PHYSICAL REVIEW B VOLUME 48, NUMBER 5 1 AUGUST 1993-I

Density of localized states in disordered solids

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(Received 15 December 1992)

Calculations of a localized state density (DOS) are carried out in the framework of a well-known variant of the Anderson model, i.e., for the three-dimensional single-band Hamiltonian with diagonal disorder. Results of the calculations give three regions of the energies below the virtual crystal band edge E_G^{vc} characterized by different behavior of the DOS. (I) The band-edge (BE) region is placed in the vicinity of E_G^{vc}. Here the DOS on a linear scale is approximately a linear function of the localization energy. (II) At lower energies the Urbach law governs the DOS behavior. (III) At lower energies the DOS exhibits Lifshitz singularity dependence. Here the DOS has a very small value and rare deep centers (DC) can appear in the spectrum. The problem of the DC-band inhomogeneous broadening is also considered. Estimations of the number of localized states and of the mobility-edge position are presented. The data on single-electron-DOS energy dependence of α-Si:H are used to compare qualitatively the calculated DOS with the experiment results. Good agreement is reached both in DOS behavior and in the mobility-edge location. An aspect in the approach to the problem is an additional restriction of the trial-function class minimizing the one-instanton action. The additional restriction was obtained from the analysis of the localized state problem for the concrete realizations of the disordered system under consideration. A strong-scattering problem in the limit of small concentration of scatterers is studied, as well as the case of the three-component system consisting of a binary solution of weak scatterers with a third component comprising rare deep centers. In all of the cases considered the general expressions for the DOS including prefactors are found, as well as their approximate forms. It is shown that there are limits which allow for single-instanton solution of the problem to coincide with the exact one.

I. INTRODUCTION

Modern experiments give detailed information on the behavior of both spectral density and single-electron density of states (DOS) for many different disordered systems, see Refs. 1–7 and references therein.

The single-electron DOS of amorphous silicon in the regions on the top of the valence band and in the band gap was studied in detail in Refs. 4 and 5. The DOS obtained in Refs. 4 and 5 in these regions can be characterized by the following interesting features.

(1) In the region of relatively high values of the DOS near the top of the valence band, the DOS energy dependence is linear; i.e., it can be described by the formula

$$\rho(\epsilon)=\rho_{\mathrm{BE}}\left\{1-\frac{E_G-\epsilon}{E_{\mathrm{BE}}}\right\}. \tag{1}$$

Parameters ρ_{BE} and E_{BE} can be found by a simple fitting procedure taking the energy E_G as the frame of reference to be equal to the experimentally known position of the mobility edge. We prefer a slightly different definition of E_G which is more convenient for the theoretical approach and put it equal to the edge of the band in a virtual-crystal approximation. After the other parameters of Eq. (1) are calculated for the model Hamiltonian we should estimate the position of the mobility edge in order to reconcile the theoretical and experimental results. Equation (1) remains correct until the linear term is small compared with the constant one.

(2) For increasing energy, Eq. (1) transforms into the well-known Urbach law,[8–10] which probably always appears in disordered solids (see Refs. 1–10 and references therein). The Urbach law for the DOS taken in the logarithmical scale leads to a linear function of energy,

$$\ln\rho(\epsilon)=\ln\rho_U-\left\{\frac{E_G-\epsilon}{E_U}\right\}. \tag{2}$$

Here again the value of the parameter ρ_U depends upon the chosen frame of reference of the energy. The magnitude of the Urbach parameter E_U obtained in Ref. 4 satisfies the inequality $E_U < E_{\mathrm{BE}}$.

(3) At lower energies the DOS behavior is influenced to a great extent by the presence of deep centers in the samples of Ref. 4. Here we can speak about the superposition of two tails of different origin. One of them is the decreasing Urbach tail, while the other is due to the inhomogeneously broadened deep-center band. The results of Ref. 4 show the Gaussian form of the band near the band center and, therefore, we write for it

$$\rho_I(\epsilon)\frac{c_I}{[2\pi\gamma_I^2]^{1/2}}\exp\left\{-\frac{(\epsilon_I-\epsilon)^2}{2\gamma_I^2}\right\}, \tag{3}$$

where c_I is the deep-center concentration and γ_I is the band half-width. The wings of the band are considerably asymmetrical. There are a number of data giving evidence for more complicated structure of the deep-center bands in the literature.[11–14] A removal of degeneracy due to fluctuation of the nearest neighborhood,[11,12] appearance of the clusters consisting of the deep centers,[13,14] as well as a homogeneous broadening lead to complexity of

0163-1829/93/48(5)/3100(16)/$06.00

the structure. We do not touch on these problems in this work.

All of the above listed features of the DOS are observed in different samples of amorphous silicon. The absolute value of the DOS accurate to a factor of 2 was reported in Ref. 4 and, therefore, the general number of states below the mobility edge can also be found as well as the number of deep centers.

The purpose of our work is a theoretical investigation of the possibility of describing the observed features of the DOS behavior. We proceed from the premise that only very general characteristics of the fluctuation potential are essential for the explanation of DOS features, and we exploit for the calculation of the DOS the simple three-dimensional single-band Hamiltonian with diagonal disorder resulting from random distribution of two kinds of atoms A (attractive centers) and B (repulsive ones) and the continuum analog of the model. It is the well-known variant of the so-called Anderson model.

The model to be used here has been extensively studied in the context of perturbation theory and in the coherent potential approximation to describe many properties of disordered solid solutions (see Refs. 15 and 16 and references therein). The problem of localized states applying a calculation method lying beyond both mentioned approaches was considered in the framework of this model earlier in Ref. 17. The results obtained there give the Urbach dependence like Eq. (2) within an energy interval which is wide enough to describe the experimental data for different disordered systems. The observed values of the Urbach parameter as well as its composition dependence for the solid solutions A_2B_6 given in Ref. 6 can be explained. However, the behavior of the DOS above the Urbach region in Ref. 17 differs from both the experimental data of Ref. 4 and Eq. (1). This problem is the subject of the present investigation.

The other question to be considered here is the strong-scattering limit, i.e., the situation of a small concentration of deep centers. Two aspects of this problem are of interest.

First, we have the limit of small but finite values of the attractive center concentration c in the two-component Hamiltonian. This question is closely related with the strong local perturbation problem solved in Ref. 18 for the electron system and in Ref. 19 for the phonon system (see also Refs. 20 and 21 and references therein). As a result, we know the answer described by the Koster-Slater-Lifshitz equation in the limit $c \rightarrow 0$, which could be used for checking the calculations.

The second variant of the problem concerns rare deep centers in the relatively shallow sea of the random potential; the actual situation for amorphous silicon and, probably, for other disordered systems. The necessary additional complication of the model Hamiltonians described above is easily incorporated. A solution of the problem could be applied to the experimental data of Ref. 4.

Another problem of interest for the experiment is concerned with a preexponential factor of the Green function which makes it possible to normalize the calculated DOS. For the purpose of checking upon the prefactor both strong-scattering cases are especially important.

We describe the model Hamiltonian in the lattice representation in Sec. II. The Hamiltonian contains three parameters. Two of them are the amplitude of the fluctuation potential equal to the difference of diagonal tight-binding matrix elements of attractive and repulsive atoms and the averaged number of attractive centers per unit volume or their concentration. The third parameter is related with the dispersion of the electronic band and in compressed form is presented by the critical value of single-lattice-site perturbation leading to a splitting off the bound state with binding energy equal to zero.

In Sec. III the Green-function representation is introduced using anti-commutating variables. The first problem appearing here is concerned with the zero fermionic modes of the determinants, leading to the disappearance of the single-instanton result for the Green function and to a DOS which looks unreasonable in the context of the problem studied. To revolve this question we accent rather a difference between the field-theory instanton approach[22–25] and that in the problem of the DOS calculation for the random system.

In the last case, the spectrum of the disordered system can be represented as a superposition of a great number of spectra calculated for each of the possible realizations of the system in definite volume taken with weights equal to the probability of the appearance of the given realization. This procedure is applied usually in numerical calculations (see Refs. 16 and 26–29 and references therein). A calculation of eigenfunctions and eigenvalues for the concrete realization is purely linear in the mathematical sense. Using all eigenstates and eigenvalues for all possible realizations we discover the supersymmetry of the problem and obtain an expression for the averaged Green function of the disordered system convenient for exact calculation of the determinants by means of a formula given by Parisi and Sourlas in Ref. 30.

After a calculation of the determinants is performed the problem is reduced to a variational procedure under the action describing the averaged Green function. This idea and many details of this procedure coincide with ones in earlier works.[17,31–44] The new element introduced here is an additional restriction on the behavior of the trial function $\varphi_{\mathrm{tr}}(R)$, presenting a solution of the saddle-point equation.

The restrictions on the trial function undertaken in previous investigations were concerned with (i) consideration of only the ground state of the fluctuation well, (ii) restriction by spherically symmetrical functions, and (iii) postulation of the decreasing law of the trial function $\varphi_{\mathrm{tr}}(R)$ at great distances R from the fluctuation, consistent with a demand of short-range potential wells. The new restriction is concerned with the coordinate dependence of the trial function in the limit of small distances from the center of the fluctuation well and appears as a result of adjusting the latter to the behavior of the most probable solutions in concrete realizations.

The general scheme of the averaging procedure is given in the last part of Sec. III, which also illustrates the fact that all of the results of Ref. 17 are contained in the new form of the Green-function representation if the additional restriction is omitted.

Section IV is devoted to the strong-scattering problem in the two-component system at small concentrations of the attractive centers. Here an additional restriction on the behavior of $\varphi_{\mathrm{tr}}(R)$ at $R \rightarrow 0$ leads to a close relation between the trial function of the variational problem and the Koster-Slater-Lifshitz solution of the point-perturbation equation. The full number of bound states appeared to be equal to the number of deep centers. The solution of the considered instanton problem coincides with exact solution of the linear problem in the limits when the binding energy goes to the Lifshitz border of the spectrum (see Refs. 45, 38–41, and 17), as well as to the upper border of the bound states in the linear approximation of attractive centers, and in the case of very strong attraction.

In Sec. V we deal with the weak-scattering situation considering the problem in a continuum limit. The equations of the paper[17] are derived again from the new representation of the Green function if the additional restriction on the behavior of the trial function is omitted.

An analysis of the linear problem is presented, showing how the additional restriction on the behavior of the trial function can be expressed in terms of properties of the admissible fluctuation wells. As a result, the R dependence of the trial function at $R \rightarrow 0$ should coincide with that of bound solutions of the linear problem containing the most probable critical cluster in the origin.

The results of numerical calculations are presented, showing a good qualitative agreement with the experimental data of Ref. 4 in regions described by both Eq. (1) and Eq. (2). The analytical expressions for the E_{BE} and for E_U are given.

The three-component system is considered when the third component is the deep centers and the Gaussian form of the deep-center band is derived. The last part of the section gives the full expression for the DOS including both exact and approximate expressions for the preexponential factors in the three-component situation.

We give also an estimation of the upper border of the single-instanton approach and of the mobility-edge position.

Section VI presents a discussion of the results and a comparison with experiential data.

II. MODEL HAMILTONIAN

We consider the macroscopic volume V of the crystal containing N lattice sites randomly filled with two sorts of atoms A and B. The averaged number of atoms A is equal to $N_A = cN$ and that of atoms B is $N_B = (1-c)N$. Atoms A are supposed to be attractive centers and c is their concentration. The single-band Hamiltonian of the system is

$$H = -\sum_{n,m} \Psi_n W_n (\Psi_{n+m} - \Psi_n) + \sum_n E_n \Psi_n^2 \ . \tag{4}$$

We can take the wave functions Ψ_n in many cases to be real. The diagonal matrix element E_n is equal to E_A if the site is occupied with atom A and to E_B in the opposite case. The off-diagonal matrix element defining the band dispersion is supposed to be independent of the composition.

If $c=0$ or $c=1$, Eq. (4) presents the Hamiltonian of regular B or A crystals with all E_n being equal to E_A or E_B. We suppose in calculations $E_B > E_A$.

Using the plane-wave representation we have in these cases

$$H_q^\alpha = \varepsilon_q + E_\alpha \ , \tag{5}$$

where α is A or B and the relation

$$\varepsilon_q = W_0 - W_q \tag{6}$$

describes the electronic band dispersion.

III. GREEN FUNCTION AND DOS REPRESENTATION

The Green function of the crystal A or B can be presented as

$$G_{nm}^\alpha(\epsilon) = \{\epsilon - H^\alpha\}_{nm}^{-1} = \frac{1}{N} \sum_q \frac{e^{iq(\mathbf{R}_n - \mathbf{R}_m)}}{\epsilon - \varepsilon_q - E_\alpha} \ , \tag{7}$$

where $\mathbf{R}_n$ gives the coordinates of lattice site n.

In the case of random filling of the lattice sites by two components the Green function is dependent on the composition realized and on the disposition of the atoms:

$$G_{nm}(\epsilon; \mathbf{R}_1 \cdots \mathbf{R}_N) = \{\epsilon - H(\mathbf{R}_1 \cdots \mathbf{R}_N)\}_{nm}^{-1} \ . \tag{8}$$

For the occasional but definite distribution of the atoms A and B the Green function looks as in Refs. 25, 46, and 47,

$$G_{nn}(\epsilon) = Z^{-1} \int D[\Psi] |\Psi_n|^2 \exp\{-iA[\Psi]\} \ , \tag{9}$$

where Z is normalizing factor equal to

$$Z = \int D[\Psi] \exp\{-iA[\Psi]\} \ , \tag{10}$$

and

$$\begin{aligned} A[\Psi] &= -\sum_{nm} \Psi_n (H_{nm} - \epsilon \delta_{nm}) \Psi_m \ , \\ H_{nm} &= -W_{m-n} + \delta_{nm} \left[\sum_l W_l + E_n \right] \ . \end{aligned} \tag{11}$$

Here δ_{nm} is the Kronecker symbol.

We introduce for the energies the frame of reference connected with the averaged value of E_n in a lattice site:

$$\langle E \rangle_{\mathrm{av}} = cE_A + (1-c)E_B \ . \tag{12}$$

The value $\langle E \rangle_{\mathrm{av}}$ coincides with the bottom of the band in a virtual-crystal approximation and, therefore, with the mobility edge in this approach $E_G \equiv E_G^{\mathrm{VC}} = \langle E \rangle_{\mathrm{av}}$. Introducing the new variables

$$\omega = E_G - \epsilon, \Delta_n = E_n - E_G \ , \tag{13}$$

we transform the action $A[\Psi]$ to the expression

$$A[\Psi] = A_{\mathrm{VC}}[\Psi] + \Delta A[\Psi] \ , \tag{14}$$

where

$$A_{\mathrm{VC}}[\Psi]=-\sum_{n,m}\Psi_n(H_{nm}+\omega\delta_{nm})\Psi_m\ , \tag{15}$$

$$\Delta A[\Psi]=\sum_n \Delta_n\Psi_n^2\ . \tag{16}$$

Note that ω is positive in the region of bound states. The problem of the eigenfunction and eigenvalue calculation for the crystal with disordered but definite disposition of constituent atoms is linear and its solution is obtained by means of diagonalization of the N-rank matrix. Each of the N lines of the corresponding equation looks as

$$\omega_\lambda\varphi_\lambda^\Delta+\sum_m (H_{nm}^{\mathrm{VC}}-\Delta_n\delta_{nm})\varphi_\lambda^\Delta(m)=0\ . \tag{17}$$

Equation (17) gives a full set of eigenfunctions for a given realization characterized by the definite disposition of the atoms. Let us rewrite the integral (9) using the eigenfunctions and eigenvalues of Eq. (17) and introducing Grassmann variables $\zeta,\bar{\zeta}$ in order to carry over the normalization factor Z into the numerator of equation (see Refs. 25, 46 and 48–51). We obtain

$$G_{nn}(\omega)=\int\prod_\lambda[dz_\lambda^* dz_\lambda d\zeta_\lambda d\bar{\zeta}_\lambda]\sum_\lambda|z_\lambda\varphi_\lambda^\Delta(n)|^2\exp\left\{-i\sum_\lambda[\omega+H^{\mathrm{VC}}-\Delta]_{\lambda\lambda}(z_\lambda^* z_\lambda+\bar{\zeta}_\lambda\zeta_\lambda)\right\}\ , \tag{18}$$

where

$$[\omega+H^{\mathrm{VC}}-\Delta]_{\lambda\lambda}=\sum_{n,m}\varphi_\lambda^\Delta(n)[(\omega-\Delta_n)\delta_{nm}+H_{nm}^{\mathrm{VC}}]\varphi_\lambda^\Delta(m)\ . \tag{19}$$

We suppose the Grassmann variables to be normalized according to

$$\int d\zeta_\lambda d\bar{\zeta}_\lambda=1/\pi\ . \tag{20}$$

The quantity of physical interest is an averaged Green function which can be obtained summing over the full set of Green functions (18) corresponding to all possible variants of filling the lattice sites in a considered volume of the crystal.

Before the averaging procedure is carried out we simplify the representation of the Green function (18) in each of the possible configurations, exploiting the very general properties of the full set of eigenfunctions used and the fact that the exponential expression in Eq. (18) in the space of variables z,ζ remains invariant under all transformations conserving the form

$$(z_\lambda^* z_\lambda+\bar{\zeta}_\lambda\zeta_\lambda)\ . \tag{21}$$

This fact is evidence for the supersymmetry of the expression and we can use the Parizi-Sourlas formula[30] for the exact calculation of the integrals over the variables $z_\lambda^*, z_\lambda, \bar{\zeta}_\lambda$, and ζ_λ.

In the sum of Eq. (18) over λ only one of an infinite number of integrals over z_λ, z_λ^* cannot be calculated explicitly. Namely, the integral

$$\begin{aligned}1/\pi\int dz_\lambda^* dz_\lambda|z_\lambda\varphi_\lambda^\Delta(n)|^2 M'_{|z_\lambda|^2}(|z_\lambda|^2)&=\int_0^\infty d\tau_\lambda M(\tau_\lambda)|\varphi_\lambda^\Delta(n)|^2\\&\equiv\int_0^\infty d\tau_\lambda|\varphi_\lambda^\Delta(n)|^2\exp\{-i[\omega+H^{\mathrm{VC}}-\Delta]_{\lambda\lambda}\tau_\lambda\}\ ,\end{aligned} \tag{22}$$

where

$$M'_{|z_\lambda|^2}(|z_\lambda|^2)=\frac{\partial}{\partial(|z_\lambda|^2)}M(|z_\lambda|^2)$$

and

$$M(|z_\lambda|^2)=\exp\{-i[\omega+H^{\mathrm{VC}}-\Delta]_{\lambda\lambda}|z_\lambda|^2\}\ .$$

As a result the partial DOS at a fixed atomic configuration (and, therefore, at a definite set of values Δ_n) and at a given quantum number λ can be presented as

$$\rho_{\Delta,\lambda}(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau_\lambda\sum_n|\varphi_\lambda^\Delta(n)|^2\times\exp\{-i[\omega+H^{\mathrm{VC}}-\Delta]_{\lambda\lambda}\tau_\lambda\}\ . \tag{23}$$

The full DOS can be written as a sum over all λ and over all possible sets of Δ taken with the weight P_Δ equal to the normalized probability of the appearance of a given configuration at random filling of the lattice:

$$\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\sum_\Delta P_\Delta\sum_\lambda d\tau_\lambda\sum_n|\varphi_\lambda^\Delta(n)|^2\exp\{-i[\omega+H^{\mathrm{VC}}-\Delta]_{\lambda\lambda}\tau_\lambda\}\ . \tag{24}$$

We are interested mainly in the partial DOS where only the states of spherical symmetry are taken into account. In that case the sum over λ in Eq. (24) should be omitted.

The physical sense of Eq. (24) is rather transparent; namely, we should look over all possible variants of the lattice filling and find the eigenfunctions and eigenvalues in each case. After that, we should calculate the integrals in (23) and perform the summing in (24). The integrals in Eqs. (23) and (24) over τ_λ can be taken in general form and the expression for the $\rho(\omega)$ is transformed to the simple formula

$$\rho(\omega)=\sum_{\Delta} P_{\Delta} \sum_{\lambda} \sum_{n} |\varphi_{\lambda}^{\Delta}(n)|^2 \delta(\omega-\omega_{\lambda}^{\Delta}) \ . \qquad (25)$$

We have denoted the eigenvalues of Eq. (17) for the fixed set of Δ_n as $\omega_{\lambda}^{\Delta}$. Functions $\varphi_{\lambda}^{\Delta}$ for the bound states can always be taken to be normalized to unity. Equation (25) presents an exact expression for the DOS of the disordered system described by the Hamiltonian (4), i.e., for the two-component solid solution $A_cB_{(1-c)}$. An analogous expression was used earlier in Ref. 31. Numerical methods of the DOS calculation for disordered systems are reduced to the procedure of Eqs. (17), followed by summing over all configurations and over all states in each configuration. Such an approach can be called an exact one. Our purpose is to obtain an approximate but realistic solution of the problem, avoiding the process of Eq. (17).

A. Restrictions of the trial-function class

The exact expression (24) could not be calculated if the eigenfunctions $\varphi_{\lambda}^{\Delta}$ and the corresponding eigenvalues are not known. The procedure of approximate calculations implies, as the first step, the introduction of the trial functions independent of the variants of the lattice-site filling. This action allows one to sum over all possible configurations. Calculations of integrals over all τ_{λ} except one, fulfilled in general form in the previous section allows one to get rid of the problem of determinant calculations[33,35,36] and, therefore, to simplify the following calculations.

The question of the choice of trial functions and their relation with solutions of Eq. (17) is one of the key issues of this work. Let us enumerate the restrictions defining the class of trial functions.

(I) We shall take into account only the ground state of the fluctuation well in spite of the fact that Eq. (24) allows one, at least in principle, to include into consideration the excited states as well. Therefore, the problem is reduced to choice of one function.

(II) The important question is about the symmetry of the trial function. We suppose that the spherical symmetry for it is in a continual limit as was done in many early calculations and the full symmetry of the lattice site of the averaged crystal in the lattice variant of the model.[17]

(III) The Hamiltonian (4) leads to short-range fluctuation wells and we suppose that a trial function that decreases with increasing distance R obeys the law

$$1/R \exp[-\kappa(\omega)R] \ , \qquad (26)$$

where $\kappa(\omega)$ is defined by the depth of the bound state (ω). It is easy to establish exactly that this behavior characterizes the localized solutions of Eq. (17) at $R \rightarrow \infty$ for the possible realization and this is the only reason why we prefer to constrain the trial function in the given form.

All the above-mentioned restrictions were used in previous investigations of the problem as well.

(IV) We introduce in this work the additional condition to constrain the behavior of the trial function at small distances from the center of the fluctuation well,

$$\lim_{R\rightarrow 0} \varphi_{\mathrm{tr}}(R) \ .$$

The purpose of this restriction is to obtain a behavior of φ_{tr} at small R which does not contradict the solutions of Eq. (17) in possible realizations. Therefore, we try to optimize the choice of φ_{tr} with a view of obtaining not only the greatest magnitude for the $\rho(\omega)$ but also the similarity between φ_{tr} and the real solutions of Eq. (17).

It is convenient to define φ_{tr} as a solution of the equation

$$\omega\varphi_{\mathrm{tr}}(n)-\sum_{m}[H_{nm}^{\mathrm{VC}}+U_{\mathrm{tr}}(n)\delta_{nm}]\varphi_{\mathrm{tr}}(m)=0 \ , \qquad (27)$$

where $U_{\mathrm{tr}}(n)$ is the averaged fluctuation well to be defined consistent with φ_{tr} by the steepest-descent procedure. It should describe the optimal configuration of the fluctuation well with or without an additional restriction.

The restrictions mentioned above influence the form of the fluctuation well. It is more convenient to rewrite condition (IV) as a restriction on the behavior of $U_{\mathrm{tr}}(n)$ at $R \rightarrow 0$ as soon as the φ_{tr} behavior in this region is completely defined by the potential energy in the saddle-point equation. We perform this procedure in the following sections considering the strong- and weak-scattering limits separately.

Here we note that the substitution of the trial function into Eq. (24) gives the expression

$$\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau \sum_{\Delta} P_{\Delta} \exp\left\{ i \sum_{n,m} \varphi_{\mathrm{tr}}(n)[(\omega-\Delta_n)\delta_{n,m}+H_{nm}^{\mathrm{VC}}]\varphi_{\mathrm{tr}}(m)\tau \right\} . \qquad (28)$$

As a rule, the φ_{tr} does not coincide with any solution of Eq. (17) in any configuration. Therefore, the integral over τ will give nonzero results for variants of the lattice-site filling which satisfy only the integral equation

$$\sum_{n,m} \varphi_{\mathrm{tr}}(n)[(\omega-\Delta_n)\delta_{n,m}+H_{nm}^{\mathrm{VC}}]\varphi_{\mathrm{tr}}(m)=0 \ . \qquad (29)$$

As a matter of fact, Eq. (29) can be fulfilled probably for any arbitrary function φ_{tr} due to the great number of variants of the random filling of the lattice resulting in a finite answer for the DOS. We face here the problem which lies in the fact that the functions φ_{tr}, which have nothing in common with the solutions of Eq. (17), can even overestimate reliable DOS values in some energy region. Examples of this will be obtained in following sections. The additional condition (IV) is called up to avoid such a situation.

B. General scheme of averaging

In this part of the section we consider the general scheme of the averaging procedure irrespective of the problem of the additional condition (IV) for $U_{\mathrm{tr}}(n)$ or φ_{tr}.

As soon as φ_{tr} does not depend on the atomic configuration we are able to sum over all possible sets of Δ.

We see from Eqs. (18), (19), and (23) that the function

$$\exp\{-i\Delta A[\tau]\}=\exp\left\{-i\sum_n \Delta_n \varphi_{\mathrm{tr}}^2(n)\tau\right\}$$

is the subject of averaging. The fluctuating item of the action $\Delta A[\tau]$ depends on the variants of the lattice-site filling. At a random distribution of constituent atoms an atom A appears in each of the lattice sites with a probability equal to c and a probability $(1-c)$ an atom B does. Taking into account that the exponent subjected to averaging can be presented as the product of independently averaging exponents we get

$$\langle\exp\{-i\Delta A[\tau]\}\rangle=\left\langle\exp\left\{-i\sum_n \Delta_n \varphi_{\mathrm{tr}}^2(n)\tau\right\}\right\rangle$$
$$=\prod_{n=1}^{N}\{c\exp[-i\Delta_A\varphi_{\mathrm{tr}}^2(n)]+(1-c)\exp[-i\Delta_B\varphi_{\mathrm{tr}}^2(n)\tau]\}\ . \qquad (30)$$

Here

$$\Delta_A=E_A-E_G=-(1-c)\Delta\ ,$$
$$\Delta_B=E_B-E_G=c\Delta\ , \qquad (31)$$
$$\Delta=E_B-E_A>0\ .$$

The averaged expression for the DOS can be presented now as

$$\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\left\{i\tau\sum_{n,m}\varphi_{\mathrm{tr}}(n)[\omega\delta_{nm}+H_{nm}^{\mathrm{VC}}]\times\varphi_{\mathrm{tr}}(m)+\sum_n\ln[R_n(\tau)]\right\}\ , \qquad (32)$$

where

$$R_n(\tau)=c\exp[i\Delta(1-c)\varphi_{\mathrm{tr}}^2(n)\tau]+(1-c)\exp[-i\Delta\varphi_{\mathrm{tr}}^2(n)\tau]\ . \qquad (33)$$

1. Laplace representation

For the convenience of further analysis we go from the Fourier integral (32) to the Laplace transformation of the DOS,

$$\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\left\{-i\sum_{n,m}\varphi_{\mathrm{tr}}(n)[\omega\delta_{nm}+H_{nm}^{\mathrm{VC}}]\times\varphi_{\mathrm{tr}}(m)(\tau-it)+\sum_n\ln[R_n(\tau-it)]\right\}\ , \qquad (34)$$

where

$$R_n(\tau-it)=c\exp[i\Delta(1-c)\varphi_{\mathrm{tr}}^2(n)(\tau-it)]+(1-c)\exp[-i\Delta c\varphi_{\mathrm{tr}}^2(n)(\tau-it)]\ . \qquad (35)$$

The equation obtained is completely equivalent to Eq. (32). The free parameter of the Laplace transformation t can take any positive or negative values.

Picking out the exponential factor we transform the expression for the DOS into a form

$$\rho(\omega)=\exp\{-A^0[\varphi_{\mathrm{tr}}^2 t]\}\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\{-\mathcal{A}^0(\tau)\}\ , \qquad (36)$$

where

$$A^0[\varphi_{\mathrm{tr}}^2 t]=(\omega+H^{\mathrm{VC}})_{\varphi,\varphi}t-\sum_n\ln R_n(-it)\ ,$$
$$\mathcal{A}^0(\tau)=i(\omega+H^{\mathrm{VC}})_{\varphi,\varphi}\tau-\sum_n\ln\left[\frac{R_n(\tau-it)}{R_n(-it)}\right]\ , \qquad (37)$$

and

$$(\omega+H^{\mathrm{VC}})_{\varphi,\varphi}=\sum_{n,m}\varphi_{\mathrm{tr}}(n)[\omega\delta_{nm}+H_{nm}^{\mathrm{VC}}]\varphi_{\mathrm{tr}}(m)\ . \qquad (38)$$

The saddle-point equation without an additional restriction has been studied earlier in Ref. 17. It results from a minimization procedure

$$\frac{\delta A[\varphi_{\mathrm{tr}}^2 t]}{\delta\varphi_{\mathrm{tr}}(n)}=0\ ; \qquad (39)$$

therefore, it looks like Eq. (27),

$$\sum_m[H_{nm}^{\mathrm{VC}}+\omega\delta_{nm}]\varphi_{\mathrm{tr}}(m)+U_{\mathrm{tr}}(n)\varphi_{\mathrm{tr}}(n)=0\ , \qquad (40)$$

where in the case without additional restriction the potential energy $U_{\mathrm{tr}}(n)$ should have the form[17]

$$U_{\mathrm{tr}}(n)=-\frac{\partial\ln R_n(-it)}{\partial t\varphi_{\mathrm{tr}}^2(n)}=-(1-c)\Delta\left[1-\frac{\exp[-\Delta t\varphi_{\mathrm{tr}}^2(n)]}{c+(1-c)\exp[-\Delta t\varphi_{\mathrm{tr}}^2(n)]}\right]\ . \qquad (41)$$

The following scheme of calculations of the DOS is the same in all cases and reduces to (i) solution of the saddle-point equation, the form of which depends on restriction (IV), (ii) calculation of the exponential index (in this case it is equal to $A^0[\varphi_{\mathrm{tr}}^2]t]$), and (iii) calculation of the τ-dependent part of the action (here it is expressed by $\mathcal{A}^0[\tau]$) and of the integral over τ which gives the preexponential multiplier. Note that the saddle-point equation gives both the function φ_{tr} and the value of the Laplace transformation parameter t.

IV. STRONG-SCATTERING LIMIT

Let us consider the situation of small concentration

$$c \ll 1$$

of strongly attractive centers when the depth of the potential well in lattice sites occupied by atoms A is great compared with its critical magnitude, i.e.,

$$(1-c)\Delta \gg |G_{nn}^{\mathrm{VC}}(0)|^{-1} . \tag{42}$$

If both conditions are fulfilled, the largest portion of atoms A is disposed on distances from each other considerably exceeding the radius of the bound state appearing at each lattice site occupied by atoms A. In this case, the solution of Eq. (17) in the region of bound states with accuracy up to terms of order of c^2 reduces to the problem of a strong local perturbation (see Refs. 18–21).

A. Additional restriction in strong-scattering limit

We see now that any fluctuation well leading to an appearance of the bound state includes at least one atom of kind A. We can transform this observation into an additional condition constraining the $U_{\mathrm{tr}}(m)$ to coincide in one of lattice sites with the potential of atom A:

$$U_{\mathrm{tr}}(n) = -(1-c)\Delta . \tag{43}$$

Choosing this lattice site as the frame of reference for φ_{tr} we collect all variants of the lattice filling satisfying this condition, neglecting the remaining ones. As a result we obtain instead of Eq. (26)

$$\rho(\omega) = \exp\{-A[\varphi_{\mathrm{tr}}^2 t]\}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau \exp\{-\mathcal{A}[\tau]\} , \tag{44}$$

where

$$A[\varphi_{\mathrm{tr}}^2 t] = (\omega + H^{\mathrm{VC}})_{\varphi,\varphi} t - \sum_{m\neq n} \ln R_m(-it) - t(1-c)\Delta\varphi_{\mathrm{tr}}^2(n) + \ln(1/c) \tag{45}$$

and

$$\mathcal{A}[\tau] = i(\omega + H^{\mathrm{VC}})_{\varphi,\varphi}\tau - \sum_{m\neq n} \ln\left[\frac{R_m(\tau - it)}{R_m(-it)}\right] - i\tau(1-c)\Delta\varphi_{\mathrm{tr}}^2(n) . \tag{46}$$

Minimizing the exponential index $A[\varphi_{\mathrm{tr}}^{p2}]$ we get the saddle-point equation in the form of Eq. (40), where now in accordance with Eq. (43)

$$U_{\mathrm{tr}}(m) = \begin{cases} -(1-c)\Delta, & m = n \\ -\dfrac{\partial}{\partial t\varphi_{\mathrm{tr}}^2(m)}[\ln R_m(-it)], & m \neq n . \end{cases} \tag{47}$$

Here

$$\frac{\partial}{\partial t\varphi_{\mathrm{tr}}^2(m)}[\ln R_m(-it)] = -[\ln R_m(-it)]'_{t\varphi_{\mathrm{tr}}^2} = -(1-c)\Delta\left[1 - \frac{\exp[-t\varphi_{\mathrm{tr}}^2(m)]}{c + (1-c)\exp[-t\varphi_{\mathrm{tr}}^2(m)]}\right] . \tag{48}$$

Multiplying the equation by the Green function of the virtual crystal we get

$$\left\{[1 + (1-c)\Delta G_{nn}^{\mathrm{VC}}(\omega)]\varphi_{\mathrm{tr}}(n) + \sum_{m\neq n} G_{nm}^{\mathrm{VC}} U_{\mathrm{tr}}(m)\varphi_{\mathrm{tr}}(m)\right\} = 0 , \tag{49}$$

where $U_{\mathrm{tr}}(m)$ is given by Eqs. (47) and (48).

B. Approximate consideration

If condition (42) is fulfilled, Eq. (49) coincides with the Koster-Slater-Lifshitz equation at $t=0$ and $\varphi_{\mathrm{tr}}(m)$ at $\omega = \omega_{\mathrm{loc}}$ coincides with eigenfunction of this equation, i.e.,

$$[1 + (1-c)\Delta G_{nn}^{\mathrm{VC}}(\omega)]\psi_{\mathrm{loc}}(n) = 0 , \tag{50}$$

which can be presented at $\omega = \omega_{\mathrm{loc}}$ as

$$\psi_{\mathrm{loc}}(m) = -G_{nm}^{\mathrm{VC}}(\omega_{\mathrm{loc}})|G_{nn}'^{\mathrm{VC}}(\omega_{\mathrm{loc}})|^{-1/2} , \quad G_{nn}'^{\mathrm{VC}}(\omega_{\mathrm{loc}}) = \frac{\partial}{\partial\omega}G_{nn}^{\mathrm{VC}}(\omega)|_{\omega=\omega_{\mathrm{loc}}} . \tag{51}$$

For deeply localized states $\psi_{\mathrm{loc}}(m)$ has nonzero value practically only at one lattice site, i.e.,

$$\psi_{\mathrm{loc}}(m) \approx \delta_{mn} ,$$

$$\psi_{\mathrm{loc}}(m \neq n) \ll 1 .$$

In the region $\omega \approx \omega_{\mathrm{loc}}$ we can use the fact that Eq. (49) has a solution at small t. Expanding $U_{\mathrm{tr}}(m \neq n)$ given by Eq. (47) in a Taylor series and conserving the linear in t power term we transform Eq. (49) to the form

$$[1 + G_{nn}^{\mathrm{VC}}(\omega)(1-c)\Delta]\chi_{\mathrm{tr}}(n) - c(1-c)\Delta^2 \sum_{m\neq n} G_{nm}^{\mathrm{VC}}(\omega)\varphi_{\mathrm{tr}}^3(m)t = 0 . \tag{52}$$

Using as a zero approximation

$$\varphi_{\mathrm{tr}}(m) \approx \psi_{\mathrm{loc}}(m)$$

and representing $G_{nn}^{\mathrm{VC}}(\omega)$ in the vicinity of ω_{loc} as

$$G_{nn}^{\mathrm{VC}}(\omega) = G_{nn}^{\mathrm{VC}}(\omega_{\mathrm{loc}}) + G_{nn}'^{\mathrm{VC}}(\omega_{\mathrm{loc}})(\omega - \omega_{\mathrm{loc}}) , \tag{53}$$

where

$$G_{nn}^{\mathrm{VC}}(\omega_{\mathrm{loc}}) = -[(1-c)\Delta]^{-1} , \tag{54}$$

we get the value of t satisfying Eq. (52):

$$t=\frac{(\omega-\omega_{\mathrm{loc}})}{c(1-c)\Delta^2}\left\{\sum_{m\neq n}\left[\frac{|G_{nm}^{\mathrm{VC}}(\omega_{\mathrm{loc}})|^2}{G_{nn}{}'^{\mathrm{VC}}(\omega_{\mathrm{loc}})}\right]^2\right\}^{-1} .$$

For $A[\varphi_{\mathrm{tr}}^2 t]$, in turn, we obtain

$$\begin{aligned}A[\varphi_{\mathrm{tr}}^2]=-\sum_{l,m}&[\psi_{\mathrm{loc}}(l)(\omega\delta_{l,m}+H_{lm}^{\mathrm{VC}})\psi_{\mathrm{loc}}(m)\\&-(1-c)\Delta\psi_{\mathrm{loc}}^2(n)\delta_{l,n}\delta_{n,m}]t\\&-\frac{c(1-c)\Delta^2}{2}\sum_{m\neq n}[\psi_{\mathrm{loc}}^2(m)]^2t^2 .\end{aligned}\tag{55}$$

Substituting ψ_{loc} into Eq. (55) in the form given by Eq. (51) and the value of t obtained from Eq. (52) we transform $\exp\{-A[\varphi_{\mathrm{tr}}^2]t\}$ to the form

$$\exp\{-A[\varphi_{\mathrm{tr}}^2]t\}=\exp\left\{-\frac{(\omega-\omega_{\mathrm{loc}})^2}{2\delta L_{\omega_{\mathrm{loc}}}c(1-c)\Delta^2}-\ln(1/c)\right\} ,\tag{56}$$

where

$$\delta L_{\omega_{\mathrm{loc}}}=L_{\omega_{\mathrm{loc}}}-[\varphi_{\mathrm{tr}}^2(n)]^2\tag{57}$$

and $L_{\omega_{\mathrm{loc}}}$ is so-called localization index,

$$L_{\omega_{\mathrm{loc}}}=\sum_m[\varphi_{\mathrm{tr}}^2(n)]^2=\sum_m\left[\frac{|G_{nm}^{\mathrm{VC}}(\omega_{\mathrm{loc}})|^2}{G_{nn}{}'^{\mathrm{VC}}(\omega_{\mathrm{loc}})}\right]^2 .\tag{58}$$

The value of the localization index L_ω characterizes the space extent of the wave function of the bound state with binding energy equal to ω. If the localization depth is great enough and inequality (42) is satisfied with a good providence the wave function is localized at the single site and $\delta L_{\omega_{\mathrm{loc}}} \ll 1$.

For the preexponential factor calculating we consider as the first step the simplified expression for the $\mathcal{A}[\tau]$ which can be obtained from expressions given by Eq. (44) when the functions $R_m(\tau-it)$ are presented by the first three terms of the Taylor-series expansion:

$$\begin{aligned}\mathcal{A}[\tau]=i\tau[(\omega-H^{\mathrm{VC}})_{\varphi,\varphi}&-(1-c)\Delta\varphi_{\mathrm{tr}}^2(n)]\\+\sum_{m\neq n}&\{i\tau[\ln R_m(-it)]'_\tau-(\tau^2/2)\\&\times[\ln R_m(-it)]''_{\tau\tau}+\cdots\} ,\end{aligned}\tag{59}$$

where

$$[\ln R_m(-it)]'_\tau=\frac{\partial}{\partial\tau}[\ln R_m(\tau-it)]\Big|_{\tau=0}$$

and

$$[\ln R_m(-it)]''_{\tau\tau}=\frac{\partial^2}{\partial\tau^2}[\ln R_m(\tau-it)]\Big|_{\tau=0} .$$

Substituting Eq. (59) into the integral over τ in the expression given by Eq. (46) for $\mathcal{A}[\tau]$ we come to the Gaussian integral which gives after a simple calculation

$$\rho(\omega)=[2\pi\delta L_{\omega_{\mathrm{loc}}}c(1-c)\Delta^2]^{-1/2}\times\exp\left\{-\frac{(\omega-\omega_{\mathrm{loc}})^2}{2\delta L_{\omega_{\mathrm{loc}}}c(1-c)\Delta^2}-\ln(1/c)\right\} .\tag{60}$$

Therefore, instead of the δ function obtained in the case of isolated deep centers in Refs. 18–21, we have for the density of localized states the Gaussian contour normalized to the probability for a given site to be occupied by an atom A. The result with the δ function can be withdrawn if the term that is quadratic in t powers in the $\mathcal{A}[\tau]$ expansion is neglected. Integrating over τ with this term leads, therefore, to a decrease of the DOS at a value $\omega=\omega_{\mathrm{loc}}$ due to the statistical dispersion of the localization energy. The value of the dispersion is characterized by the energy

$$\gamma=[\delta L_{\omega_{\mathrm{loc}}}c(1-c)\Delta^2]^{1/2} ,$$

which goes to zero at $\omega_{\mathrm{loc}}\to\infty$. The disappearance of the statistical dispersion of the localization energy means that we have got in this limit an exact solution coinciding with solution of Eq. (17) for some configurations.

Equation (60) presents the contribution of one lattice site. The full number of localized states in the considered volume of the crystal can be obtained by multiplying the given number by the full number n of lattice sites in the volume V. As a result, we get a number of localized states equal to $N_A=cN$. This natural result is obtained due to restriction (IV) and drastically changes if it is omitted. The most considerable difference occurs in the region of small ω.

C. Exact formulation of the problem and some results

The Gaussian form of the localized-state band takes place in the vicinity of the center band only. Equation (49) gives solutions within an energy interval restricted both from above and from below, while the parameter t changes within the interval $-\infty<t<\infty$. The deepest states appear when $t\to\infty$ and the potential energy given by Eq. (47) corresponds to an increase of the macroscopical cluster consisting of atoms A. The maximum binding energy at $t\to\infty$ coincides with Lifshitz border $E_L=(1-c)\Delta$. We get the smallest binding energy in the limit $t\to-\infty$ when Eq. (47) corresponds to a macroscopical cluster consisting of atoms B with a single atom A in the center of this cluster.

Some of the features of the DOS remain unchanged compared with ones described in Ref. 17. So, when the depth of the bound state goes to the Lifshitz border,

$$\omega\to(1-c)\Delta ,$$

Eq. (44) leads to the well-known singular behavior of the DOS. In the intermediate region

$$\omega_{\mathrm{loc}}<\omega<(1-c)\Delta ,$$

the DOS dependence on the ω obeys the Urbach rule as was shown in Ref. 17. However, it drastically changes compared with one from Ref. 17 within the interval

$$0<\omega<\omega_{\text{loc}}\ .$$

Equation (49) with the potential energy given by Eq. (47) leads to the appearance of a minimal binding energy at $t\rightarrow-\infty$, which can be defined from the equation

$$[1+\Delta G_{nn}^{B}(\omega_{\min})]\varphi_{\text{tr}}(n)=0\ , \tag{61}$$

where $G_{nn}^{B}(\omega)$ is the Green function of the crystal consisting of atoms B. With accuracy up to terms proportional to c^2 the value $\omega_{\min}$ can be considered as the upper border of the bound states. The DOS decreases within interval

$$\omega_{\min}<\omega<\omega_{\text{loc}}$$

when ω moves toward the $\omega_{\min}$ and goes to zero when

$$\omega\rightarrow\omega_{\min}$$

according to a singular law. The difference in the DOS behavior compared with Ref. 17 results from the additional restriction (IV). The DOS expression in the whole region

$$\omega_{\min}<\omega<(1-c)\Delta \tag{62}$$

can be written in the form of Eq. (44) where $A[\varphi_{\text{tr}}^2t]$ is transformed with the help of Eq. (49) to the formula

$$A[\varphi_{\text{tr}}^2t]=-\sum_{m\neq n}\{\ln R_m(-it)-t\varphi_{\text{tr}}^2(m)[\ln R_m(-it)]'_{t\varphi_{\text{tr}}^2}\}+\ln(1/c) \tag{63}$$

and $\mathcal{A}[\tau]$ can be presented in the form

$$\mathcal{A}[\tau]=\sum_{m\neq n}\left\{\ln\left[\frac{R_m(\tau-it)}{R_m(-it)}\right]-i\tau[\ln R_m(-it)]'_{\tau}\right\}. \tag{64}$$

Here φ_{tr} and t are defined by Eq. (49) together with Eqs. (47) and (48). For the approximate calculation of the preexponential factor we can again expand $\mathcal{A}[\tau]$ in a Taylor series and reduce the integral (44) to the Gaussian form. As a result we have

$$\rho(\omega)=\left\{2\pi\sum_{m\neq n}[\ln R_m(-it)]''_{\tau\tau}\right\}^{-1/2}\times\exp\{-A[\varphi_{\text{tr}}^2t]\}\ , \tag{65}$$

where $A[\varphi_{\text{tr}}^2t]$ is given by Eq. (63) and φ_{tr} is normalized to unity.

The solution in the strong-scattering regime described in this section in general terms obviously resembles the one of the Koster-Slater-Lifshitz problem. In distinction from the last, the shift of the band edge given by $\langle E\rangle_{\text{av}}$ and the inhomogeneous broadening of localized states leading to an asymmetrical form of the deep-center band of Eq. (65) are taken into account.

We consider in more detail the variant of the strong-scattering problem in the context of the three-component system, consisting of Nc atoms A, $(1-c-c_I)N$ atoms B, and c_IN deep centers by the condition $c_I\ll c,(1-c)$ supposing the depth of the potential well of atom A to be considerably less than one of deep center I and using the continual approach to the problem.

V. CONTINUAL LIMIT, A WEAK SCATTERING

In this section we consider a situation which, probably, is encountered in experiments much more often than the strong-scattering limit. Now, the concentration will not be considered as a small value, but we will suppose that the perturbation concerned with attractive centers is not strong; i.e., it is considered to be less than the critical value of the single-site binding potential. The signs showing the weakness of the perturbation are a small width of the region of bound states compared with the whole band and a small number of localized states compared with their full quantity in the band.

The importance of this limit is concerned with the fact that a great number of solid solutions for a certainty and, as it seems now, the amorphous silicon in the major part of its valence-band tail can be attributed to weak-scattering systems.

In weak-scattering disordered systems the scale of bound states is supposed to exceed the lattice constant considerably and, therefore, an appropriate method to deal with is the continual approximation.

A. DOS in the continual approximation

To go over to a continual representation we should use the effective-mass approximation for the electron zone (6) and transform the summing over discrete lattice sites to the integral in accordance with equation

$$\sum_{n}\rightarrow(1/v_0)\int d^3R\ ,$$

where integrating should be expanded into the whole considered volume of the crystal. Here v_0 is the volume per lattice site.

It is convenient to use in the calculations the dimensionless variables. We take the de Broglie wavelength $(\hbar^2/2M\omega)^{1/2}$ to scale the length and the depth of the bound state ω as an energy unit. Accordingly, we change the variables $(\tau\Delta)/\omega\rightarrow\tau$ and $(t\Delta)/\omega\rightarrow t$.

Analogously to (26), we write down the expression for the density of states without the additional restriction (IV),

$$\rho(\omega)=\left(\frac{\omega}{\Delta}\right)\left(\frac{1}{\omega}\right)\left(\frac{E_0}{\omega}\right)^{3/2}\exp\{-\tilde{A}^0[\varphi_{\text{tr}}^2t]\}\times\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\{-\tilde{\mathcal{A}}^0(\tau)\}\ . \tag{66}$$

Here the new—compared with Eq. (26)—multipliers are produced by the introduction of dimensionless variables.

The continual analog of the action written in Eq. (37) is given by the expression

$$\tilde{A}^0[t\varphi_{\mathrm{tr}}^2]=\left[\frac{\omega}{\Delta}\right]\left[\frac{E_0}{\omega}\right]^{3/2}\int d^3x[(\nabla\varphi_{\mathrm{tr}})^2+\varphi_{\mathrm{tr}}^2]t-\left[\frac{E_0}{\omega}\right]^{3/2}\int d^3x\,\ln\mathcal{R}(-it)\;, \tag{67}$$

where the energy $E_0=\hbar^2/2Mv_0^{3/2}$ is related to the critical depth of the potential well of volume v_0 by means of the equation $E_0=(6/\pi^4)^{2/3}E_{\mathrm{cr}}$, and M is the effective mass of the electron band defined by the disposition of Eq. (6).

The function $\mathcal{A}^0[\tau]$ can be written as

$$\mathcal{A}^0[\tau]=\left[\frac{\omega}{\Delta}\right]\left[\frac{E_0}{\omega}\right]^{3/2}\int d^3x\; i\tau[(\nabla\varphi_{\mathrm{tr}})^2+\varphi_{\mathrm{tr}}^2]-\left[\frac{E_0}{\omega}\right]^{3/2}\int d^3x\left\{\ln\left[\frac{\mathcal{R}(\tau-it)}{\mathcal{R}(-it)}\right]\right\}. \tag{68}$$

The expression $\mathcal{R}(\tau-it)$ is given by the formula

$$\mathcal{R}(\tau-it)=(\exp\{i(\tau-it)(1-c)\varphi_{\mathrm{tr}}^2\}\times[c+(1-c)\exp\{i(\tau-it)\varphi_{\mathrm{tr}}^2\}])\;.$$

The analog of Eq. (40) has the form

$$(-\nabla^2+1)\varphi(x)+U_{\mathrm{tr}}(x)\varphi_{\mathrm{tr}}(x)=0\;, \tag{69}$$

where

$$U_{\mathrm{tr}}(x)=-\frac{(1-c)\Delta}{\omega}\times\left[1-\frac{\exp\{-t\varphi_{\mathrm{tr}}^2(x)\}}{c+(1-c)\exp\{-t\varphi_{\mathrm{tr}}^2(x)\}}\right]. \tag{70}$$

A detailed analysis and the results of the numerical solution of this equation are given in Ref. 17.

B. Separation of the critical cluster

In the case of weak scattering the bound state can appear in any configuration if atoms A aggregate at some point in a cluster the potential well of which exceeds the critical power. As soon as the depth of the potential well is restricted in the considered model by the value $(1-c)\Delta$, we obtain from Eq. (17) a criterion for the radius of the spherical critical cluster consisting of atoms A in the form

$$\varphi_{1s}(R)+(1-c)\Delta\int_0^{R_{\mathrm{cr}}}d^3R_1G^{\mathrm{VC}}_{|\mathbf{R}-\mathbf{R}_1|}(0)\varphi_{1s}(R_1)=0\;. \tag{71}$$

The probability of formation of such a cluster at random filling of the lattice sites is

$$\exp\left\{-\frac{\ln(1/c)}{v_0}\int_0^{R_{\mathrm{cr}}}d^3R\right\}.$$

Here the Green function of the virtual crystal in the continual limit can be written as

$$G_R^{\mathrm{VC}}(\omega)=-\frac{2Mv_0}{4\pi\hbar^2R}\exp\{-\kappa(\omega)R\} \tag{72}$$

and

$$\kappa(\omega)=\left[\frac{2M\omega}{\hbar^2}\right]^{1/2}. \tag{73}$$

The radial part of the wave function within the cluster at $R\le R_{\mathrm{cr}}$ has the form

$$\varphi_{1s}(R)\sim\frac{\sin\{[2M(1-c)\Delta/\hbar^2]^{1/2}R\}}{R}\;. \tag{74}$$

After integrating in Eq. (71) over R_1 at $R=0$ we get the condition of the bound-state appearance as

$$R_{\mathrm{cr}}=(\pi/2)\left[\frac{\hbar^2}{2M(1-c)\Delta}\right]^{1/2}, \tag{75}$$

which gives us the radius of the critical cluster. The probability of the appearance of this cluster is

$$\exp\left\{-\frac{4\pi R_{\mathrm{cr}}^3\ln(1/c)}{v_0}\right\}. \tag{76}$$

Such critical clusters could be called compact, because they have a minimal size. They have the maximal probability of appearing among the critical clusters. The critical spherical clusters of greater size containing the atom B or the cluster of atoms B within themselves are less probable because the atoms B, being the repulsive centers, lead to a decrease in the integral in the corresponding analog of Eq. (71) and, therefore, to an increase in the region of the integrating compared with Eq. (71) for the critical situation to be reached and to a decrease in the probability of the appearance.

The fluctuations responsible for the formation of the bound states with finite localization energy have well powers certainly exceeding those of the critical cluster. Therefore, they should contain one of the variants of the critical clusters within themselves. At a given localization energy the most probable fluctuation wells should contain the most probable critical cluster, i.e., the compact cluster consisting of atoms A. This condition we will consider as an additional restriction (IV) in the case of weak scattering.

C. Solution with exponential energy accuracy for fluctuations containing the critical cluster

Let us consider the changes of Eqs. (67)–(70) due to restriction by the fluctuation wells containing the compact spherical critical cluster. The depth of the potential well within the volume of the critical cluster (sphere of the radius X_{cr}) is equal to $(1-c)\Delta$, as a result of the filling of this volume by atoms A. Picking out configurations consistent with this demand we get instead of Eq. (67)

$$\tilde{A}[t\varphi_{\rm tr}^2]=\left[\frac{\omega}{\Delta}\right]\left[\frac{E_0}{\omega}\right]^{3/2}\int d^3x\{[\nabla\varphi_{\rm tr}(x)]^2+\varphi_{\rm tr}^2(x)\}t$$
$$-\left[\frac{E_0}{\omega}\right]^{3/2}\left[\int_0^{X_{\rm cr}}d^3x[(1-c)t\varphi_{\rm tr}^2(x)-\ln(1/c)]+\int_{X_{\rm cr}}^{\infty}d^3x\,\ln\mathcal{R}(-it)\right], \tag{77}$$

where

$$X_{\rm cr}=(\pi/2)\sqrt{\omega/(1-c)\Delta}\ .$$

Minimizing the action obtained we derive the equation

$$(-\nabla^2+1)\varphi(x)+U_{\rm tr}(x)\varphi(x)=0\ , \tag{78}$$

where the potential energy now has the form

$$U_{\rm tr}(x)=\begin{cases}-\dfrac{(1-c)\Delta}{\omega}, & x\le X_{\rm cr}\\ -\dfrac{(1-c)\Delta}{\omega}\left[1-\dfrac{\exp[-t\varphi_{\rm tr}^2(x)]}{c+(1-c)\exp[-t\varphi_{\rm tr}^2(x)]}\right], & x>X_{\rm cr}\ .\end{cases} \tag{79}$$

Equation (78) has the spherically symmetrical solution within the whole interval of energies $0<\omega<(1-c)\Delta$. Substitution of Eq. (78) into Eq. (77) gives for the DOS with exponential accuracy the expression

$$\rho(\omega)=\exp\left\{-(E_0/\omega)^{3/2}\int_{X_{\rm cr}}d^3x\{\ln\mathcal{R}(-it)-t\varphi_{\rm tr}^2(x)[\ln\mathcal{R}(-it)]'_{t\varphi_{\rm tr}^2(x)}\}\right.$$
$$\left.-(E_0/\omega)^{3/2}(4\pi/3)X_{\rm cr}^3\ln 1/c\right\}[\ln\mathcal{R}(-it)]'_{t\varphi_{\rm tr}^2(x)}=\frac{\partial}{\partial(t\varphi_{\rm tr}^2(x))}[\ln\mathcal{R}(-it)]\ . \tag{80}$$

1. Lifshitz and Urbach regions

Note that at $X_{\rm cr}\to 0$ expressions (77)–(80) transform to the corresponding equations of Ref. 17. In the limit $\omega\to(1-c)\Delta$, Eq. (80) gives for the DOS dependence the Lifshitz singularity law

$$\rho(\omega)\sim\exp\left[-\left\{\frac{E_{\rm cr}}{(1-c)\Delta-\omega}\right\}^{3/2}\right]\ .$$

At $\omega<(1-c)\Delta$ they lead to a Urbach character of the DOS decreasing as in Ref. 17 with the Urbach parameter E_U, which with good accuracy can be described by the equation

$$E_U=\frac{1}{\beta^3\ln(1/c)}\frac{[(1-c)\Delta]^{5/2}}{E_{\rm cr}^{3/2}},\quad \beta\approx 2\ . \tag{81}$$

2. Band-edge region

In the limit $\omega\to 0$ expression (80) can be simplified in so far as the potential wells are defined in this limit by the compact critical cluster. In this case Eq. (78) has solutions at small t, which allows us to expand the exponential expressions of Eqs. (77) and (79) into a series in t powers. Therefore, we have

$$\tilde{A}[t\varphi_{\rm tr}^2]=\left[\frac{\omega}{\Delta}\right]\left[\frac{E_0}{\omega}\right]^{3/2}\int d^3x\{[\nabla\varphi_{\rm tr}(x)]^2+\varphi_{\rm tr}^2(x)\}t$$
$$-\left[\frac{E_0}{\omega}\right]^{3/2}\int_0^{X_{\rm cr}}d^3x[(1-c)\varphi_{\rm tr}^2(x)t-\ln(1/c)]$$
$$-\frac{c(1-c)t^2}{2}\left[\frac{E_0}{\omega}\right]^{3/2}\int_{X_{\rm cr}}^{\infty}d^3x[\varphi_{\rm tr}^2(x)]^2\ . \tag{82}$$

The potential energy is transformed to the equation

$$U_{\rm tr}(x)=\begin{cases}-\dfrac{(1-c)\Delta}{\omega}, & x\le X_{\rm cr}\\ -\dfrac{c(1-c)\Delta}{\omega}t\varphi_{\rm tr}^2(x), & x>X_{\rm cr}\ .\end{cases} \tag{83}$$

As an approximate solution of Eq. (78) with the potential energy (83) we can use the solution of the equation

$$(-\nabla^2+1)\varphi_\omega(x)+U_\omega(x)\varphi_\omega(x)=0\ , \tag{84}$$

with the potential energy being equal to

$$U_\omega(x)=\begin{cases}-\dfrac{(1-c)\Delta}{\omega}, & x\le X_\omega\\ 0, & x>X_\omega\ ,\end{cases} \tag{85}$$

where

$$X_\omega=\left[\frac{\omega}{(1-c)\Delta-\omega}\right]^{1/2}$$
$$\times\left[\pi-\arctan\left[\frac{(1-c)\Delta-\Omega}{\omega}\right]^{1/2}\right]$$

and

$$\varphi_\omega(x)=\begin{cases}\dfrac{1}{\sqrt{\mathcal{N}}}\dfrac{\sin[\chi(\omega)x]}{x}, & x\le X_\omega\\[2ex] \dfrac{\mu}{\sqrt{\mathcal{N}}}\dfrac{\exp[-x]}{x}, & x>X_\omega\ .\end{cases}\tag{86}$$

Here also are

$$\chi(\omega)=\left[\frac{(1-c)\Delta-\omega}{\omega}\right]^{1/2},$$
$$\mu=\left[\frac{1-c)\Delta-\omega}{(1-c)\Delta}\right]^{1/2}\exp(x)\ ,$$

and

$$\mathcal{N}=\int d^3x\,\varphi_\omega^2(x)\ .$$

Substitution of Eq. (83) and $\varphi_\omega(x)$ into Eq. (84) leads to a value of t equal to

$$t=\frac{\omega\int_{X_{\rm cr}}^{X_\omega}d^3x\,\varphi_\omega^2(x)}{c(1-c)\Delta\int_{X_{\rm cr}}^{\infty}d^3x[\varphi_\omega^2(x)]^2}\ .\tag{87}$$

Simple calculations give in this limit

$$\rho(\omega)\sim\exp\left\{-\frac{\omega}{c\Delta}\left[\frac{E_{\rm cr}}{(1-c)\Delta}\right]^{3/2}\frac{6}{\pi^2}\frac{1}{I_4^{\rm cr}}-\left[\frac{E_{\rm cr}}{(1-c)\Delta}\right]^{3/2}\ln(1/c)\right\},\tag{88}$$

where

$$I_4^{\rm cr}=\int_0^\infty\frac{\exp(-4X_{\rm cr}Y)}{(1+Y)^2}dY\ .\tag{89}$$

The last expression gives at small ω the dependence

$$\rho(\omega)\sim\exp\left\{-\frac{\omega}{E_{\rm BE}}\right\},\tag{90}$$

with the value

$$E_{\rm BE}=c\Delta\left[\frac{(1-c)\Delta}{E_{\rm cr}}\right]^{3/2}\frac{\pi^2 I_4^{\rm cr}}{6}\tag{91}$$

weakly dependent on the ω due to the integral $I_4^{\rm cr}$. Neglecting the weak dependence of the $I_4^{\rm cr}$ at $\omega\ll E_{\rm BE}$ we can expand the exponential expression, which leads to the linear function of $\rho(\omega)$ coinciding with the one in Eq. (1).

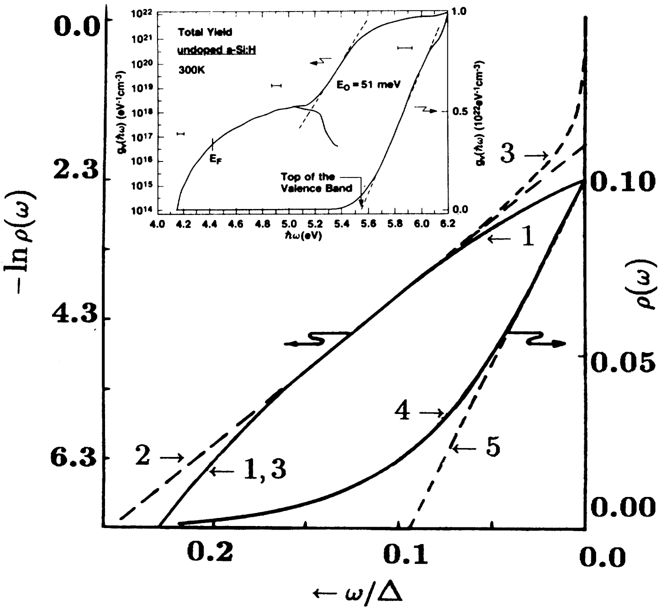

FIG. 1. Energy dependence with exponential accuracy of the calculated DOS. Curve 1 is obtained as result of Eq. (78) solution with help of Eq. (80), curve 2 obtained using the Urbach approximation, curve 3 is the result of Eq. (69) and calculations according to Eq. (67) and coincides with data of Ref. 17, curve 4 is the same as curve 1 in linear scale, and curve 5 is linear approximation of the DOS dependence in the region of the band edge. Calculation results are given at $c=0.1$; the common multiplier $\nu_{\rm cr}=[E_{\rm cr}/(1-c)\Delta]^{3/2}$ is taken as the scale unit for $\ln[\rho(\omega)]$. The inset gives one of the experimental curves for the single-electron DOS of amorphous silicon taken from Ref. 4.

3. *Results of numerical calculations*

The numerical solution of Eq. (76) gives the exponential part of the $\rho(\omega)$ dependence presented in Fig. 1. In the figure the data obtained as a result of the solution of Eq. (69) without separation of the compact critical cluster are also given. They coincide with the data of Ref. 17.

As the unit of $\ln[\rho(\omega)]$ we get the common multiplier equal to $[E_{\rm cr}/(1-c)\Delta]^{3/2}$ persistent in all expressions.

In Fig. 1 it is easily recognized that $\rho(\omega)$ presented in linear scale have almost linear dependence on ω within the interval $0<\omega<0.07\Delta$. At greater values of ω it transforms into Urbach's law, which, in turn, goes to the Lifshitz singularity at ω approaching the border of the bound states.

The results of the given calculations coincide with the previous ones of Ref. 17 with high accuracy beginning from the values $\omega\approx0.1\Delta$. This results from the fact that the form of the fluctuation wells at given localization energies is already insensitive to restriction (IV) because these energies demand for the wells size to exceed considerably a critical size in any case. The difference between the DOS values obtained with and without restriction (IV) (curves 1 and 3 in Fig. 1) is again considerable in the region of small ω. As a result, the DOS found without the additional restriction overestimate the full number of states below E_G.

D. Solution for three-component system with exponential accuracy

We consider here the situation often met in experiments when the disordered system contains a small number of deeply localized centers influencing the form of the deep tail of the band.

To describe the desirable situation we use the binary solid solution $A_cB_{(1-c)}$ where a small fraction of lattice sites is occupied by deep centers I. The concentration of the centers c_I is supposed to obey the condition $c_I \ll c,(1-c)$. The chemical formula of the solution could be written now as $A_cI_{c_I}B_{(1-c-c_I)}$. We suppose the depth of the fluctuation wells of the solid solution to be restricted by the value $(1-c)\Delta < E_{\rm cr}$ as before, neglecting the influence of deep centers on the value of averaged potential $\langle E \rangle_{\rm av}$.

The deep center itself is supposed to be described by a spherical potential well of a volume equal to v_0 with a depth Δ_I considerably exceeding the critical energy $\Delta_I \gg E_{\rm cr}$.

Taking into account restriction (IV) for fluctuation wells consisting of atoms A, we conclude that now bound states of two kinds are possible. The first ones are states in the fluctuation wells containing the compact critical cluster of atoms A, while the second ones are deeply localized states initiated by the centers I surrounded with a fluctuation potential of the binary solution $A_cB_{(1-c)}$. Therefore, we neglect the possibility for the deep center to appear within a critical cluster. The action describing the fluctuation states of the first kind is given by Eq. (77). The additional item of the Green function and DOS is concerned with deep centers and can be characterized by the action which we present in the form

$$\tilde{A}_I[t\varphi_{\rm tr}^2]=\left[\frac{\omega}{\Delta}\right]\left[\frac{E_0}{\omega}\right]^{3/2}\int d^3x\{[\nabla\varphi_{\rm tr}(x)]^2+\varphi_{\rm tr}^2(x)\}t - \left[\frac{E_0}{\omega}\right]^{3/2}\left[\int_0^{X_0} d^3x[\Delta_I t\varphi_{\rm tr}^2(x)+\ln(c_I)]+\int_{X_0}^{\infty} d^3x\,\ln\mathcal{R}(-it)\right] . \tag{92}$$

Here

$$X_0=\left[\frac{2M\omega}{\hbar^2}\right]^{1/2}\left[\frac{3v_0}{4\pi}\right]^{1/3} .$$

Equations (77)–(82) do not change their form in the approximation under consideration, while the minimization of the action of Eq. (92) leads to equation

$$(-\nabla^2+1)\varphi_{\rm tr}(x)+U_{\rm tr}^I(x)\varphi_{\rm t}(x)=0 , \tag{93}$$

where the potential energy takes the form

$$U_{\rm tr}^I(x)=\begin{cases} -\dfrac{\Delta_I}{\omega}, & x\le X_0 \\ -\dfrac{(1-c)\Delta}{\omega}\left[1-\dfrac{\exp[-t\varphi_{\rm tr}^2(x)]}{c+(1-c)\exp[-t\varphi_{\rm tr}^2(x)]}\right], & x>X_0 . \end{cases} \tag{94}$$

Properties of Eq. (94) have much in common with the strong-scattering situation considered in Sec. IV. At $t=0$ the problem is reduced to the Schrödinger equation with spherical potential well which contains a deep level at $\omega=\omega_I$. At small deviations from ω_I we accept approximately that $\varphi_{\rm tr}(x)\approx\varphi_I(x)$, where $\varphi_I(x)$ is the eigenfunction of the Schrödinger equation for the spherical potential well with radius equal to X_0 and depth equal to Δ_I.

The behavior of the DOS in the vicinity of the level is much analogous to the one in the case of the strong-scattering situation. With exponential accuracy we have in a Gaussian approximation

$$\rho_I(\omega)\sim\exp\{-A_I[\varphi_{\rm tr}]^2t\} =\exp\left\{-\frac{(\omega-\omega_I)^2}{2\delta L_{\omega_I}c(1-c)\Delta^2}-\ln(1/c_I)\right\} , \tag{95}$$

where

$$\delta L_{\omega_I}=\left[\frac{E_0}{\omega_I}\right]^{3/2}\left[\frac{\Delta_I}{\omega_I}\right]I_4^I , \qquad I_4^I=\int_{X_0}^{\infty}d^3x[\varphi_I^2(x0]^2 . \tag{96}$$

The normalization integral is

$$\int d^3x\,\varphi_I^2(x)=1 .$$

The form of the deep-center band is related to the fluctuation potential and, therefore, experimental data in the form of the band can give additional information on the fluctuation potential parameters which can be used together with data on the Urbach parameter E_U and on the DOS slope in the region of the band edge $E_{\rm BE}$. Unfortunately, it appears to be impossible to avoid the calculation of the integral I_4^I. The value of the integral is rather sensitive to the kind of wave function used for the calculation and, probably, the spherical well approximation will not always give the best result.

E. Preexponential factors, estimation of the mobility-edge position

The expression for the DOS in the whole interval of energies

$$0<\omega<(1-c)\Delta$$

can now be written as a sum of two items,

$$\rho(\omega)+\rho_I(\omega)\ .$$

Here we have the expression with a preexponential factor

$$\rho(\omega)=\frac{1}{\omega}\left[\frac{\omega}{\Delta}\right]\left[\frac{E_0}{\omega}\right]^{3/2}\exp\{-\tilde{A}[\varphi_{\rm tr}^2 t]\}\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\{-\tilde{A}[\tau]\}\ , \tag{97}$$

where with the help of Eqs. (78)–(79) $\tilde{A}[\varphi_{\rm tr}^2 t]$ transforms to the formula

$$\tilde{A}[\varphi_{\rm tr}^2 t]=\left[\frac{E_0}{\omega}\right]^{3/2}\int_{X_{\rm cr}}^{\infty}d^3x\,\{\ln\mathcal{R}(-it)-t\varphi_{\rm tr}^2(x)[\ln\mathcal{R}(-it)]'_{t\varphi_{\rm tr}^2}\}+(E_0/\omega)^{3/2}(4\pi/3)X_{\rm cr}^3\ln(1/c) \tag{98}$$

and $\tilde{\mathcal{A}}[\tau]$ can be written as

$$\tilde{\mathcal{A}}[\tau]=\left[\frac{E_0}{\omega}\right]^{3/2}\int_{X_{\rm cr}}^{\infty}d^3x\left\{\ln\left[\frac{\mathcal{R}(\tau-it)}{\mathcal{R}(-it)}\right]-i\tau[\ln\mathcal{R}(\tau-it)]'_\tau\right\}\ , \tag{99}$$

where

$$[\ln\mathcal{R}(\tau-it)]'_\tau=\frac{\partial}{\partial\tau}[\ln\mathcal{R}(\tau-it)]\bigg|_{\tau=0}\ .$$

The deep centers result in

$$\rho_I(\omega)=\frac{1}{\omega}\left[\frac{\omega}{\Delta}\right]^{3/2}\exp\{-A_I[\varphi_{\rm tr}]^2 t\}(1/2\pi)\int_{X_0}d^3x\,\exp\{-\mathcal{A}_I(\tau)\}\ , \tag{100}$$

where $A_I[\varphi_{\rm tr}^2]$ can be written in the general case as

$$\tilde{\mathcal{A}}_I[\varphi_{\rm tr}^2 t]=\left[\frac{E_0}{\omega}\right]^{3/2}\int_{X_0}^{\infty}d^3x\,\{\ln\mathcal{R}(-it)-t\varphi_{\rm tr}^2(x)[\ln\mathcal{R}(-it)]'_{t\varphi_{\rm tr}^2}\}+\ln(1/c_I) \tag{101}$$

and

$$\tilde{\mathcal{A}}_I[\tau]=\left[\frac{E_0}{\omega}\right]^{3/2}\int_{X_0}^{\infty}d^3x\left\{\ln\left[\frac{\mathcal{R}(\tau-it)}{\mathcal{R}(-it)}\right]-i\tau[\ln\mathcal{R}(\tau-it)]'_\tau\right\}\ . \tag{102}$$

Expanding $\tilde{\mathcal{A}}[\tau]$ and $\tilde{\mathcal{A}}_I[\tau]$ in a Taylor series in τ powers and restricting by the second-order term we get after calculation of the Gaussian integral

$$\begin{aligned}\rho(\omega)+\rho_I(\omega)=&\frac{1}{\omega}\left[\omega\Delta\right]\left[\frac{E_0}{\omega}\right]^{3/2}\left\{2\pi\int_{X_{\rm cr}}d^3x[\ln\mathcal{R}(-it)]''_{\tau\tau}\right\}^{-1/2}\exp\{-\tilde{A}[\varphi_{\rm tr}^2 t]\}\\&+\frac{1}{\omega}\left[\frac{\omega}{\Delta}\right]\left[\frac{E_0}{\omega}\right]^{3/2}\left\{2\pi\int_{X_0}d^3x[\ln\mathcal{R}(-it)]''_{\tau\tau}\right\}^{-1/2}\exp\{-\tilde{A}_I[\varphi_{\rm tr}^2 t]\}\ ,\end{aligned} \tag{103}$$

where

$$[\ln\mathcal{R}(-it)]''_{\tau\tau}=\frac{\partial^2}{\partial\tau^2}[\ln\mathcal{R}(\tau-it)]\bigg|_{\tau=0}\ .$$

Using for the calculation of the integral

$$\int_{X_{\rm cr}}d^3x[\ln\mathcal{R}(-it)]''_{\tau\tau}$$

an approximate solution $\varphi_\omega(x)$ given in the limit $\omega\to 0$ by Eq. (86) we get the value of the energy which describes the statistical dispersion of the localization energy:

$$\gamma_\omega=\sqrt{\langle(\delta\omega)^2\rangle_{\rm av}}=\sqrt{\omega E_{\rm BE}/2}=\sqrt{c(1-c)\Delta^2\delta L_\omega}\ . \tag{104}$$

The last expression can be rewritten in the form

$$c(1-c)\Delta^2\delta L_\omega\equiv\omega c\Delta\left[\frac{(1-c)\Delta}{E_{\rm cr}}\right]^{3/2}\frac{\pi^2 I_4^{\rm cr}}{12}\ . \tag{105}$$

For deep centers we get

$$\gamma_I=\sqrt{c(1-c)\Delta^2\delta L_{\omega_I}}\ , \tag{106}$$

with δL_{ω_I} given by Eq. (96). To estimate the order of the magnitude of the last expression we can use the wave function of the spherical well with the volume equal to v_0 and with the depth given by Δ_I.

As we can see from Eq. (105) at $\omega\to 0$ the value of the γ_ω will reach the value of ω at $\omega=\omega_{\mathrm{ME}}$ given by equation

$$\omega_{\mathrm{ME}}=E_{\mathrm{BE}}/2=c\Delta\left[\frac{(1-c)\Delta}{E_{\mathrm{cr}}}\right]^{3/2}\frac{\pi^2 I_4^{\mathrm{cr}}}{12}\ . \tag{107}$$

We already cannot consider the states with $\omega\le\omega_{\mathrm{ME}}$ as localized ones and, therefore, we can take the value ω_{ME} as an estimation of the mobility edge in the single-instanton approximation. It has an obvious resemblance to the well-known Ioffe-Regel criterion, but in distinction from the last it is obtained for the states supposed to be localized and has more chances to succeed in the approximate definition of the mobility-edge position.

The value $\omega=\omega_{\mathrm{ME}}$ also gives us the upper border of the single-instanton approximation because wave functions of states above the ω_{ME} should be changed by the interaction between the overlapping states.

VI. DISCUSSION AND COMPARISON WITH EXPERIMENT

Using for the approximate calculation of the first item in Eq. (103), Eqs. (88) and (104), obtained in the limit of the small localization energies we get the estimation of the full number of states below the E_G per lattice site as

$$\mathcal{N}(0)=\int_0^{E_L}\rho(\omega)d\omega\approx c^{\nu_{\mathrm{cr}}}\ , \tag{108}$$

where

$$\nu_{\mathrm{cr}}=\left[\frac{E_{\mathrm{cr}}}{(1-c)\Delta}\right]^{3/2}\ .$$

These states have appeared as a result of fluctuations of the binary solution and it looks quite natural that their number is restricted by the possible number of the most probable critical clusters. Analogous calculations for the second item of Eq. (103) using Eqs. (95) and (106) give a value equal to c_I for the number of deep centers per lattice site. We shall note that both results are obtained with restriction (IV) being incorporated into the calculations. Without a given restriction the number of the states appeared to be independent of the properties of the fluctuation potential, which looks unreasonable.

The full number of localized states can be estimated with help of Eq. (107) by means of the numerical evaluation of the integral

$$\mathcal{N}(\omega_{\mathrm{ME}})=\int_{\omega_{\mathrm{ME}}}^{E_L}\rho(\omega)d\omega\ . \tag{109}$$

Both estimations given by Eqs. (108) and (109) have the same order of magnitude and can be compared with the experimental number of localized states below the mobility edge. From the experimental data of Ref. 4 and references therein we can see that the number of localized states is rather small compared with the full number of states in valence bands. This fact can be interpreted in terms of Eq. (108) and the expression for ν_{cr} as resulting in the inequality $\nu_{\mathrm{cr}}>1$ for these fluctuation potentials which have a maximum depth of the single-site well of less than the critical value E_{cr}. We can consider these potentials as weakly scattering ones. At these estimations we shall have in mind that expression (108) overestimates the number of the localized states and Eq. (109) is preferable.

There are another two values convenient for a comparison with the experiment. They are the slope of the linear region E_{BE} defined by Eq. (91) and the Urbach parameter E_U presented in Eq. (81). From the relation of these two quantities the most pronounced dependence on E_{cr} disappears.

Totally, the three mentioned quantities give a chance to find the three parameters of the theory, namely, the concentration of the attractive centers, c, the random potential amplitude Δ, and the critical depth of the single site perturbation, E_{cr}. If the possibility exists to find one of the parameters from the independent sources, then the knowledge of the mentioned experimental data allows one to check the theoretical relations quantitatively.

The most suitable parameter for the independent estimation is, probably E_{cr}. For its estimation it is necessary to know the effective mass of the carrier and the volume v_0. The estimation of the E_{cr} is, probably, possible for amorphous silicon and glasses. The amplitude of the random potential and the concentration are known as a rule for isoelectronic solid solutions, which makes these objects a very good prospect for use in an investigation of the behavior of the single-electron density of states in the region of localization.

Additional information can be obtained from the investigation of deep-center bands. In the case of amorphous silicon fitting of the theory parameters with help of the data on the band tail makes it possible to predict the broadening of the deep-center band and even its form if the preexponential factor is calculated more accurately.

The comparison of the qualitative level of the experimental data of Ref. 4 on the single-electronic density of states with our calculations is given in Fig. 1. Here the DOS calculated within exponential accuracy without the deep-center band is presented. The inset reproduces one of the experimental figures of Ref. 4. According to Ref. 4 the experimental mobility edge is disposed at energy 5.7 eV (see the inset in Fig. 1). That means that almost the whole linear region obtained in the linear scale for the DOS is disposed above the mobility edge. The estimation of the mobility edge (107) also gives its position just above the Urbach region at the very beginning of the linear region of Eq. (1). The calculated spectrum has an obvious likeness with the experimental one.

The preexponential factor cannot change the DOS dependence in the region $\omega \geq \omega_{\mathrm{ME}}$ and therefore the qualitative agreement between the theory and the experiment. While in the interval $0 \leq \omega \leq \omega_{\mathrm{ME}}$ we cannot use the energy dependence of the preexponential factor obtained above because of the localization index energy dependence. Taking into account that the DOS does not have any discontinuities at the mobility edge and so is the exponential part of the DOS we can use the obtained exponential part of the DOS dependence to extrapolate the DOS dependence into the region above the estimated mobility edge.

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