuum analogue of the action (19) can be written in the form

$$\tilde{A}[\Phi]=\left(\frac{\tilde{\omega}}{\Delta}\right)\left(\frac{E_0}{\tilde{\omega}}\right)^{3/2}\int d^3x[(\nabla\Phi)^2+\Phi^2]$$
$$-\left(\frac{E_0}{\tilde{\omega}}\right)^{3/2}\int d^3x\ln\{\exp[(1-c)\Phi^2][c+(1-c)\exp(-\Phi^2)]\}. \tag{29}$$

Here, we introduce the units $(\hbar^2/2M\tilde{\omega})^{1/2}$ and $\tilde{\omega}=|\varepsilon|$ for measuring length and energy, respectively. The energy $E_0=\hbar^2/2Mv_0^{-2/3}$, where v_0 is the volume of an elementary scatterer, i.e., the volume of crystal required by a single atom. We will use a spherical potential well with volume v_0 as the potential of such a scatterer. Then we can match the parameters of the lattice Hamiltonian and the continuum limit, by requiring that their critical energies be equal for a single scatterer. This implies

$$\frac{2M}{\hbar^2}\left(\frac{2}{\pi}\right)^2\left(\frac{3v_0}{4\pi}\right)^{2/3}=\frac{1}{E_{cr}},\quad\text{i.e. } E_0=\left(\frac{6}{\pi^4}\right)^{2/3}E_{cr}, \tag{30}$$

where E_{cr} is expressed in terms of the parameters of the lattice Hamiltonian in the usual way

$$E_{cr}^{-1}=G_{00}^{vc}(0)=\frac{v_0}{(2\pi)^3}\int_{BZ}\frac{d^3\mathbf{q}}{\varepsilon_{\mathbf{q}}} \tag{31}$$

(the integration extends over the Brillouin zone). The continuum analogue of Eq. (22) has the form

$$(-\nabla^2+1)\Phi_{cl}(x)+u(\Phi_{cl})\Phi_{cl}(x)=0, \tag{32}$$

where

$$u(\Phi_{cl})=-\frac{E_g-E_L}{\tilde{\omega}}\left\{1-\frac{\exp[-\Phi_{cl}^2(x)]}{c+(1-c)\exp[-\Phi_{cl}^2(x)]}\right\}. \tag{33}$$

By substituting the solution (32) into (29), we obtain for the density of states, within a constant coefficient

$$\rho(\omega)\propto\exp\{-\tilde{A}[\Phi_{cl}]\}$$
$$=\exp\left\{\left(\frac{E_0}{\tilde{\omega}}\right)^{3/2}\int d^3x[F-F'_{\Phi_{cl}^2}\Phi_{cl}^2]\right\},$$
$$F=\ln[c+(1-c)\exp(-\Phi_{cl}^2(x))]. \tag{34}$$

Equation (32) has an exponentially decaying solution over the entire interval

$$0<\tilde{\omega}<E_g-E_L. \tag{35}$$

1. Lifshits singularity and approximate solution

Let us consider the situation for $\tilde{\omega}\lesssim E_g-E_L$. In order that a solution to Eq. (32) exist in this case, it is necessary to choose the absolute value of the function Φ_{cl}^2 sufficiently large. Substituting a solution of the form $\Phi_{cl}^2=\lambda\Phi_{cl}^2$ into (32), where φ_{cl}^2 is a normalized function, we see that the depth of the potential well $u(\lambda^{1/2}\varphi)$ is bounded by the quantity $(E_g-E_L)/\tilde{\omega}$; however, its width can increase without bound as λ increases. This also allows us to obtain a solution that corresponds to a bound state for any $\omega<E_g-E_L$. For a

well with sufficiently large radius, we can neglect the contribution from the region of the walls of the potential well, which are not strictly vertical, by replacing them with vertical walls. The radius x_0 of a well with depth $(E_g - E_L)/\tilde{\omega}$ large enough to ensure a bound state with energy equal to unity is given by the well-known expression

$$x_0=\left(\frac{1}{\Omega}-1\right)^{1/2}\left[\pi-\operatorname{arctg}\left(\frac{1}{\Omega}-1\right)^{1/2}\right], \quad \Omega=\frac{\tilde{\omega}}{E_g-E_L}. \tag{36}$$

Keeping in mind that the probability of forming a cluster of radius x_0 consisting of atoms of type A equals

$$\exp\left[\frac{4\pi}{3}x_0^3\left(\frac{\hbar^2}{2M\tilde{\omega}}\right)^{3/2}\frac{1}{v_0}\ln c\right], \tag{37}$$

after substituting (36) into (37) we obtain the Lifshits result (1) in the limit $\tilde{\omega}\to E_g - E_L$. However, (37) is too crude an approximation for the case $\tilde{\omega} < E_g - E_L$. We can significantly improve this result in the region $\Omega < 1$ if we take into account the contributions of the walls. In order to do this, we make use of the following procedure.

Let us write the solution $\Phi_{cl}(x)$ in the form $\Phi_{cl}(x) = \lambda^{1/2}\varphi_0(x)$, where φ_0 is the normalized eigenfunction of a bound state with unit energy in a potential well with vertical walls, i.e.,

$$u^0(x)=\begin{cases}-(E_g-E_L)/\tilde{\omega}, & x\leqslant x_0\\ 0, & x>x_0\end{cases}. \tag{38}$$

Let us substitute this test function into $\tilde{A}[\Phi]$, and find λ from the condition that the action be an extremum

$$\frac{\delta\tilde{A}[\lambda^{1/2}\varphi_0]}{\delta\lambda}=0. \tag{39}$$

Keeping in mind that $\varphi_0(x)$ is an eigenfunction of the linear equation

$$[-\nabla^2+1+u^0(x)]\varphi_0(x)=0, \tag{40}$$

we transform (39) to the form

$$\int d^3x\, u[\lambda^{1/2}\varphi_0(x)]\varphi_0^2(x)=\int d^3x u^0(x)\varphi_0^2(x), \tag{41}$$

where the left-hand side contains the potential energy from (33). This equation has a solution over the entire interval (35). The substitution $\Phi_{cl} = \lambda^{1/2}\varphi_0$ into (34) gives a result that agrees very well with the exact solution (32).

2. The Halperin-Lax limit and the Lorentz model

Let us consider the solution to Eq. (32) in the region $\tilde{\omega}\ll E_g - E_L$. A solution exists in this region when the absolute value of Φ_{cl}^2 is small compared to unity. Expanding $u(\Phi_{cl})$ in a series of powers of Φ_{cl}^2, and keeping the first term, we obtain after some transformations an equation which corresponds in form to the $g\psi^4$ problem,[21,22] i.e.,

$$[-\nabla^2+1-\psi_{cl}^2(x)]\psi_{cl}(x)=0. \tag{42}$$

The action, including the first-order correction, takes the form

$$\tilde{A}[\psi_{cl}]=\frac{I_4}{4g}-c(1-c)(1-2c)\left(\frac{\Delta}{E_0}\right)^3\frac{I_6}{48g^3}, \tag{43}$$

where

$$I_n=\int d^3x\psi^n(x), \quad I_4=75{,}585, \quad I_6=659{,}928 \tag{44}$$

and g is the coupling constant of the theory:

$$g=\frac{c(1-c)\Delta^2}{2\tilde{\omega}^2}\left(\frac{\tilde{\omega}}{E_0}\right)^{3/2}. \tag{45}$$

We note that in the region $c\approx 1/2$ it is necessary to include the next terms in the expansion of the action as well.

In order to estimate the region of ω where (43) is correct, we recall that not only the action itself but also its derivative with respect to $\tilde{\omega}$ is forbidden to change sign. From this we obtain a bound on the quantity $\tilde{\omega}$:

$$\tilde{\omega}\ll\omega_0, \quad \omega_0=\Delta\frac{c(1-c)}{1-2c}\frac{I_4}{I_6}. \tag{46}$$

This being the case, the value of the coupling constant g is bounded by the inequality

$$g\gg{}^1/_2[c(1-c)(1-2c)]^{1/2}(I_6/I_4)^{1/2}. \tag{47}$$

Keeping in mind that the region of the single-instanton approximation for the $g\psi^4$ theory is limited by the requirement $g < 1$, we may conclude that the behavior of the density of states predicted by this theory

$$\rho(\omega)\propto\exp\left(-\frac{I_4}{4g}\right)=\exp\left[-\frac{I_4}{16\pi}\left(\frac{\tilde{\omega}}{\omega_{HL}}\right)^{1/2}\right], \tag{48}$$
$$\omega_{HL}^{7/2}=\frac{c(1-c)\Delta^2}{8\pi E_0^{3/2}},$$

can occur only in an extremely narrow region

$$\omega_{HL}<\tilde{\omega}\ll\omega_0 \tag{49}$$

for values of $\min(c,1 - c)\ll 1$, and also in the limit of weak scattering $\Delta\ll E_0$. In the remaining cases, i.e., for $\Delta\lesssim E_0$ and not-too-small values of c and $1 - c$, the quantity ω_0 may be regarded as an upper limit for the applicability of the single-instanton approximation in the Anderson model under discussion here.

The Lorentz model i.e., a dilute gas of scattering centers with repulsive potentials, has been investigated in a number of papers.[9-12] The action corresponding to this model is obtained from (29) by expanding in powers of $1 - c$ and preserving the first term

$$\tilde{A}[\Phi]=\left(\frac{\tilde{\omega}}{\Delta}\right)\left(\frac{E_0}{\tilde{\omega}}\right)^{3/2}\int d^3x\left[(\nabla\Phi)^2+\Phi^2-\frac{E_g-E_L}{\tilde{\omega}}(1-\exp(-\Phi^2))\right]. \tag{50}$$

The equation of motion has the form

$$(-\nabla^2+1)\Phi_{cl}-\frac{E_g-E_L}{\tilde{\omega}}[1-\exp(-\Phi_{cl}^2)]\Phi_{cl}=0, \tag{51}$$

and the expression for the density of states is

$$\rho(\omega)\propto\exp\left\{-\left(\frac{E_0}{\tilde{\omega}}\right)^{3/2}\times\int d^3x(1-c)[1-(1+\Phi_{cl}^2)\exp(-\Phi_{cl}^2)]\right\} \tag{52}$$

which also leads to a Lifshits singularity as $\tilde{\omega}\to E_g - E_L$, as in the exact expression (32)–(34).

3. Results of numerical calculations

Equation (32) depends on two parameters: $\Omega = \tilde{\omega}/(E_g - E_L)$, i.e., the relative depth of the bound state, and c, i.e., the concentration of atoms A. In the interval of values $0 < \Omega < 1$ we obtain a family of solutions corresponding to different values of the other parameter c. Keeping in mind that $E_0 = (6/\pi^4)^{2/3} E_{\rm cr}$, we write $\rho(\omega)$ in the form

$$\rho(\omega) \propto \exp \{\nu_{cr}^{3/2} J(\Omega, c)\}, \tag{53}$$

where

$$\nu_{cr} = \frac{E_{cr}}{E_g - E_L}, \quad J(\Omega, c) = \frac{6}{\pi^4} \frac{1}{\Omega^{3/2}} \int d^3x \, [F - F'_{\Phi^2_{cl}} \Phi_{cl}{}^2]. \tag{54}$$

For comparison let us write (37) in the same units

$$\rho(\omega) \propto \exp \Big\{ -\nu_{cr}^{3/2} \left(\ln \frac{1}{c}\right) \left(\frac{1}{1-\Omega}\right)^{3/2} \times \left[2 - \frac{2}{\pi} \operatorname{arctg}\left(\frac{1}{\Omega} - 1\right)^{1/2} \right]^3 \Big\}, \tag{55}$$

where $\nu_{\rm cr}^{3/2}$ is the number of attractive centers necessary to form a bound state with zero energy. From this it is clear that if $E_g(c) - E_L$ coincides with $E_{\rm cr}$, then the maximum value satisfies $\rho(\omega) \sim c$. Expression (55) makes it possible for us to estimate $\rho(\omega)$ over the entire interval of Ω and c with the exception of the region $\Omega \ll 1$.

In Fig. 1 we show the results of a calculation of $\tilde{A}\,[\Phi_{cl}]$ using the exact formula (53), the approximate solution (41), the approximation (55), and the limiting Halperin-Lax formula (48). It is clear from the figure that the exact solution of Eq. (32) and the approximate solution (41) give results that practically coincide. This implies that the exact solution can be usefully approximated by the solution to Eq. (40), and that the shape of the fluctuation-induced well does not differ too greatly from rectangular. In Fig. 2 we show the potential wells for various values of Ω. From this figure we can conclude that with the exception of the region $\Omega \ll 1$ the fluctuation-induced wells are actually close to rectangular.

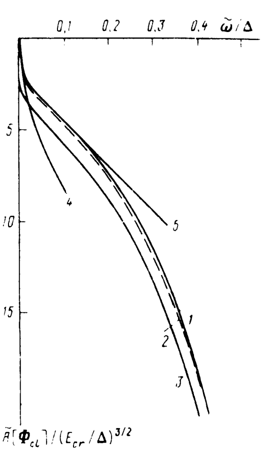

FIG. 1. Dependence of the exponential of the density of states on the depth of the state: *1*—results of exact solution to Eq. (32), *2*—computation using the approximate solution (41), *3*—approximate fluctuation-induced well for spherical and vertical walls (37), (55), *4*—approximation of Gaussian white noise (48), and *5*—approximation of a portion of the dependence of $\tilde{A}\,[\phi_{\rm cl}]$ on $\tilde{\omega}$ by the Urbach rule. All computations were carried out for $c = 0.1$.

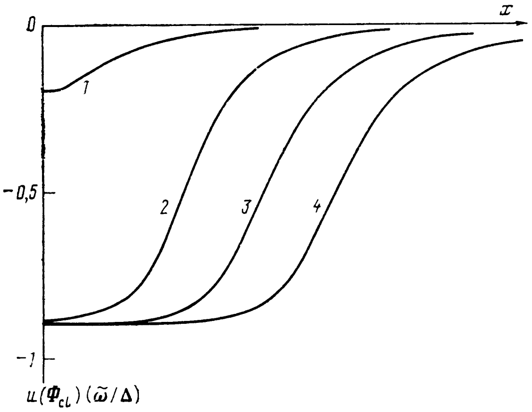

FIG. 2. Dependence of the shape of the potential well (33) on the depth of the state. Curves *1–4* correspond to values $\tilde{\omega}/\Delta = 0.005, 0.055, 0.105$, and 0.155.

Let us turn now to the dependence of $\tilde{A}\,[\Phi_{cl}]$ on Ω. It is clear from Fig. 1 that in the region $\Omega < 1$ there is a sizable interval of Ω below the mobility edge over which the behavior of curves *1–3* is close to linear. Analogous portions appear for other values of concentration as well. The presence of segments of Urbach behavior of $\tilde{A}\,[\Phi_{cl}]$ is a property that is intrinsic to the Anderson model, and probably to other models of random potentials where the depth of the potential contour is bounded by some limiting value. It is clear from Fig. 1 (curve *4*) that such segments are absent for a potential with the statistics of Gaussian white noise.

4. The Urbach rule

It follows from Sec. 2 that the function $\tilde{A}\,[\Phi_{cl}]$ has a singularity of the form $\Omega^{1/2}$ as $\Omega \to 0$. Thus, even the first derivative of the action with respect to frequency satisfies $\tilde{A}'_\Omega[\Phi_{cl}] \to \infty$ as $\Omega \to 0$. As we move away from the upper boundary of the spectrum, $\tilde{A}'_\Omega[\Phi_{cl}]$ decreases. In the vicinity of the point $\Omega_0 = \omega_0/(E_g - E_L)$, the character of the frequency dependence of $\tilde{A}'_\Omega$ changes considerably. This is because it is not valid to expand $u(\Phi_{cl})$ in powers of Φ^2_{cl} in this region, since all the terms of the series begin to play a role. As we depart further from the mobility edge, $\tilde{A}'_\Omega[\Phi_{cl}]$ begins to increase once more, since its behavior in this region is dominated by the approach to the Lifshits boundary where the function itself and all of its derivatives are singular. These considerations imply that the derivative $\tilde{A}'_\Omega[\Phi_{cl}]$ has a minimum whose position is given by the equation

$$\tilde{A}_{\Omega=\Omega_u}[\Phi_{cl}] = 0 \tag{56}$$

The expansion of $\tilde{A}\,[\Phi_{cl}]$ in a Taylor series at this point has the form

$$\tilde{A}[\Phi_{cl}] = \tilde{A}_{\Omega_u}[\Phi_{cl}] + \tilde{A}'_{\Omega_u}(\Omega-\Omega_u) + {}^1/_6 \tilde{A}'''_{\Omega_u}(\Omega-\Omega_u)^3 + \ldots \tag{57}$$

Taking into account that for $\Omega \gtrsim \Omega_u$ the action is a function of Ω whose essential dependence is determined by the factor $(1-\Omega)^{-3/2}$, we may conclude that in this region the cubic term of the expansion will be small as long as the following condition holds:

$$(\Omega-\Omega_u)^2 \ll 1. \tag{58}$$

At the same time, in the region $\Omega < \Omega_u$ we must use the value

$\Omega = \Omega_0$, where the dependence of $\tilde{A}_\Omega[\Phi_{cl}]$ on Ω becomes sqaure-root-like, in order to estimate the limits of applicability of the expansion (57).

Thus, we conclude that, regardless of the values of the parameters of the problem, e.g., $\Delta = E_0 - E_A$, E_0 and the concentration, the function $\tilde{A}_\Omega[\Phi_{cl}]$ is dominated by the linear term in the expansion (57) over a rather wide interval of values

$$\omega_0<\tilde{\omega}<E_g-E_L. \tag{59}$$

In this region ($\varepsilon < 0$),

$$\rho(\varepsilon) \propto \exp\left(\frac{\varepsilon}{E_u}\right) = \exp\left(-\frac{E_g-\omega}{E_u}\right), \tag{60}$$

where

$$E_u = (E_g - E_L)/\tilde{A}'_{\Omega=\Omega_u}[\Phi_{cl}], \tag{61}$$

and the position of Ω_u is given by Eq. (56).

The dependence of the Urbach parameter E_u on concentration is shown in Fig. 3. It is noteworthy that the use of the exact solution to Eq. (32) and the approximate solution (41) lead to values of E_u that agree to two decimal places. Using the approximation (55) also gives a value for this parameter close to the previous two. Using this fact, we obtain an approximate formula for E_u:

$$E_u = \frac{(E_g - E_L)^{5/2}}{E_{cr}^{3/2}}\left(\beta^3 \ln\frac{1}{c}\right)^{-1}, \tag{62}$$

where by using (55) we have separated out the primary part of the dependence of E_u on c and two other parameters of the problem, while the function β with good accuracy can be set equal to a constant, i.e., $\beta \simeq 2$. The results of calculating E_u using (62) are also shown in Fig. 3.

It follows from (61) and (62) that we may expect E_U to be very sensitive to the dependence of E_g on concentration. In the approach developed in this paper, the dependence of the mobility edge on concentration turns out to be associated with the average value of the potential at a site $E_g = \bar{E} \equiv E_g^{vc}$. In practice, however, the mobility edge may differ considerably from E_g^{vc}. In Fig. 3 we show the values of E_u obtained by substituting a value of E_g of the form $E_g = E_g^{vc} - bc(1-c)\Delta^2/E_{\rm cr}$ into Eq. (32), using the values $b = 0.5$ and $b = 1$. It is clear that this change in b affects the position of the maximum E_u and its value. The question of whether or not it is possible to sequentially eliminate the fluctuation-induced corrections to E_g^{vc} remains an open one at this time.

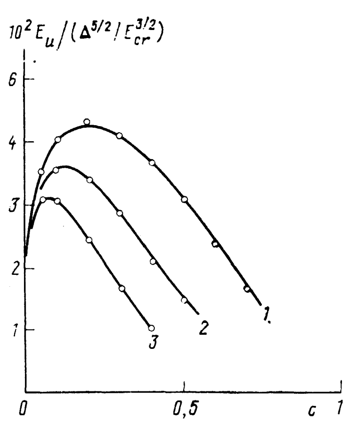

FIG. 3. Dependence of the Urbach parameter on concentration. The solid curves are the results of calculations using (61) and (56). The circles come from using (62) for $\beta = 2.025$. *1*—the approximation $E_g = E_g^{vc}$, *2,3*—results obtained from the substitution $E_g = E_g^{vc} - b \cdot c(1-c)\Delta^2/E_{\rm cr}$ for $b = 0.5$ and 1.

The calculated results given here and plotted in Fig. 3 allow us to estimate the absolute values of the Urbach parameter E_u. Analogous estimates are also possible using the expression (62). Thus, if the maximum depth of the potential perturbations associated with the insertion of an A atom into a B lattice is a number on the order of the kinetic energy $\Delta \approx E_{\rm cr}$, while the absolute value is $E_{\rm cr} \approx 1$ eV, then the maximum value satisfies $E_u \approx 50$ meV. This estimate shows that experimental data available at the present time regarding the value E_u for a large variety of disordered systems lie within the interval of values E_u predicted by the Anderson model for moderate values of the model parameters.

The strong dependence of the value of E_u on the ratio $\Delta/E_{\rm cr}$ allows us to explain the differing scales of fluctuation-induced effects in the solid solutions $\rm A_{II}B_{VI}$ during anionic and cationic replacements. When an anion is replaced, the magnitude of the effect is determined by the valence bands, for which the value of $E_{\rm cr}$ is considerably smaller than for the conduction bands, so that at least for several compounds this type of ratio $\Delta/E_{\rm cr}$ is close to unity, and the value of E_u for the valence band takes on values close to maximal.

We should also note that the concentration dependence of E_u obtained in Ref. 5 is found to be in good agreement with the results of these calculations.

It seems to us that these investigations establish a simple connection between the Urbach rule for decay of the density of localized states and the asymptotic Lifshits behavior of the latter. The limitation on the depth of the fluctuation-induced well imposed by the Lifshits bound leads to the appearance of a solution to Eq. (56) and to the expansion (57) for which the linear terms dominate over a wide range. These relations, and also the expression for E_u (61), are also applicable to crystals with dimensions $d = 1$ and 2, because they are based on properties of $\tilde{A}[\Phi_{cl}]$ that are general for all three choices of dimensionality.

The Urbach dependence we have obtained cannot be described even approximately by the Gaussian approximation. It is clear from a comparison of curves *1* and *4* of Fig. 1 that extrapolation of a Gaussian into this region leads to negligibly small values of $\rho(\omega)$. Introduction of nonlocal Gaussian statistics[23-25] also leads to the appearance of a segment of $\ln\rho(\omega)$ with linear slope; however, as shown in Ref. 25, this occurs because of a further decrease in $\rho(\omega)$.

The problem investigated here does not include temperature effects, and E_u can be compared with the low-temperature limit of the Urbach formula,[26-27] which gives $E_u = \hbar\omega_p/2\sigma_0$ (see data regarding the parameters ω_p and σ_0 in the tables of Ref. 27). At finite temperatures, interactions with lattice vibrations[28-31] can change the value of E_u considerably, both in ordered and in disordered systems. If the temperature is comparable to the melting temperature, intrinsic lattice defects may play an important role in the formation of the tail of localized states.[4]

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