Density distribution of localized states in disordered systems

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The density of localized states of a single-band diagonal-disorder Hamiltonian is calculated in three dimensions with proper regard to the pre-exponential factor. A novel feature of the theory is the imposition of an additional constraint on the class of functions minimizing the action functional in the one-instanton approximation. The rationale for this constraint is derived from the analysis of localized states for a number of realizations of the disordered system under study. The problems considered include (i) the limit of the low density of strong scatterers, and (ii) a ternary system composed of a two component solid solution with a weak scatterer at each site, plus a low density of deep impurity centers. In all cases, both general and simplified expressions are found for the pre-exponential factors. It is shown that in limiting cases the results agree with the exact solutions of the problem. The calculations agree well with the experimental data on the one-electron density of states in amorphous silicon.

1. INTRODUCTION

Modern experimental methods provide detailed information on the spectral density and the density of states in disordered systems of greatly varying physical nature.[1–7]

As of today, most extensive density-of-states studies have been made on amorphous silicon at the peak of its valence band and in the band gap.[4,5] One distinguishes in the behavior of the density of states three major features which appear to be common to diverse samples of the material:

1) In the region of relatively high densities (which we will arbitrarily call the *band-edge region*) there is an energy range where the density of states varies linearly with energy, that is, on a linear scale,

$$\rho(\varepsilon)=\rho_{\rm BE}\left\{1-\frac{E_g-\varepsilon}{E_{\rm BE}}\right\}. \tag{1}$$

The parameters $\rho_{\rm BE}$ and $E_{\rm BE}$ can be found by a simple data-processing procedure taking the mobility edge as the zero of the energy E_g. A specific model we consider below makes it possible both to illustrate the meaning and to show the order of magnitude of the parameters involved. The dependence of the type (1) is limited to the range of energies for which the second term in the braces is small compared to the first.

2) As the energy of localization is increased, there is a smooth crossover to a linear Urbach exponential dependence[8–10] which, using a logarithmic scale, may be written as

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

Here ρ_U is the density of states at some point ε_U of the Urbach region and E_U is the Urbach parameter. Note that $E_U<E_{\rm BE}$.

3) Further down in energy the density of states is strongly influenced by the presence of impurity centers, whose states undergo a considerable nonuniform broadening. Reference 4 presents a detailed study of a situation in which the band formed by deep-center states is fairly well described by the Gaussian form

$$\rho_{\rm I}(\varepsilon)=\frac{c_{\rm I}}{(2\pi\gamma_{\rm I}^2)^{1/2}}\exp\left\{-\frac{(\varepsilon_{\rm I}-\varepsilon)^2}{2\gamma_{\rm I}^2}\right\} \tag{3}$$

in the vicinity of the band maximum. Here $c_{\rm I}$ is the density of the centers and $\gamma_{\rm I}$ the half-width of the contour. The wings of the band show a considerable asymmetry, however.[1)]

The purpose of this paper is to discuss the behavior of the density of localized states for a simple model of a disordered system. We believe that only the most general features of the fluctuation-induced potential are essential for explaining the observed data, and so the system we consider is a three-dimensional two-component Anderson model described by a single-band hamiltonian with diagonal disorder caused by the random occupation of the crystal lattice sites by both types of atoms, A and B. A continuum version of this model will also be considered.

As a further complication of the model, we will also analyze the situation in which a low density $c_{\rm I}$ of deep impurity centers is added to the system.

As discussed previously,[15] application of the instanton approximation to the above model yields the Urbach behavior, Eq. (2), for an energy range sufficiently wide to explain the experimental data for a wide variety of disordered systems. In particular, this gives a correct order of magnitude of the Urbach parameter E_U as well as explaining its concentration dependence observed in solid solution experiments.[6] It turns out, however, that for band-edge energies above the Urbach region, Ref. 15 gives the density of states whose behavior departs considerably from both experimental data[4] and expression (1). This question will be examined closely in the present study.

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One further motivation for the improvement of the method of Ref. 15 comes from the problem of strong electron scattering by a deep potential well in the limit of extremely small density of such wells (i.e., of attractive centers as far as the electron is concerned). The solution for a two-component disordered system will be applicable to amorphous silicon[4] and other disordered systems with deep impurities.

Finally, the problem of the so-called pre-exponential factor of the density of localized states will be considered: its value is crucial for the comparison of the predicted *absolute* density of states with its experimental counterpart usually known to within a factor of about 2.[4] It is well known, on the other hand, that because of the presence of the Fermi zero mode in the fluctuation determinant the one-instanton contribution to the Green's function is zero, which makes a comparison of theory and experiment impossible. As a means to overcome this problem we represent the Green's function in terms of complete sets of the eigenfunction and eigenvalues of all permissible realizations of the system under study, which allows one to employ the exact transformation of the Green's function using the Parisi-Sourlas magic formula.[16] To check the results, it proves useful to address the limiting cases for which the one-instanton solution is exact. These are the behavior of the density of states near the Lifshitz bound[17] and the above-mentioned case of the low density of extremely deep centers.

We see thus that despite their apparent diversity the topics we have listed prove to be closely interrelated.

A common feature of previous approximate analyses of three-dimensional disordered systems[18–29] is that, following averaging over all possible configurations of the system, the calculation of the density of states reduces to a variational procedure. The novel feature of the present approach is a more detailed analysis of the class of functions among which to seek the solution: analysis, in fact, of the relation between the variational solution for the averaged problem and those solutions which are most probably realized in various regions of the disordered model system.

In previous analyses, one distinguishes three basic constraints imposed on the form of the variational solution: (i) in a fluctuation-induced well, only the ground state is considered, (ii) the trial function is spherically symmetric, which reduces the computational effort to a minimum, and (iii) certain assumptions concerning the decrease of the solution at large distances from the fluctuation are made. The last constraint is related to the assumption of the short-range nature of the potential fluctuation and—adopting Anderson's model with diagonal disorder as we do—is also adequate for solutions obtained for specific occupation variants.

The main difference between the present approach and that of Ref. 15 is the imposition of yet another constraint on the variational solution $\varphi_{\mathrm{tr}}(R)$ in the region of small values of R. We relate this constraint to the behavior (compatible with our model) of the potential wells occurring most frequently in actual configurations, and we find as a result that the small-R behavior of $\varphi_{\mathrm{tr}}(R)$ is identical to that exhibited by the solutions for these wells. We will consider two limiting cases for which we believe that the additional constraint is the simplest to formulate, namely low density of strong attractive centers and arbitrary density of weak scatterers. In the former case we add the requirement that there be at least one attractive center in a fluctuation producing a localized state. In the latter case we demand that such a fluctuation include the most likely critical-size cluster. The two cases will match if the single-site scattering intensity is taken to be equal to its critical value.

The need for the additional constraint is especially obvious when applied to the case of a very low density of strong attractive centers ($c \ll 1$) leading to the familiar problem of the spectrum of localized states produced by a point perturbation. In the limit $c \to 0$, the solution to this problem is well known: it was first obtained in Ref. 30 (see also Ref. 31) and since then has been the subject of extensive analyses using various versions of the tight binding model (see e.g., Lannoo and Lenglart[32] and Bernholc and Pantelides[33] as well as references therein). To linear order in c, the density of local states is described by a δ function centered at the local energy level $\varepsilon = \varepsilon_{\mathrm{loc}}$ given by the Koster–Slater–Lifshitz equation.[30–33]

Using the approach we propose, the problem at hand—essentially a model one—may be solved in an instanton formulation and gives rise to a continuous spectrum of localized states bounded by the limits $0 > \varepsilon_{\min} > \varepsilon > E_L$ and having its maximum density at the point $\varepsilon = \varepsilon_{\mathrm{loc}}$. The central portion of the line is Gaussian and for $\varepsilon = \varepsilon_{\mathrm{loc}}$ the equation of motion of the instanton is exactly the Koster–Slater–Lifshitz equation for a localized state in a virtual crystal. The quantity E_L is precisely the edge of the spectrum and the density of states in its vicinity is described by the Lifshitz singularity while $\varepsilon_{\min}$ is the position of the local level of the A atom when placed in the macroscopic cluster of B atoms. The resulting solution enables one to normalize the density of states accurate to terms of order c^2, which implies that the number of states equals the number of A atoms ($= cN$). The solution coincides with the exact one at two points, $\varepsilon = \varepsilon_{\min}$ and $\varepsilon = E_L$, is virtually identical to the solution of Ref. 15 in the range $\varepsilon_{\mathrm{loc}} < \varepsilon < E_L$, and is quite different from it for $0 > \varepsilon > \varepsilon_{\mathrm{loc}}$.

In the weak scattering regime, the additional condition is conveniently taken in the form of a restriction on the minimum power of those potential fluctuations playing the dominant role in the formation of localized states; this power may be bounded from below by that of the most probable critical cluster of spherical shape. As a result the trial function within the critical cluster, is identical to the solution of the Schrödinger equation for most probable fluctuation wells containing such a cluster. On the other hand, far away from the center of the well the behavior of the trial function is identical to that of the exact solutions for short-range potentials. Note, however, that at intermediate distances the trial function is no more than an interpolation between these two extremes, strongly smoothed as compared with those solutions actually existing in specific realizations. As in the strong scattering case, here too the maximum departure from the results of Ref. 15 occurs at small localization energies. We see thus that in both cases the additional condition provides a means for avoiding unrealistic solutions.

It should be noted that the translational symmetry of the solution is lost at the outset as a result of the above additional constraint. The averaged Green's function does preserve this property because the summation is over all possible positions of the instanton center in the course of the calculation.

Our method reproduces the basic features of the previous analyses[15,18–29] and is essentially approximate in that instead of a multitude of specific realizations of disorder we are dealing with a variational problem resulting from an approximate averaging procedure. Using the simplest possible instanton solution in the variational analysis of the averaged action imposes an additional limitation on the applicability of the method. Since three-dimensional model problems have not yet been treated numerically in the literature, it turns out that, except for the two limiting cases we mentioned, a comparison with the exact solution is not yet possible. The experimental data on the one-electron density of states of amorphous silicon show good qualitative agreement with the theory over a wide range of energies.

2. HAMILTONIAN OF THE MODEL

We consider a solid solution of macroscopic volume V containing N sites occupied at random by either A or B atoms. The mean numbers of A and B atoms are $N_A=cN$ and $N_B=(1-c)N$, respectively, c being the concentration of the A atoms. The single-band Hamiltonian of this system is taken to be

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

with Ψ_n assumed real. The diagonal matrix element E_n takes on the value E_A (E_B) if the site is an A (B) atom. In the limiting cases $c=0$ and $c=1$ the Hamiltonian (4) reduces to that for the pure B or pure A crystal, respectively, and all the E_n are replaced either by E_A or E_B.

In the plane-wave representation the matrix element of the Hamiltonian is

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

where α stands for A or B and the electronic dispersion is given by

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

3. GREEN's FUNCTION REPRESENTATION

The Green's function of a pure A or B crystal is written as

$$G_{nm}^\alpha(\varepsilon)=\{\varepsilon-H^\alpha\}_{nm}^{-1}=\frac{1}{N}\sum_q\frac{\exp[i\mathbf{q}(\mathbf{R}_n-\mathbf{R}_m)]}{\varepsilon-\varepsilon_q-E_\alpha}, \tag{7}$$

where $\vec{R}$ is the radius-vector of the site n. For a random occupation of both types of atom, the Green's function for each particular realization of the system depends on both the composition and the arrangement of the atoms,

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

Introducing the normalizing factor, and assuming the distribution of A and B atoms to be random but fixed, the diagonal matrix element of the Green's function is[34–36]

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

where

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

and

$$A[\Psi]=-\sum_{nm}\Psi_n(H_{nm}-\epsilon\delta_{nm})\Psi_m,$$
$$H_{nm}=-W_{m-n}+\delta_{nm}\Bigl(\sum_l W_l+E_n\Bigr). \tag{11}$$

Here δ_{nm} is Kronecker's symbol.

As a point of reference for ε and E_n we introduce a quantity related to the average of E_n in the site:

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

In the virtual-crystal approximation, $\langle E\rangle_{\rm av}$ coincides with the band bottom of the solid solution and also fixes its mobility threshold, $E_g\equiv E_g^{\rm vc}=\langle E\rangle_{\rm av}$. Let us introduce the new variables

$$\omega=E_g-\varepsilon,\quad \Delta_n=E_n-E_g \tag{13}$$

and represent the action as a sum of two terms,

$$A[\Psi]=A_{\rm vc}[\Psi]+\Delta A[\Psi], \tag{14}$$

where

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

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

For a random but fixed distribution of the two types of atom, finding the eigenfunctions and eigenvalues of the Hamiltonian is a linear problem solved by diagonalizing a matrix of rank N whose rows are of the form

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

We next rewrite the functional integral (9) making use of the eigenfunctions (17) and the Grassmann variables ζ and $\bar{\zeta}$[36–40] in order to raise Z to the numerator:

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

where

$$[\omega+H^{\text{vc}}-\Delta]_{\lambda\lambda}=\sum_{n,m}\varphi_{\lambda}^{\Delta}(n)[(\omega-\Delta_{n})\delta_{nm}+H_{nm}^{\text{vc}}]\varphi_{\lambda}^{\Delta}(m), \tag{19}$$

and the Grassmann variables are normalized so that

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

The spectrum of the disordered system is obtained through an averaging procedure, i.e., by summing the spectra of specific configurations weighted by their probability of occurrence; of interest here is the Green's function averaged over all possible atom distributions over the sites of the crystal.

Before we sum over the entire ensemble of realizations of the system we simplify the Green's functions for each particular configuration using only the most general properties of the representation (18). We note that the argument of the exponential in (18) is supersymmetric in the z, ζ space, i.e., remains invariant under transformations conserving the form

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

and we may therefore employ the magic formula of Parisi and Sourlas[16] when integrating over the variables z_{λ}^{*}, z_{λ}, $\bar{\zeta}_{\lambda}$, and ζ_{λ}.

In any λth term in the sum in (18), it is seen that of the infinite number of τ_{λ} integrations only one contributes nontrivially,

$$\begin{aligned}1/\pi \int dz_{\lambda}^{*}dz_{\lambda}|z_{\lambda}\varphi_{\lambda}^{\Delta}(n)|^{2}M'_{|z_{\lambda}|^{2}}(|z_{\lambda}|^{2}) &= \int_{0}^{\infty} d\tau_{\lambda}M(\tau_{\lambda})|\varphi_{\lambda}^{\Delta}(n)|^{2} \\ &\equiv \int_{0}^{\infty} d\tau_{\lambda}|\varphi_{\lambda}^{\Delta}(n)|^{2}\exp\{-i[\omega+H^{\text{vc}}-\Delta]_{\lambda\lambda}\tau_{\lambda}\},\end{aligned} \tag{22}$$

where

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

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

As a result, for a fixed set of Δ_{n}'s and a given set of quantum numbers (denoted above by λ), the density of states takes the form

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

and, summing over all λ and all the Δ realizations with their respective weighting factors P_{Δ}, the total averaged density of states is

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

If the contribution from a certain specific—say, spherical—symmetry is of interest, the summation over λ may be omitted in (24).

The meaning of the above expression is quite lucid: we list all possible configurations of the system, calculate the eigenvalues and eigenfunction for each of them, and, finally, evaluate the integrals (23).

The integration over τ_{λ} in Eqs. (23) and (24) can be done in the general form and the final expression for $\rho(\omega)$ becomes

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

where we have denoted by $\omega_{\lambda}^{\Delta}$ the eigenvalue of Eq. (17) for a fixed set Δ_{n}. The bound-state wave functions $\varphi_{\lambda}^{\Delta}$ may always be normalized to unity.

The expression above is a rigorous definition of the density of states for a disordered system described by the Hamiltonian (4)—that is, for a two-component solid solution $A_{c}B_{1-c}$. A very similar expression was employed, for example, in Ref. 18.

Numerical methods for calculating the spectra of disordered systems are usually reduced to the solution of the system (17) followed by a summation of the type (25) taking into account all occupation variants Δ and all λ at each Δ.

Our goal here is to obtain a realistic approximation for the density of localized states without resorting to a solution of the system (17).

3.1. Restrictions on the class of trial functions

The exact expression (24) cannot be summed over the ensemble of configurations unless the eigenstates $\varphi_{\lambda}^{\Delta}$ and their eigenvalues are known. The first step in the approximate calculation procedure is to replace the exact solutions by trial functions independent of the specific arrangement of atoms over the lattice sites. This permits the summation over all possible configurations to be performed. In the preceding section, integration in a general fashion over all but one τ_{λ}'s enabled us to avoid calculating the determinants involved[19–21] and thereby markedly reduced the computational effort.

The key question concerns the choice of trial functions and their relation to the solutions of the system (17) for various configurations. The restrictions on the class of trial functions may be summarized as follows:

(i) Even though the formulation in terms of the integral (24) makes it possible to include excited states if there are any, we again restrict ourselves in this paper to a single nodeless ground state in each fluctuation well. The problem thus reduces to the choice of only one trial function.

(ii) An important question is that of the symmetry of the wave function of the fluctuation bound state. As before (see Ref. 15) the trial wave function is assumed to possess either total point symmetry of the lattice (lattice Hamiltonian) or spherical symmetry (continuum limit).

(iii) The model Hamiltonian (4) leading as it does to short-range potential wells, it is assumed that at large distance R from the well the trial function falls off like

$$1/R\exp[-\varkappa(\omega)R], \tag{26}$$

where $\varkappa(\omega)$ is determined by the depth of the bound state (ω). This behavior as $R\to\infty$ is also a feature of exact bound-state solutions generated by the system (17) for specific configurations.

(iv) In the present work we introduce an additional condition which follows from the properties of exact bound-state solutions of the system (17) of the Hamiltonian (4); the effect of the new condition is to restrict the magnitude of $\varphi_{\rm tr}(R)$ as $R\to 0$, i.e., to impose some limitation on the small-R behavior of the trial function. The idea is that the small-R behavior of the solution $\varphi_{\rm tr}$ be consistent with equations (17); we wish, in other words, that $\varphi_{\rm tr}$ be optimal not only from the point of view of its contribution to $\rho(\omega)$ but, as well, from the point of view of its relation to exact eigenfunctions for specific configurations. We take for the trial function $\varphi_{\rm tr}$ an eigenfunction of the equation

$$\omega\varphi_{\rm tr}(n)-\sum_m(H^{\rm vc}_{nm}+U_{\rm tr}(n)\delta_{nm})\varphi_{\rm tr}(m)=0, \tag{27}$$

where $U_{\rm tr}(n)$ is a spherically symmetric trial fluctuation well whose shape is usually determined from the extremum of the action functional of the problem. Trying the (normalized) lowest wave function as $\varphi_{\rm tr}$ and dropping all $\lambda\neq 1s$ terms, Eq. (24) becomes

$$\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\sum_\Delta P_\Delta\exp\biggl\{i\sum_{n,m}\varphi_{\rm tr}(n)\times[(\omega-\Delta_n)\delta_{n,m}+H^{\rm vc}_{nm}]\varphi_{\rm tr}(m)\tau\biggr\}. \tag{28}$$

The important point to be made here is that $\varphi_{\rm tr}$ is not generally an eigenfunction of the system (17), so that in the course of integration over τ, it only picks up those configurations satisfying the integral relation

$$\sum_{n,m}\varphi_{\rm tr}(n)[(\omega-\Delta_n)\delta_{n,m}+H^{\rm vc}_{nm}]\varphi_{\rm tr}(m)=0. \tag{29}$$

Because of the huge number of possible configurations of the system, (29) ensures that the density of localized states will be finite for virtually any trial function $\varphi_{\rm tr}$. The difficulty we encounter is that trial functions having nothing to do with solutions realizable in specific configurations may lead to a prohibitively large density of localized states in a certain energy range. It is to exclude this possibility that we add the constraint (iv) on the shape of the trial function at $R\to 0$.

Because the shape of the wave function for R small compared with the bound-state radius is determined by the form of the potential in this region, we will formulate the constraint (iv) as a condition that the trial potential as $R\to 0$ be bounded by a certain value to be found from the system (17) for the most probable bound states. Depending on the parameters of the Hamiltonian (4), in the next sections we discuss the limiting cases of strong and weak scattering and present corresponding formulations of the above condition.

3.2. General averaging scheme

In this section we consider the averaging procedure in a general fashion, without specifying the form of the additional constraint (iv) to be imposed on $U_{\rm tr}(n)$ and $\varphi_{\rm tr}$.

Since $\varphi_{\rm tr}$ is independent of the particular configuration, it is now possible to sum over all sets Δ. From Eqs. (18), (19), and (23) it is seen that the quantity to be averaged is the function

$$\exp\{-i\Delta A[\tau]\}=\exp\biggl\{-i\sum_n\Delta_n\varphi^2_{\rm tr}(n)\tau\biggr\}.$$

The fluctuation-related term in the action $\Delta A[\tau]$ depends on the particular configuration of the system. In the case of random occupation, each site is either an A or a B atom with the respective probabilities c and $(1-c)$. Recognizing that the exponential to be averaged factorizes into exponentials each of which can be averaged independently, we obtain

$$\langle\exp\{-i\Delta A[\tau]\}\rangle=\biggl\langle\exp\biggl\{-i\sum_n\Delta_n\varphi^2_{\rm tr}(n)\tau\biggr\}\biggr\rangle=\prod_{n=1}^{N}\{c\exp(-i\Delta_{\rm A}\varphi^2_{\rm tr}(n))+(1-c)\exp(-i\Delta_{\rm B}\varphi^2_{\rm tr}(n)\tau)\}. \tag{30}$$

Here

$$\Delta_{\rm A}=E_{\rm A}-E_g=-(1-c)\Delta,\quad \Delta_{\rm B}=E_{\rm B}-E_g=c\Delta,\quad \Delta=E_{\rm B}-E_{\rm A}>0. \tag{31}$$

The averaged density of states then becomes

$$\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\biggl\{-i\tau\sum_{n,m}\varphi_{\rm tr}(n)(\omega+H^{\rm vc})\varphi_{\rm tr}(m)+\sum_n\ln R_n(\tau)\biggr\}, \tag{32}$$

where

$$R_n(\tau)=c\exp[i\Delta(1-c)\varphi^2_{\rm tr}(n)\tau]+(1-c)\exp[-i\Delta c\varphi^2_{\rm tr}(n)\tau]. \tag{33}$$

To proceed it is convenient to change from the Fourier integral (32) to the Laplace transformation

$$\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\Big\{-i\sum_{n,m}\varphi_{\rm tr}(n)(\omega+H^{\rm vc})\times\varphi_{\rm tr}(m)(\tau-it)+\sum_{n}\ln[R_n(\tau-it)]\Big\},\qquad(34)$$

where

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

This result is fully equivalent to (32) and the free parameter t may in this case assume any positive or negative value.

Separating the exponential, the above expression can be put into the form

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

where

$$A^0[\varphi_{\rm tr}^2t]=(\omega+H^{\rm vc})_{\varphi,\varphi}t-\sum_{n}\ln R_n(-it),$$
$$\mathscr{A}^0(\tau)=i(\omega+H^{\rm vc})_{\varphi,\varphi}\tau-\sum_{n}\ln\left[\frac{R_n(\tau-it)}{R_n(-it)}\right],\qquad(37)$$

and

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

In Ref. 15 the bound state equation is discussed without subjecting the trial function to the additional constraint we have introduced here. This equation can be obtained from the extremum condition for the action,

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

i.e., it takes the form of Eq. (27),

$$\sum_{m}[H_{nm}^{\rm vc}+\omega\delta_{nm}]\varphi_{\rm tr}(m)+U_{\rm tr}(n)\varphi_{\rm tr}(n)=0.\qquad(40)$$

To obtain an extremum of the action the potential $U_{\rm tr}(n)$ must in this case be taken in the form[15]

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

Thus, the calculation of the density of states for the general case proceeds like follows: 1) solve a bound-state equation, of a form determined by the additional constraint (iv) on $U_{\rm tr}$, 2) calculate the argument of the exponential (in this case, $A^0[\varphi_{\rm tr}^2])t$, and 3) calculate the τ-dependent contribution to the action (here $\mathscr{A}^0[\tau]$) and integrate over to obtain the pre-exponential factor. Note that apart from yielding the function $\varphi_{\rm tr}$ the bound-state equations also fix the the free parameter t of the Laplace transform.

4. STRONG SCATTERING

We assume that the concentration of A atoms is small and that the perturbation by an individual atom is large compared to the critical value and produces a deep level in the energy spectrum, i.e.,

$$c\ll1,\ (1-c)\Delta\gg|G_{nn}^{\rm vc}(0)|^{-1}.\qquad(42)$$

The simultaneous fulfilment of these equations implies that A–A separations are almost always larger than the radius of the bound state produced by each of these attractive centers, so that, to terms of order c^2, the solution of the system (17) in the localization region is reduced to the familiar local perturbation problem.[30–33]

Since there is at least one attractive center (i.e., an A atom) present in any bound-state-forming fluctuation, we stipulate that on a certain site of the lattice the trial function $U_{\rm tr}$ reproduce the exact value of the attractive potential of an isolated A atom,

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

Referring $\varphi_{\rm tr}$ to this particular site as the origin and ignoring the configurations failing to satisfy the above condition, (36) transforms to

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

where

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

and

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

Minimizing the exponent $A[\varphi_{\rm tr}^2]$ we arrive at an equation of the form (40) where now

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

Here

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

Multiplication of the above expression on the left by the Green's function of the virtual crystal now gives

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

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

4.1. Approximate formulation

For $t=0$ and (42) fulfilled, Eq. (49) recovers the Köster–Slater–Lifshitz equation for a single-site localized state in a virtual crystal formulation, and for $\omega=\omega_{\mathrm{loc}}$, $\varphi_{\mathrm{tr}}(m)$ is exactly the solution of this equation, i.e.,

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

which for $\omega=\omega_{\mathrm{loc}}$ may be written as

$$\begin{aligned}\psi_{\mathrm{loc}}(m)&=-G^{\mathrm{vc}}_{nm}(\omega_{\mathrm{loc}})\,|G^{\mathrm{vc}\prime}_{nn}(\omega_{\mathrm{loc}})|^{-1/2},\\ G^{\mathrm{vc}\prime}_{nn}(\omega_{\mathrm{loc}})&=\frac{\partial}{\partial\omega}G^{\mathrm{vc}}_{nn}(\omega)_{|\omega=\omega_{\mathrm{loc}}}.\end{aligned} \tag{51}$$

For deep states, $\varphi_{\mathrm{loc}}(m)$ is virtually zero everywhere except one site,

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

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

For $\omega\approx\omega_{\mathrm{loc}}$, noting that (49) is solvable only for small values of t, the quantity $U_{\mathrm{tr}}(m\neq n)$ in (47) may be expanded in powers of t and, keeping only the first nonvanishing term, (49) takes the form

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

Now taking

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

as the zeroth-order approximation and representing $G^{\mathrm{vc}}_{nn}(\omega)$ around ω_{loc} as

$$G^{\mathrm{vc}}_{nn}(\omega)=G^{\mathrm{vc}}_{nn}(\omega_{\mathrm{loc}})+(\omega-\omega_{\mathrm{loc}})G^{\mathrm{vc}\prime}_{nn}, \tag{53}$$

where

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

it is found that Eq. (52) will be satisfied if

$$t=\frac{(\omega-\omega_{\mathrm{loc}})}{c(1-c)\Delta^2}\left\{\sum_{m\neq n}\left[\frac{|G^{\mathrm{vc}}_{nm}(\omega_{\mathrm{loc}})|^2}{G^{\mathrm{vc}\prime}_{nn}(\omega_{\mathrm{loc}})}\right]^2\right\}^{-1}$$

The quantity $A[\varphi^2_{\mathrm{tr}}t]$, in turn, is found to be given by

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

We make use next of (52), with (51) for ψ_{loc} and t from (52), to transform $\exp\{-A[\varphi^2_{\mathrm{tr}}t]\}$ into

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

where

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

and $L_{\omega_{\mathrm{loc}}}$ is the localization index defined by

$$L_{\omega_{\mathrm{loc}}}=\sum_m[\varphi^2_{\mathrm{tr}}(n)]^2=\sum_m\left[\frac{|G^{\mathrm{vc}}_{nm}(\omega_{\mathrm{loc}})|^2}{G^{\mathrm{vc}\prime}_{nn}(\omega_{\mathrm{loc}})}\right]^2. \tag{58}$$

The value of the localization index L_ω characterizes the size of the bound-state wave function with binding energy ω. If the localization depth is large and inequality (42) satisfied with sufficient margin, the wave function is very nearly localized on one site of the lattice, and $\delta L_{\omega_{\mathrm{loc}}}\ll 1$.

Before evaluating the pre-exponential factor, let us consider $\mathscr{A}[\tau]$ in its simplified form obtainable from (46) by keeping only the first three terms in the Taylor expansions of the functions $R_m(\tau-it)$:

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

where

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

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

Substitution of (59) for $\mathscr{A}[\tau]$ into the integral over τ in (44) yields a Gaussian integral giving

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

Thus, instead of the δ-functional expression[30-33] we have obtained a Gaussian contour normalized to the probability of a given site being A. Integration over τ, retaining the quadratic term in the $\mathscr{A}[\tau]$ expansion, has decreased the density of states at $\omega \approx \omega_{\mathrm{loc}}$ because of the statistical scatter in localization energies. The amount of the scatter is characterized by the energy parameter

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

which vanishes as $\omega_{\mathrm{loc}} \to \infty$. We note that in this limit the problem affords an exact solution against which to check the validity of the method.

Since (60) represents a contribution from only one lattice site—of which there are N in the volume under study—it follows that summing over all possible positions of the A atom yields the total of $N_A = cN$ terms, each corresponding to a localized state at $\omega \approx \omega_{\mathrm{loc}}$.

4.2. Exact formulation

It will be recognized that the Gaussian behavior is actually limited to the vicinity of the band maximum. Results obtained from Eq. (49) are finite everywhere in the range $-\infty < t < \infty$. At the extremes $t \to \infty$ and $t \to -\infty$, the effective potential energy represents, respectively, a cluster of pure A atoms and a cluster of pure B atoms with a single A atom at the center. The energy limit determining the maximum depth of the level at $t \to \infty$ is just the Lifshitz limit $E_L = (1-c)\Delta$.

Close to the Lifshitz limit,

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

(44) yields a characteristic singular behavior, whereas in the intermediate range

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

we return to the Urbach behavior.^{15} A markedly modified situation obtains, however, in the range

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

Equation (49) with potential (47) leads to the appearance of the minimum binding energy, which is attained at $t \to -\infty$ and is given by the equation

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

$G^{\mathrm{B}}_{nn}(\omega)$ denoting the Green's function of the B crystal. To terms of order c^2, ω_{min} may be considered as the upper edge of the spectrum of localized states. The density of states decreases in the range

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

and singularly vanishes for

$$\omega \to \omega_{\mathrm{min}}.$$

In the range

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

the density of states takes the form (44), where $A[\varphi^2_{\mathrm{tr}} t]$ transforms into

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

by using (49), and $\mathscr{A}[\tau]$ may be written as

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

Here φ_{tr} and t are calculated from (49) using (47) and (48). As before, we may approximate the pre-exponential factor by Taylor expansion of $\mathscr{A}[\tau]$, and thereby reduce the integral (44) to a Gaussian form. As a result, the density of states takes the form

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

where $A[\varphi^2_{\mathrm{tr}} t]$ is given by (63) and φ_{tr} is normalized to unity. The present solution shares all properties of the instanton solution with the only exception of translational symmetry which, as far as the density of states and the Green's function are concerned, can be restored only by summing the contributions from all possible ways of separating a factor in (44) or, in other words, by summing over all possible positions of the given A atom. The obtained solution agrees closely with that for isolated attractive centers with deep states in their spectra. The existing differences arise, first, from systematically accounting for the lowering of the band edge by $\langle E \rangle_{\mathrm{av}}$, and, second, from the broadening of the level due to the interaction with other attractive centers that happen, by some chance, to be around. The solution is readily extended to a ternary system containing Nc A atoms, $(1-c-c_{\mathrm{I}})N$ B atoms, and $c_I N$ deep attractive centers, provided that $c_{\mathrm{I}} \ll c$, $(1-c)$ and the A-atom potential well is much shallower than its deep-center counterpart. We will address this case after first examining the continuous limit.

5. CONTINUOUS LIMIT, WEAK SCATTERING

We assume that the concentration c of A atoms is arbitrary and that the perturbation potential associated with one atom is much less than its critical value. This problem is conveniently treated in the continuous limit.

5.1. Density of states in the continuum approximation

To change to the continuum model we adopt the effective-mass approximation in the electron band, Eq. (6), and replace the lattice summation by an integration,

$$\sum_n \to (1/v_0) \int d^3R,$$

where the integral extends over the entire crystal and v_0 is the atomic volume. It is also convenient to employ nondimensional length and energy units [de Broglie wavelength $(\hbar^2/2M\omega)^{1/2}$ and ω, respectively] and to change to the new variables $(\tau\Delta)/\omega \to \tau$ and $(t\Delta)/\omega \to t$.

By analogy with (36)—and postponing the imposition of our new constraint on the functions being varied—the density of states may be written as

$$\rho(\omega)=\frac{\omega}{\Delta}\,\frac{1}{\omega}\left(\frac{E_0}{\omega}\right)^{3/2}\exp\{-\tilde{A}^0[\varphi_{\rm tr}^2 t]\}$$

$$\times\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\{-\tilde{\mathscr{A}}^0(\tau)\},\qquad(66)$$

the use of nondimensional variables giving rise to factors that are absent in (36).

The continuum analog of the action (37) is

$$\tilde{A}^0[t\varphi_{\rm tr}^2]=\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\int d^3x[(\nabla\varphi_{\rm tr})^2+\varphi_{\rm tr}^2]t$$

$$-\left(\frac{E_0}{\omega}\right)^{3/2}\int d^3x\ln\mathscr{R}(-it),\qquad(67)$$

where $E_0=\hbar^2/2Mv_0^{3/2}$ and also $E_0=(6/\pi^4)^{2/3}E_{\rm cr}$, $E_{\rm cr}$ being the critical depth of the potential well of volume v_0; M is the electron effective mass as defined by the dispersion law (6).

The function $\tilde{\mathscr{A}}[\tau]$ may be written as

$$\tilde{\mathscr{A}}[\tau]=\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\int d^3x i\tau[(\nabla\varphi_{\rm tr})^2+\varphi_{\rm tr}^2]$$

$$-\left(\frac{E_0}{\omega}\right)^{3/2}\int d^3x\left\{\ln\left[\frac{\mathscr{R}(\tau-it)}{\mathscr{R}(-it)}\right]\right\},\qquad(68)$$

and the combination $\mathscr{R}(\tau-it)$ is defined by

$$\mathscr{R}(\tau-it)=[\exp\{i(\tau-it)(1-c)\varphi_{\rm tr}^2\}$$

$$\times(c+(1-c)\exp\{i(\tau-it)\varphi_{\rm tr}^2\})].$$

The analog of Eq. (40) is

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

where

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

The solution of this equation is given in Ref. 15.

5.2. Critical Cluster Separation

It is now of interest to analyze conditions for bound-state formation from the viewpoint of the system (17). For a bound state to exist in the case we consider it is necessary that attracting centers (i.e., A atoms) form a cluster whose strength equals or exceeds the critical value of the attractive potential. Noting that the potential depth is bounded by $(1-c)\Delta$ in the present model, Eq. (17) yields the following criterion for the existence of a zero-energy bound state in a spherical A cluster:

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

The probability of occurrence of such a cluster is

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

The quantity

$$G_R^{\rm vc}(\omega)=-\frac{2Mv_0}{4\pi\hbar^2R}\exp\{-\varkappa(\omega)R\}\qquad(72)$$

with

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

is the Green's function of the virtual crystal in the continuous limit. For $R\leqslant R_{\rm cr}$, the radial wave function behaves like

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

The requirement for a bound state to exist is obtained from (71) by integrating over R_1 at $R=0$ to give

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

and the probability of a minimum-size critical cluster in the case of random occupation is

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

Compact clusters of radius $R_{\rm cr}$ will occur with the highest probability. Larger critical clusters are less probable because of the B atoms they incorporate: these acting as repulsive centers, the integral in (71) is reduced in magnitude, and a larger domain of integration is required to achieve the critical situation.

There is an important point to note about the fluctuations producing localized states with finite localization energy as different configurations are counted: these must necessarily be stronger than the critical cluster and so are bound to include one version of a critical cluster as their part. All other things being equal, the most probable fluctuations incorporate the most probable critical cluster, that is, a compact A cluster. We will take this condition to play the role of constraint (iv) in the weak scattering case.

5.3. Exponentially accurate solution for fluctuations with a critical cluster

An important question is how the solution will change if only fluctuations with a compact critical cluster are included. Obviously, the potential depth in a volume of radius $X_{\rm cr}$ will become $(1-c)\Delta$ because of the volume being filled by A atoms. When only those configurations satisfying this condition are considered, then the action (67) is replaced by

$$\tilde{A}[t\varphi_{\rm tr}^2]=\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\int d^3x[(\nabla\varphi_{\rm tr}(x))^2+\varphi_{\rm tr}^2(x)]t$$

$$-\left(\frac{E_0}{\omega}\right)^{3/2}\left[\int_0^{X_{\rm cr}}d^3x[(1-c)t\varphi_{\rm tr}^2(x)\right.$$

$$\left.-\ln(1/c)]+\int_{X_{\rm cr}}^{\infty}d^3x\ln\mathscr{R}(-it)\right],\qquad(77)$$

where

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

Minimizing this action yields the equation

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

with the potential energy

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

Equation (78) has spherically symmetric solutions over the entire energy range $0<\omega<(1-c)\Delta$. On substituting the solution into (77), the density of states follows (apart from the pre-exponential factor) as

$$\begin{aligned}\rho(\omega)=\exp\Big\{&-(E_0/\omega)^{3/2}\int_{X_{\rm cr}}^{\infty}d^3x\{\ln\mathscr{R}(-it)\\&-t\varphi_{\rm tr}^2(x)[\ln\mathscr{R}(-it)]'_{t\varphi_{\rm tr}^2(x)}\}-(E_0/\omega)^{3/2}\\&\times(4\pi/3)X_{\rm cr}^3\ln 1/c\Big\}[\ln\mathscr{R}(-it)]'_{t\varphi_{\rm tr}^2(x)}\\&=\frac{\partial}{\partial(t\varphi_{\rm tr}^2(x))}[\ln\mathscr{R}(-it)].\end{aligned} \tag{80}$$

Note that as $X_{\rm cr}\to 0$, Eqs. (77)–(80) go over to the corresponding formulas of Ref. 15. In the limit $\omega\to(1-c)\Delta$, Eq. (80) yields the Lifshitz singularity

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

For lower energies $\omega<(1-c)\Delta$ we retrieve the Urbach decrease with parameter E_U accurately representable by

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

As $\omega\to 0$, we can again simplify Eq. (80) by noting that the potential wells produced by the fluctuations are in this limit mainly determined by the critical-size spherical cluster we have defined. Equation (78) then turns out to be solvable at small values of t, so that the exponentials in (77) and (79) can be expanded in powers of t to obtain

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

The potential energy transforms to

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

The solution to Eq. (78) with potential (83) will be approximated with the solution of the equation

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

with the potential energy

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

where

$$X_\omega=\sqrt{\frac{\omega}{(1-c)\Delta-\omega}}\left[\pi-\arctan\sqrt{\frac{(1-c)\Delta-\omega}{\omega}}\right],$$

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

in which

$$\chi(\omega)=\sqrt{\frac{(1-c)\Delta-\omega}{\omega}},$$

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

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

Substitution of (83) and $\varphi_\omega(x)$ into (84) now yields

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

We find, after some manipulation, that in this limit

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

where

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

For small values of ω, the last expressions yield the dependence

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

with the quantity

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

slowly varying with ω on account of the integral I_4^{cr}. For $\omega\ll E_{\mathrm{BE}}$, we may expand the exponential—neglecting the slow variation of I_4^{cr}—to obtain $\rho(\omega)$ with the same linear dependence as given in (1).

5.4. Numerical calculation

Figure 1 presents the results of the numerical solution of Eq. (76) for the exponential part of $\rho(\omega)$. For comparison, we also show the results which were obtained from Eq. (69) without invoking the critical-size cluster concept and are in fact identical to the results of Ref. 15.

The quantity ln $[\rho(\omega)]$ is measured in units of $[E_{\mathrm{cr}}/(1-c)\Delta]^{3/2}$, the common multiplier to all the terms involved.

With increasing energy, $\rho(\omega)$ plotted on a linear scale is seen to first vary almost linearly in the range $0<\omega<0.07\Delta$. Following this it goes over to the Urbach falloff behavior which gradually gives way to the characteristic Lifshitz singularity.

Starting from $\omega\approx 0.1\Delta$, our results are virtually identical to those of Ref. 15.

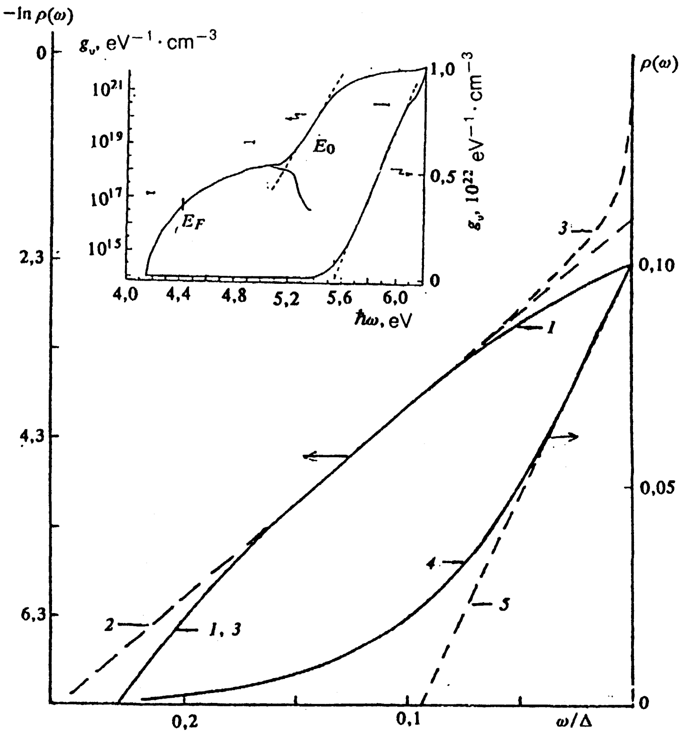

FIG. 1. Exponential part of $\rho(\omega)$. Curve *1*: solution of Eq. (78) in accordance with (80); Curve *2*: Urbach approximation; Curve *3*: solution of Eq. (69) and calculation of expression (67) (agrees with the results of Ref. 15); Curve *4*: curve *1* in a linear scale; Curve *5*: linear approximation for the band-edge region, the calculations were made for the concentration $c=0.1$ using the common multiplier $\nu_{\mathrm{cr}}=[E_{\mathrm{cr}}/(1-c)\Delta]^{3/2}$ as the unit for $\ln[\rho(\omega)]$ (this holds also for curve *5*). Inset: experimental data[4] on the one-electron density of states near the band edge and in the band gap of amorphous silicon ($E_0=51$ MeV).

5.5. Exponentially accurate solution for a three-component system

In a frequent experimental situation a disordered system contains some relatively small number of deep centers which produce a characteristic tail in the density of states. We model such a three-component system by a disordered solid solution A_cB_{1-c} with addition of a small number $c_I\ll c$, $(1-c)$ of deep substitutional centers of type I. The composition of such a solution may be written as $A_cI_{c_I}B_{1-c-c_I}$. We ignore the formation of deep-center clusters as well as the effect of the deep centers on the average potential $\langle E\rangle_{\mathrm{av}}$ and we assume, as before, that the depth of binding fluctuation-induced potential wells is $(1-c)\Delta<E_{\mathrm{cr}}$. We visualize a deep center as a spherical potential well of volume v_0, whose depth is much greater than its critical value, $\Delta_I\gg E_{\mathrm{cr}}$. In this situation, two types of localized states can occur: first, states having an critical A cluster at their center and, second, deep centers surrounded by the potential fluctuation of the solid solution A_cB_{1-c}. (The probability of finding a deep center within a critical cluster is assumed to be negligibly small). The action describing the first type of states is given by Eq. (77), whereas the additional terms in the Green's function and in the density of states are characterized by a deep-center-related action representable as

$$\tilde{A}_{\mathrm{I}}[t\varphi_{\mathrm{tr}}^2]=\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\int d^3x[(\nabla\varphi_{\mathrm{tr}}(x))^2+\varphi_{\mathrm{tr}}^2(x)]t-\left(\frac{E_0}{\omega}\right)^{3/2}\left[\int_0^{X_0}d^3x[\Delta_{\mathrm{I}}t\varphi_{\mathrm{tr}}^2(x)+\ln(c_{\mathrm{I}})]+\int_{X_0}^\infty d^3x\ln\mathscr{R}(-it)\right],\tag{92}$$

where

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

In the approximation considered, Eqs. (77)–(82) remain unchanged and minimization of the action (92) leads to the equation

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

with a potential energy of the form

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

For $t=0$ the problem reduces to that of solving the Schrödinger equation for a spherical potential well with a deep level at $\omega=\omega_{\rm I}$. For small departures from $\omega_{\rm I}$ we let $\varphi_{\rm tr}(x)\approx\varphi_{\rm I}(x)$, the solution of the Schrödinger equation for a spherical potential well of radius X_0 and of depth $\Delta_{\rm I}$.

The behavior of the density of states in this vicinity is analogous to that in the strong scattering case. Under the Gaussian assumption it is found that, to exponential accuracy,

$$\rho_{\rm I}(\omega)\propto\exp\{-A_{\rm I}[\varphi_{\rm tr}]^2t\}$$

$$=\exp\left\{-\frac{(\omega-\omega_{\rm I})^2}{2\delta L_{\omega_{\rm I}}c(1-c)\Delta^2}-\ln(1/c_{\rm I})\right\}, \tag{95}$$

where

$$\delta L_{\omega_{\rm I}}=\left(\frac{E_0}{\omega_{\rm I}}\right)^{3/2}\left(\frac{\omega_{\rm I}}{\Delta_{\rm I}}\right)I^{\rm I}_4,$$

$$I^{\rm I}_4=\int_{X_0}^{\infty}d^3x[\varphi^2_{\rm I}(x)]^2, \tag{96}$$

with the normalization condition

$$\int_0^{\infty}d^3x\varphi^2_{\rm I}(x)=1.$$

Since the shape of the deep-center band also depends on the fluctuation-induced potential in the binary solution, it contains some information about this potential, to be usefully added to that obtainable from the Urbach parameter E_U and from the slope of the linear dependence near the band edge $E_{\rm BE}$. However, in the practical use of this additional information one cannot avoid encountering the integral $I^{\rm I}_4$, which is unfortunate because $I^{\rm I}_4$ is determined by the shape of the deep-center wave function and is not always describable well enough by that of a spherical potential well.

5.6. Pre-exponential factors and an estimate of the range of validity of the theory

Everywhere in the range

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

the density of states may now be written as a sum of two terms,

$$\rho(\omega)+\rho_{\rm I}(\omega).$$

Taking account of the pre-exponential factor we have

$$\rho(\omega)=\frac{1}{\omega}\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\exp\{-\tilde{A}[\varphi^2_{\rm tr}t]\}$$

$$\times\frac{1}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\{-\tilde{\mathscr{A}}[\tau]\}, \tag{97}$$

where, using (78) and (79), $\tilde{A}[\varphi^2_{\rm tr}t]$ is transformed into

$$\tilde{A}[\varphi^2_{\rm tr}t]=\left(\frac{E_0}{\omega}\right)^{3/2}\int_{X_{\rm cr}}^{\infty}d^3x\{\ln\mathscr{R}(-it)-t\varphi^2_{\rm tr}(x)$$

$$\times[\ln\mathscr{R}(-it)]'_{t\varphi^2_{\rm tr}}\}$$

$$+(E_0/\omega)^{3/2}(4\pi/3)X^3_{\rm cr}\ln 1/c, \tag{98}$$

and $\tilde{\mathscr{A}}[\tau]$ takes the form

$$\tilde{\mathscr{A}}[\tau]=\left(\frac{E_0}{\omega}\right)^{3/2}\int_{X_{\rm cr}}^{\infty}d^3x\left\{\ln\left[\frac{\mathscr{R}(\tau-it)}{\mathscr{R}(-it)}\right]\right.$$

$$\left.-i\tau[\ln\mathscr{R}(\tau-it)]'_{\tau}\right\}. \tag{99}$$

Here

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

The deep-centers contribution is

$$\rho_{\mathrm{I}}(\omega)=\frac{1}{\omega}\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\exp\{-A_{\mathrm{I}}[\varphi_{\mathrm{tr}}]^2 t\}$$

$$\times(1/2\pi)\int_{X_0}^{\infty}d^3x\exp\{-\mathscr{A}_{\mathrm{I}}(\tau)\},\qquad(100)$$

where $A_{\mathrm{I}}[\varphi_{\mathrm{tr}}^2]$ is generally

$$\tilde{A}_{\mathrm{I}}[\varphi_{\mathrm{tr}}^2 t]=\left(\frac{E_0}{\omega}\right)^{3/2}\int_{X_0}^{\infty}d^3x\{\ln\mathscr{R}(-it)-t\varphi_{\mathrm{tr}}^2(x)$$

$$\times[\ln\mathscr{R}(-it)]'_{t\varphi_{\mathrm{tr}}^2}\}+\ln 1/c_{\mathrm{I}},\qquad(101)$$

and where

$$\tilde{\mathscr{A}}_{\mathrm{I}}[\tau]=\left(\frac{E_0}{\omega}\right)^{3/2}\int_{X_0}^{\infty}d^3x\left\{\ln\left[\frac{\mathscr{R}(\tau-it)}{\mathscr{R}(-it)}\right]\right.$$

$$\left.-i\tau[\ln\mathscr{R}(\tau-it)]'_{\tau}\right\}.\qquad(102)$$

Expanding $\tilde{\mathscr{A}}[\tau]$ and $\tilde{\mathscr{A}}_{\mathrm{I}}[\tau]$ in powers of τ, retaining only second-order terms, we obtain after calculating the Gaussian integrals

$$\rho(\omega)+\rho_{\mathrm{I}}(\omega)=\frac{1}{\omega}\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\left\{2\pi\int_{X_{\mathrm{cr}}}^{\infty}d^3x\right.$$

$$\left.\times[\ln\mathscr{R}(-it)]''_{\tau\tau}\right\}^{-1/2}\exp\{-\tilde{A}[\varphi_{\mathrm{tr}}^2 t]\}$$

$$+\frac{1}{\omega}\frac{\omega}{\Delta}\left(\frac{E_0}{\omega}\right)^{3/2}\left\{2\pi\int_{X_0}^{\infty}d^3x\right.$$

$$\left.\times[\ln\mathscr{R}(-it)]''_{\tau\tau}\right\}^{-1/2}\exp\{-\tilde{A}_{\mathrm{I}}[\varphi_{\mathrm{tr}}^2 t]\},$$

$$(103)$$

where

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

The integral

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

can be evaluated, using the approximate solution for $\varphi_\omega(x)$ [Eq. (86)] as $\omega\to 0$. This gives the energy indicative of the statistical scatter of the localization energies.

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

The last expression may also be written as

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

Similarly, we may estimate the deep-center contribution:

$$\gamma_{\mathrm{I}}=\sqrt{c(1-c)\Delta^2\delta L_{\omega_{\mathrm{I}}}},\qquad(106)$$

where the quantity $\delta L_{\omega_{\mathrm{I}}}$ is defined by Eq. (96). An order-of-magnitude estimate for $\delta L_{\omega_{\mathrm{I}}}$ may be obtained using the wave function of a spherical well of volume v_0, with depth given by the deep center perturbation potential Δ_{I}.

Letting $\omega\to 0$ in (105) we see that γ_ω becomes equal to and exceeds the localization energy when $\omega=\omega_{\mathrm{ME}}$, where

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

States with $\omega\leqslant\omega_{\mathrm{ME}}$ cannot be regarded as localized, so that the quantity ω_{ME} actually gives an estimate of the position of the mobility edge as well as defines the range of applicability of the instanton approximation.

6. DISCUSSION AND COMPARISON WITH EXPERIMENT

The total density of states per lattice site for energies below E_g is estimated by using Eqs. (88) and (104) for small localization energies in the approximate calculation of the first term in (103). We find

$$\mathscr{N}(0)=\int_0^{E_L}\rho(\omega)d\omega\approx c_{\mathrm{cr}}^{\nu},\qquad(108)$$

where

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

These states are due to compositional fluctuations in the system and their number is naturally limited by the number of compact—i.e., most probable—critical clusters. Similarly, using (95) and (106) in the second terms in (103) we obtain c_{I} as the number of deep centers per lattice site.

Expression (108) also provides a rough estimate of the number of localized states in the system, which in a more rigorous treatment is estimated by numerically evaluating the integral

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

Both these estimates may be compared with the experimentally measured number of states below the mobility edge. Experimental data show (see Winer *et al.*[4] and references therein) that the number of (localized) gap states is much smaller than the total number of band states. This is easy to understand if we note that expression (108) turns out to be greater than unity in the weak scattering case, when the maximum depth of a potential well is less than the critical value E_{cr} of the potential.

Two other quantities which give a ready comparison with experiment are the slope of the linear dependence near the band edge $E_{\mathrm{BE}}(91)$ and the Urbach parameter $E_U(81)$. The ratio of these has the advantage of being free of the most sensitive part of the dependence on E_{cr}.

The above three characteristics of the energy spectrum can yield three major parameters of the theory: the concentration (c), the amplitude of the random potential (Δ), and the critical depth of the site perturbation potential (E_{cr}). If one of these can be determined independently, the above experimental data are quite sufficient for the quantitative verification of the theory. The parameter $E_{\rm cr}$ seems to be the easiest to determine independently because to estimate it all we must know is the effective mass of the carrier and v_0. Estimates of this kind seem to be possible both for amorphous silicon and for glass. In isoelectronic solid solutions usually the amplitude of the random potential and the concentrations are known with good accuracy, which makes these materials excellent candidates for the study of the (one-electron) density of localized states.

The study of the shape of the deep center band also yields valuable insights. In amorphous silicon, the amount of broadening of the band can already be predicted if only the first three quantities characterizing the density-of-states tail are taken as fitting parameters; in a more accurate calculation, the whole of the band shape can be reconstructed.

In Fig. 1 our results are compared, in a qualitative manner, with experimental data on the one-electron density of states in amorphous silicon.[4] The calculations are limited to the exponential part of $\rho(\omega)$ and neglect the presence of the deep center band. According to Ref. 4, the mobility edge of the material is at 5.7 eV, which means that the linear region we have near the band edge lies almost entirely above the mobility edge. The estimate (107) also suggests that the mobility edge is above the Urbach region while at the same time remaining in the lower part of the linear portion of the spectrum (1). As a whole, there is a undeniable resemblance between the theoretical and experimental spectra.

Accounting for the pre-exponential factor in the range $\omega \geqslant \omega_{\rm ME}$ cannot worsen the qualitative agreement with experiment. In the range $0 \leqslant \omega \leqslant \omega_{\rm ME}$ the localization index in the pre-exponential factor clearly prevents the use of the latter energy dependence in the form we have obtained. However, noting that the density of states has no singularities at the mobility edge, it may be justifiable to consider the exponential factor (90) alone when interpolating to these energies.

[1)] There exists evidence[11–14] for a more complex behavior of the density of states in deep-impurity bands. The complicating factors include the degeneracy lifting by fluctuations in the closest environment;[11,12] the formation of complex clusters of impurity centers;[13,14] and uniform broadening. These questions will not be pursued in the present paper.

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